Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:45 PM GMT

PDB ID	:	4ACQ
Title	:	Alpha-2 Macroglobulin
Authors	:	Marrero, A.; Duquerroy, S.; Trapani, S.; Goulas, T.; Guevara, T.; Andersen, G.R.; Navaza, J.; Sottrup-Jensen, L.; Gomis-Ruth, F.X.
Deposited on	:	2011-12-17
Resolution	:	4.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

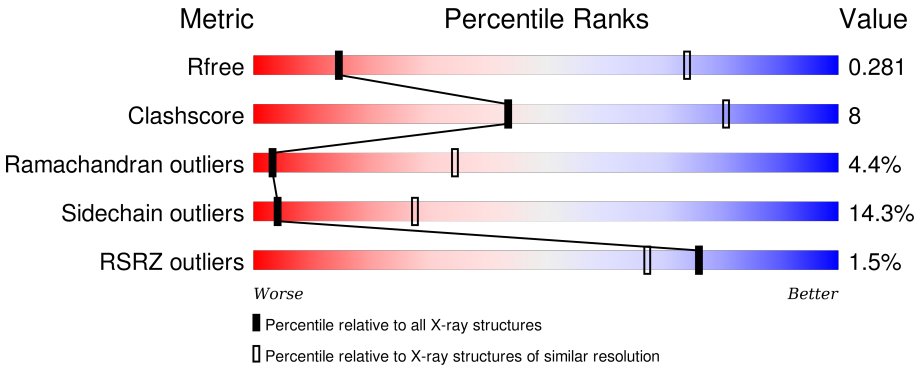
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1451	% 61% 22% • 12%
1	B	1451	% 61% 22% • 12%
1	C	1451	% 67% 25% • •
1	D	1451	% 61% 23% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	2002	X	-	-	-
2	NAG	A	2401	-	-	-	X
2	NAG	A	2402	X	-	-	-
2	NAG	A	2502	X	-	-	-
2	NAG	B	2001	-	-	-	X
2	NAG	B	2002	X	-	-	-
2	NAG	B	2402	X	-	-	-
2	NAG	B	2502	X	-	-	-
2	NAG	C	2001	-	-	-	X
2	NAG	C	2002	X	-	-	-
2	NAG	C	2402	X	-	-	-
2	NAG	C	2502	X	-	-	-
2	NAG	D	2001	-	-	-	X
2	NAG	D	2002	X	-	-	-
2	NAG	D	2402	X	-	-	-
2	NAG	D	2502	X	-	-	-
4	NAG	A	2602	X	-	-	-
4	NAG	B	2602	X	-	-	-
4	MAN	B	2603	-	X	-	-
4	NAG	C	2602	X	-	-	-
4	MAN	C	2603	-	X	-	-
4	NAG	D	2602	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 39900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALPHA-2-MACROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			
1	B	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			
1	C	1403	Total	C	N	O	S	0	0	0
			10582	6729	1774	2032	47			
1	D	1270	Total	C	N	O	S	0	0	0
			9548	6067	1606	1833	42			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		

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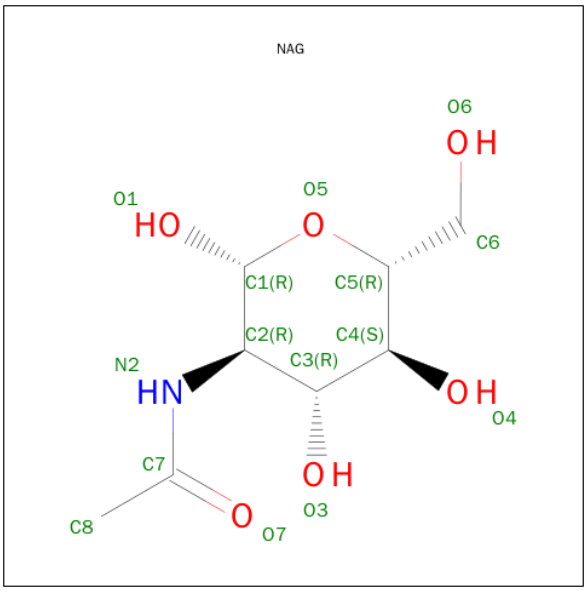
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total C N O 28 16 2 10	0	0
2	D	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

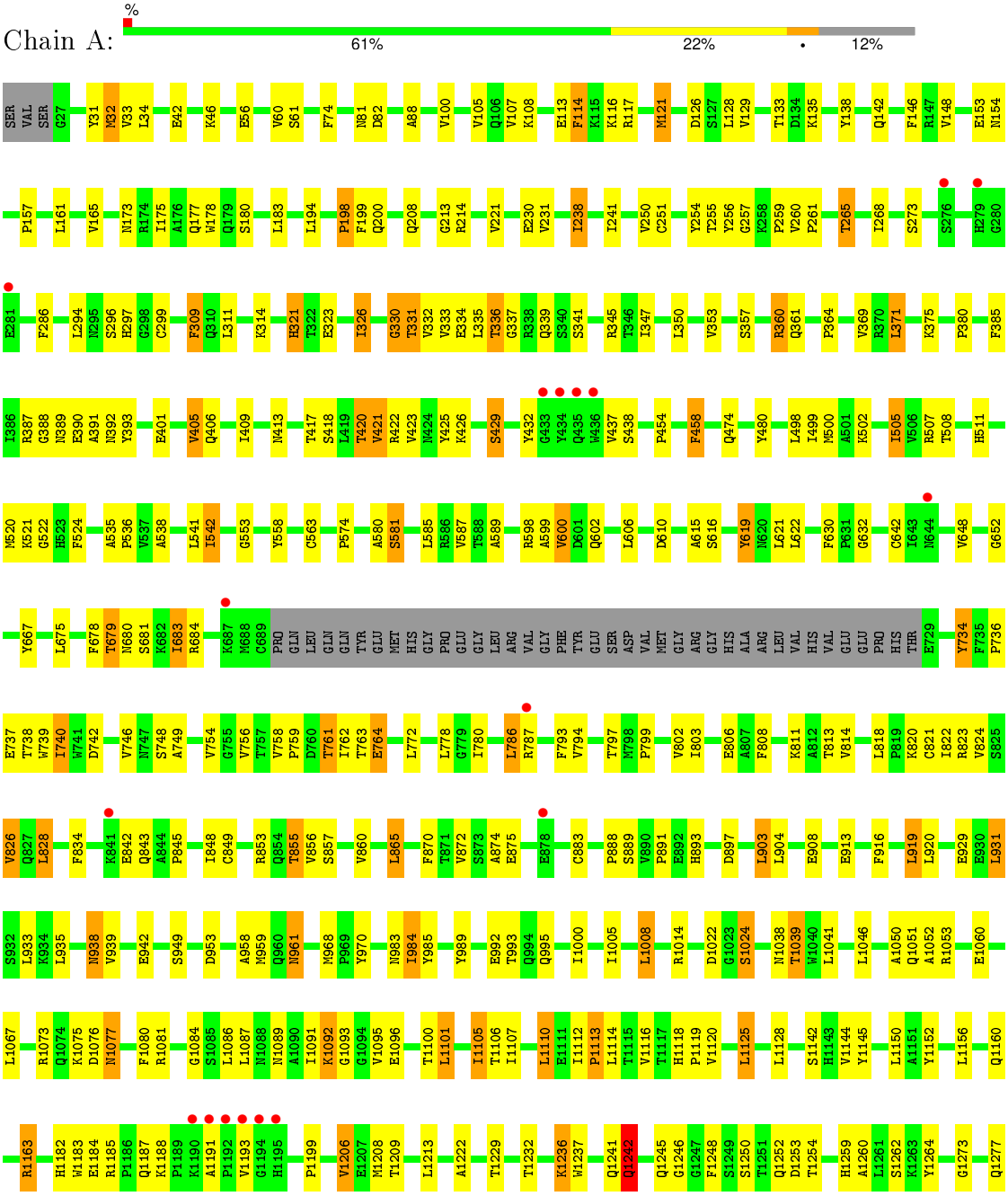
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

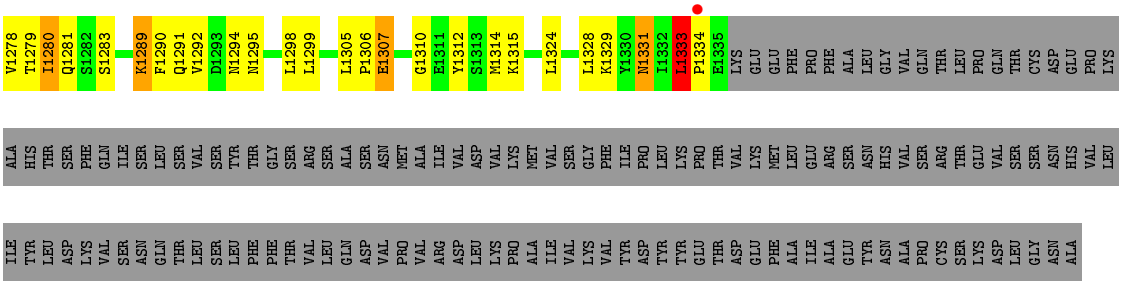
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ALPHA-2-MACROGLOBULIN

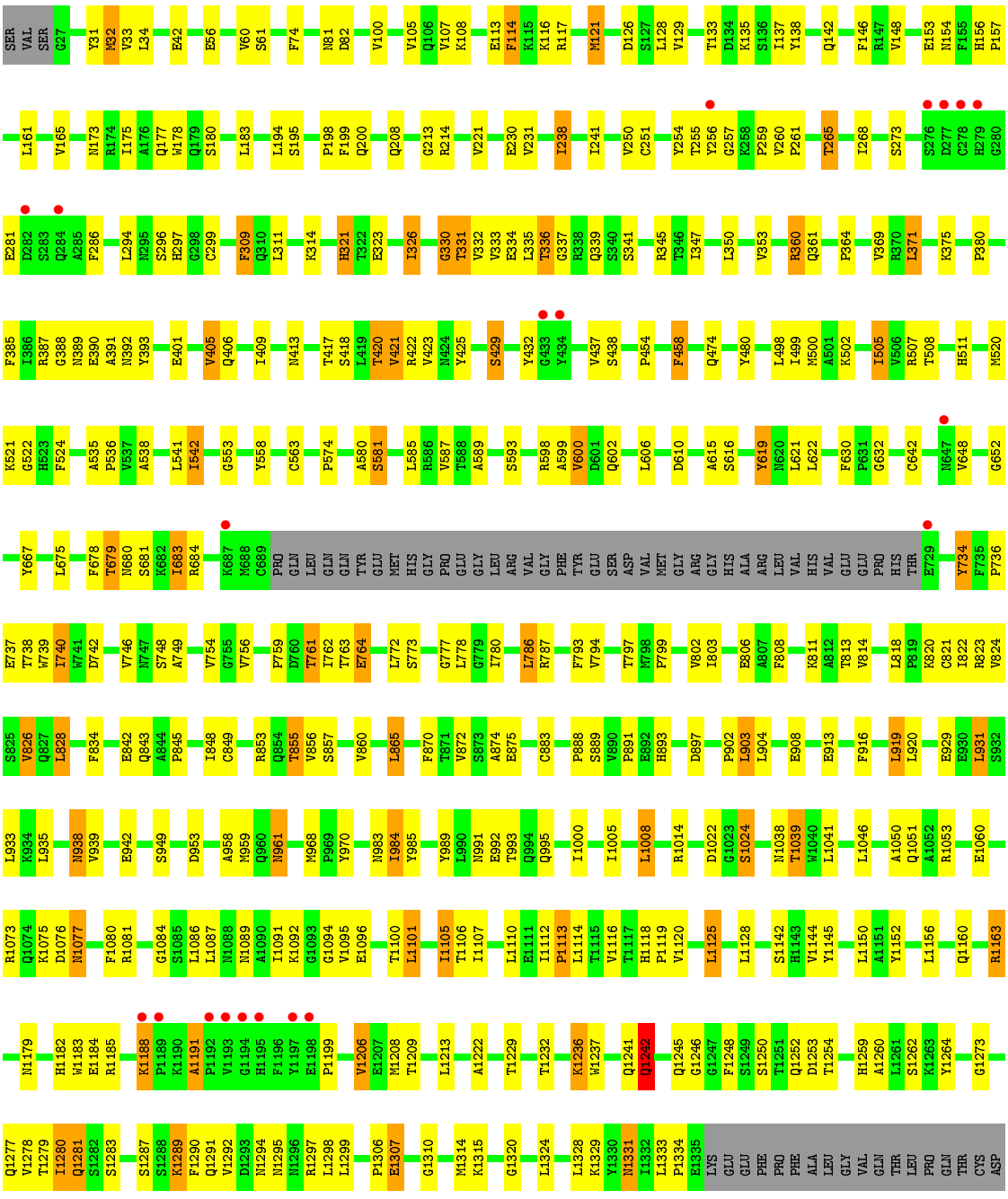
Chain A:

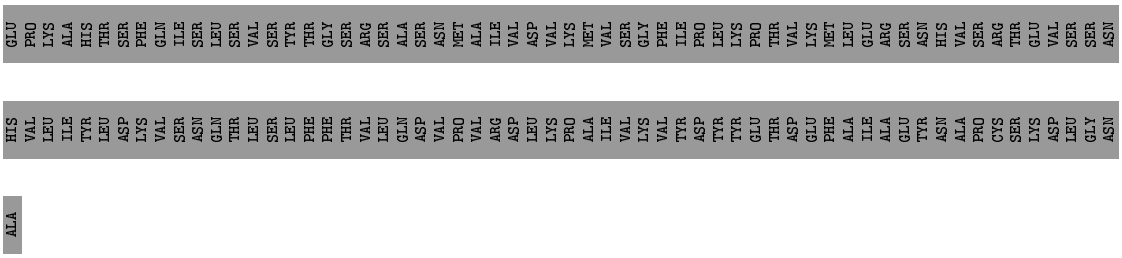




• Molecule 1: ALPHA-2-MACROGLOBULIN

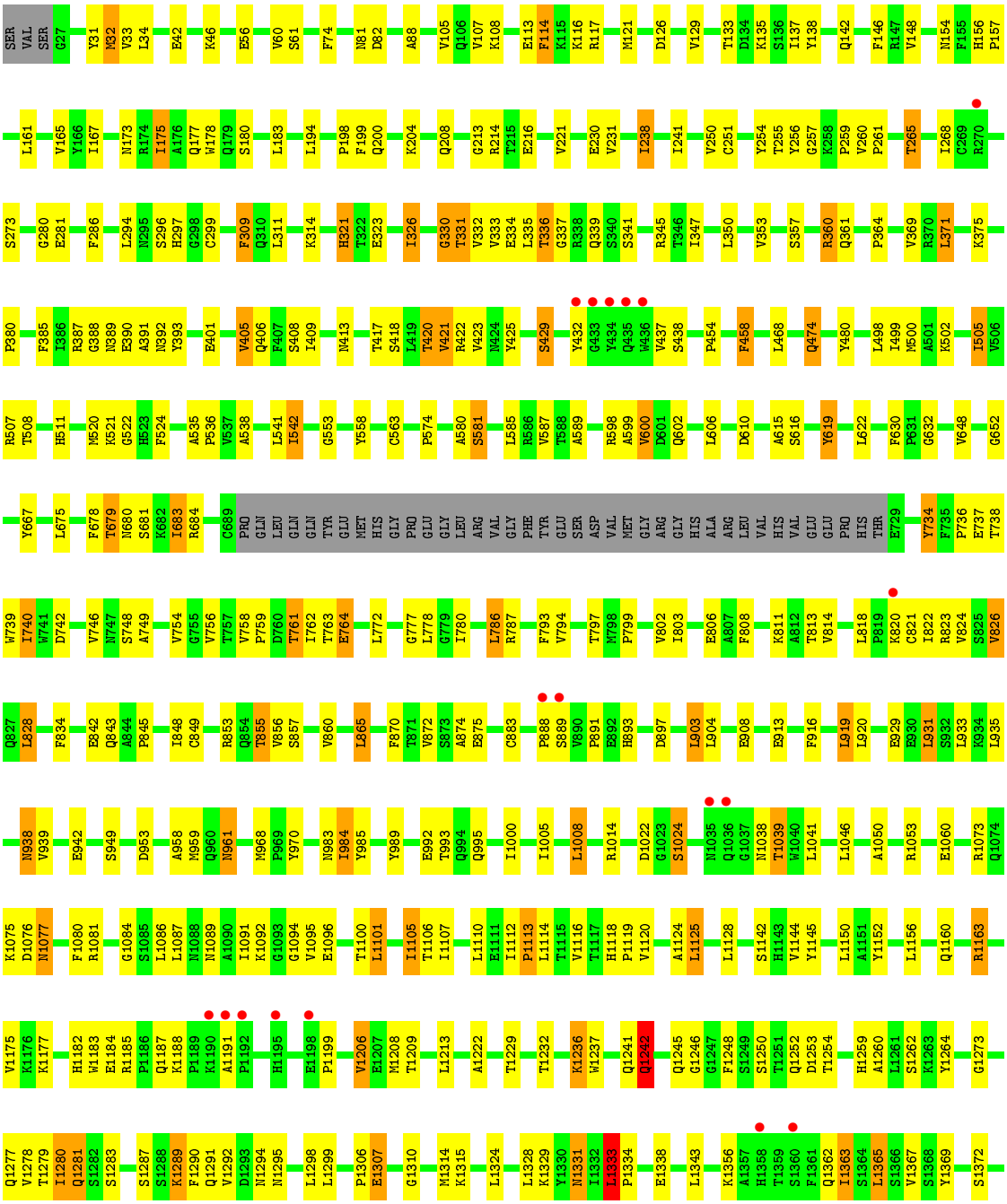
Chain B:

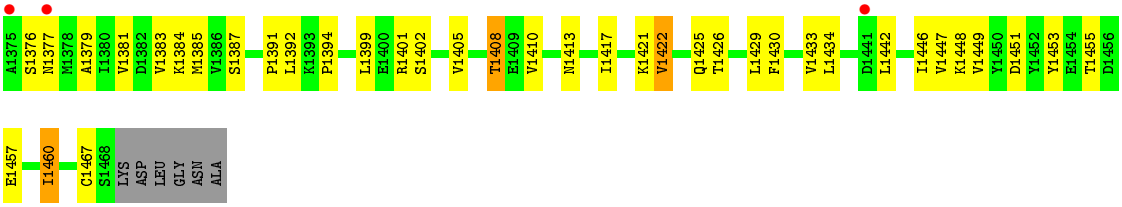




• Molecule 1: ALPHA-2-MACROGLOBULIN

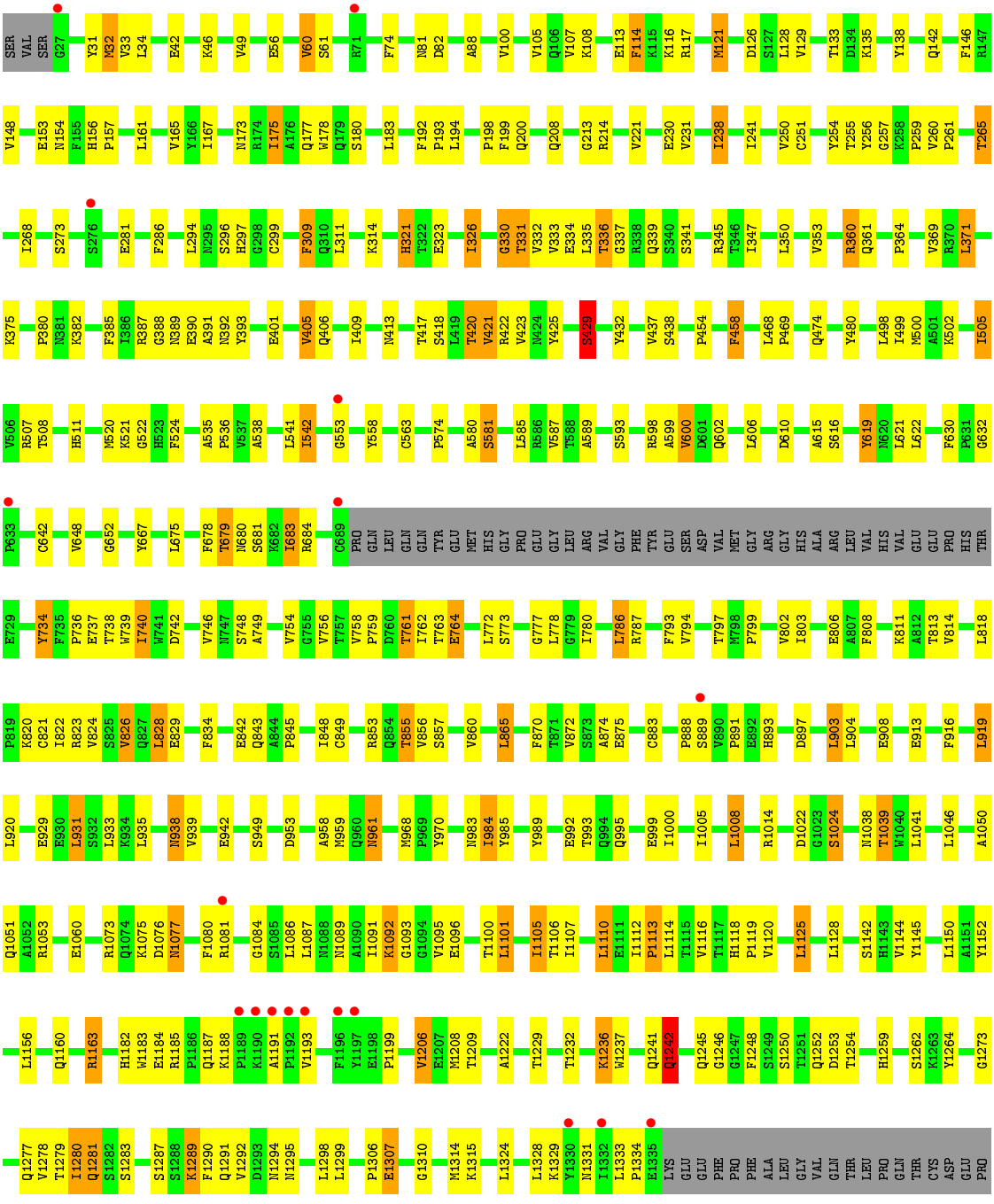
Chain C:





- Molecule 1: ALPHA-2-MACROGLOBULIN

Chain D:



LYS ALA HIS THR SER PHE GLN ILE SER LEU SER VAL SER TYR THR GLY SER ARG SER ALA SER ASN MET ALA ILE VAL ASP VAL LYS MET VAL SER GLY PHE ILE PRO LEU LYS PRO THR VAL LYS MET LEU GLU ARG SER ASN HIS VAL SER ARG THR GLU VAL SER SER ASN HIS VAL

LEU ILE TYR LEU ASP LYS VAL SER ASN GLN THR LEU SER LEU PHE PHE THR VAL LEU GLN ASP VAL PRO VAL ARG ASP LEU LYS PRO ALA ILE VAL LYS VAL TYR ASP TYR TYR GLU THR ASP GLU PHE ALA ILE ALA GLU TYR ASN ALA PRO CYS SER LYS ASP LEU GLY ASN ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	130.69Å 260.30Å 281.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 4.30 24.95 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.00-4.30) 99.0 (24.95-4.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 4.24Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.238 , 0.260 0.263 , 0.281	Depositor DCC
R_{free} test set	3303 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	205.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 154.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 65058 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	39900	wwPDB-VP
Average B, all atoms (Å^2)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEQ, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/9743	0.72	0/13275
1	B	0.42	0/9743	0.72	0/13275
1	C	0.44	0/10801	0.73	0/14718
1	D	0.41	0/9743	0.72	0/13275
All	All	0.43	0/40030	0.72	0/54543

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
2	A	3	0
2	B	3	0
2	C	3	0
2	D	3	0
4	A	1	0
4	B	1	0
4	C	4	0
4	D	1	0
All	All	19	8

There are no bond length outliers.

There are no bond angle outliers.

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	NAG	C1
2	A	2402	NAG	C1
2	A	2502	NAG	C1
4	A	2602	NAG	C1
2	B	2002	NAG	C1
2	B	2402	NAG	C1
2	B	2502	NAG	C1
4	B	2602	NAG	C1
2	C	2002	NAG	C1
2	C	2402	NAG	C1
2	C	2502	NAG	C1
4	C	2602	NAG	C2,C5,C1,C4
2	D	2002	NAG	C1
2	D	2402	NAG	C1
2	D	2502	NAG	C1
4	D	2602	NAG	C1

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	SER	Mainchain,Peptide
1	B	429	SER	Mainchain,Peptide
1	C	429	SER	Mainchain,Peptide
1	D	429	SER	Mainchain,Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9548	0	9181	153	0
1	B	9548	0	9181	152	0
1	C	10582	0	10201	174	0
1	D	9548	0	9181	153	0
2	A	84	0	75	3	0
2	B	84	0	75	3	0
2	C	84	0	75	3	0
2	D	84	0	75	2	0
3	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	39	0	0
3	C	56	0	52	0	0
3	D	42	0	39	0	0
4	A	39	0	34	1	0
4	B	39	0	34	2	0
4	C	39	0	32	1	0
4	D	39	0	34	1	0
All	All	39900	0	38347	633	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (633) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2501:NAG:H83	2:D:2502:NAG:H82	1.65	0.79
2:C:2501:NAG:H83	2:C:2502:NAG:H82	1.65	0.78
2:B:2501:NAG:H83	2:B:2502:NAG:H82	1.65	0.78
1:C:280:GLY:HA3	1:D:429:SER:HA	1.65	0.77
1:C:535:ALA:HB1	1:C:536:PRO:HD2	1.65	0.76
2:A:2501:NAG:H83	2:A:2502:NAG:H82	1.66	0.76
1:C:1280:ILE:HG23	1:C:1314:MET:HB3	1.69	0.74
1:A:1280:ILE:HG23	1:A:1314:MET:HB3	1.70	0.74
1:D:535:ALA:HB1	1:D:536:PRO:HD2	1.68	0.74
1:D:1280:ILE:HG23	1:D:1314:MET:HB3	1.69	0.74
1:B:535:ALA:HB1	1:B:536:PRO:HD2	1.68	0.73
1:B:1280:ILE:HG23	1:B:1314:MET:HB3	1.70	0.73
1:B:502:LYS:HG3	1:B:535:ALA:HB2	1.72	0.71
1:A:535:ALA:HB1	1:A:536:PRO:HD2	1.71	0.71
1:D:502:LYS:HG3	1:D:535:ALA:HB2	1.73	0.70
1:C:502:LYS:HG3	1:C:535:ALA:HB2	1.71	0.70
1:A:502:LYS:HG3	1:A:535:ALA:HB2	1.73	0.70
1:A:919:LEU:H	1:A:1229:THR:HG22	1.57	0.70
1:B:919:LEU:H	1:B:1229:THR:HG22	1.57	0.69
1:C:938:ASN:HD22	1:C:1334:PRO:HG2	1.59	0.67
1:C:865:LEU:H	1:C:865:LEU:HD13	1.60	0.67
1:D:574:PRO:HA	1:D:786:LEU:HD12	1.76	0.67
1:A:616:SER:HA	1:A:619:TYR:CE2	2.30	0.67
1:C:574:PRO:HA	1:C:786:LEU:HD12	1.77	0.67
1:B:679:THR:HG22	1:B:681:SER:H	1.61	0.66
1:A:865:LEU:HD13	1:A:865:LEU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:LEU:HD13	1:D:865:LEU:H	1.61	0.66
1:B:865:LEU:HD13	1:B:865:LEU:H	1.61	0.66
1:B:260:VAL:HG23	1:B:853:ARG:HH22	1.61	0.65
1:C:616:SER:HA	1:C:619:TYR:CE2	2.31	0.65
1:A:574:PRO:HA	1:A:786:LEU:HD12	1.78	0.65
1:B:574:PRO:HA	1:B:786:LEU:HD12	1.79	0.65
1:D:679:THR:HG22	1:D:681:SER:H	1.62	0.65
1:A:250:VAL:O	1:A:299:CYS:HB3	1.97	0.65
1:B:157:PRO:HB3	1:B:772:LEU:HD23	1.78	0.65
1:B:616:SER:HA	1:B:619:TYR:CE2	2.32	0.65
1:B:107:VAL:HB	1:B:114:PHE:HB2	1.78	0.65
1:C:1118:HIS:CD2	1:C:1120:VAL:HG22	2.32	0.64
1:D:157:PRO:HB3	1:D:772:LEU:HD23	1.79	0.64
1:A:931:LEU:HD11	1:A:1314:MET:SD	2.38	0.64
1:A:679:THR:HG22	1:A:681:SER:H	1.62	0.64
1:B:938:ASN:HD22	1:B:1334:PRO:HG2	1.61	0.64
1:D:616:SER:HA	1:D:619:TYR:CE2	2.32	0.64
1:D:260:VAL:HG23	1:D:853:ARG:HH22	1.62	0.64
1:C:165:VAL:HG13	1:C:178:TRP:HB2	1.79	0.64
1:D:107:VAL:HB	1:D:114:PHE:HB2	1.80	0.63
1:B:1118:HIS:CD2	1:B:1120:VAL:HG22	2.33	0.63
1:C:679:THR:HG22	1:C:681:SER:H	1.61	0.63
1:C:260:VAL:HG23	1:C:853:ARG:HH22	1.62	0.63
1:A:107:VAL:HB	1:A:114:PHE:HB2	1.80	0.63
1:D:799:PRO:HD2	1:D:903:LEU:HD11	1.81	0.63
1:B:364:PRO:HG3	2:B:2401:NAG:H81	1.80	0.63
1:A:1118:HIS:CD2	1:A:1120:VAL:HG22	2.34	0.63
1:C:919:LEU:H	1:C:1229:THR:HG22	1.64	0.63
1:A:499:ILE:HD12	1:A:507:ARG:HB3	1.82	0.62
1:B:250:VAL:O	1:B:299:CYS:HB3	1.98	0.62
1:D:165:VAL:HG13	1:D:178:TRP:HB2	1.81	0.62
1:A:260:VAL:HG23	1:A:853:ARG:HH22	1.64	0.62
1:C:157:PRO:HB3	1:C:772:LEU:HD23	1.80	0.62
1:D:1118:HIS:CD2	1:D:1120:VAL:HG22	2.34	0.62
1:C:799:PRO:HD2	1:C:903:LEU:HD11	1.81	0.62
1:B:165:VAL:HG13	1:B:178:TRP:HB2	1.80	0.62
1:C:107:VAL:HB	1:C:114:PHE:HB2	1.80	0.62
1:D:499:ILE:HD12	1:D:507:ARG:HB3	1.81	0.62
1:C:250:VAL:O	1:C:299:CYS:HB3	2.00	0.62
1:A:938:ASN:HD22	1:A:1334:PRO:HG2	1.65	0.62
1:A:165:VAL:HG13	1:A:178:TRP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:VAL:O	1:D:299:CYS:HB3	2.00	0.62
1:B:499:ILE:HD12	1:B:507:ARG:HB3	1.81	0.62
1:A:157:PRO:HB3	1:A:772:LEU:HD23	1.80	0.61
1:A:1182:HIS:NE2	1:A:1237:TRP:HB3	2.16	0.61
1:D:931:LEU:HD11	1:D:1314:MET:SD	2.41	0.61
1:C:33:VAL:HG11	1:C:105:VAL:HG11	1.82	0.61
1:A:117:ARG:HH22	1:D:1119:PRO:HB2	1.65	0.61
1:C:364:PRO:HG3	2:C:2401:NAG:H81	1.82	0.61
1:B:117:ARG:HH22	1:C:1119:PRO:HB2	1.66	0.61
1:D:364:PRO:HG3	2:D:2401:NAG:H81	1.81	0.61
1:D:938:ASN:HD22	1:D:1334:PRO:HG2	1.64	0.61
1:A:364:PRO:HG3	2:A:2401:NAG:H81	1.82	0.61
1:B:799:PRO:HD2	1:B:903:LEU:HD11	1.83	0.61
1:C:499:ILE:HD12	1:C:507:ARG:HB3	1.82	0.61
1:C:931:LEU:HD11	1:C:1314:MET:SD	2.41	0.61
1:C:32:MET:HG2	1:C:679:THR:HG23	1.83	0.61
1:A:426:LYS:HA	1:B:1191:ALA:HB3	1.83	0.61
1:A:32:MET:HG2	1:A:679:THR:HG23	1.81	0.60
1:D:919:LEU:H	1:D:1229:THR:HG22	1.65	0.60
1:D:32:MET:HG2	1:D:679:THR:HG23	1.82	0.60
1:D:764:GLU:HB3	1:D:787:ARG:HG3	1.84	0.60
1:B:989:TYR:HA	1:B:1262:SER:HB3	1.83	0.60
1:A:799:PRO:HD2	1:A:903:LEU:HD11	1.83	0.60
1:B:32:MET:HG2	1:B:679:THR:HG23	1.82	0.60
1:D:989:TYR:HA	1:D:1262:SER:HB3	1.83	0.60
1:B:931:LEU:HD11	1:B:1314:MET:SD	2.42	0.59
1:D:1182:HIS:NE2	1:D:1237:TRP:HB3	2.17	0.59
1:B:1182:HIS:NE2	1:B:1237:TRP:HB3	2.17	0.59
1:C:1182:HIS:NE2	1:C:1237:TRP:HB3	2.16	0.59
1:A:989:TYR:HA	1:A:1262:SER:HB3	1.85	0.59
1:C:989:TYR:HA	1:C:1262:SER:HB3	1.83	0.59
1:D:33:VAL:HG11	1:D:105:VAL:HG11	1.85	0.59
1:C:600:VAL:HG12	1:C:738:THR:HA	1.84	0.58
1:C:616:SER:HA	1:C:619:TYR:CD2	2.38	0.58
1:A:764:GLU:HB3	1:A:787:ARG:HG3	1.85	0.58
1:C:764:GLU:HB3	1:C:787:ARG:HG3	1.85	0.58
1:D:273:SER:HB2	1:D:314:LYS:HA	1.85	0.58
1:C:138:TYR:HB2	1:C:221:VAL:HG22	1.85	0.58
1:D:600:VAL:HG12	1:D:738:THR:HA	1.86	0.58
1:B:33:VAL:HG11	1:B:105:VAL:HG11	1.86	0.58
1:C:273:SER:HB2	1:C:314:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:764:GLU:HB3	1:B:787:ARG:HG3	1.85	0.58
1:A:138:TYR:HB2	1:A:221:VAL:HG22	1.85	0.58
1:A:33:VAL:HG11	1:A:105:VAL:HG11	1.85	0.57
1:A:1119:PRO:HB2	1:D:117:ARG:HH22	1.69	0.57
1:C:385:PHE:HB2	1:C:422:ARG:HB2	1.86	0.57
1:A:616:SER:HA	1:A:619:TYR:CD2	2.40	0.57
1:B:958:ALA:HA	1:B:961:ASN:HD21	1.69	0.57
1:A:273:SER:HB2	1:A:314:LYS:HA	1.86	0.57
1:B:385:PHE:HB2	1:B:422:ARG:HB2	1.86	0.57
1:D:1248:PHE:HB2	1:D:1254:THR:HG23	1.86	0.57
1:C:1248:PHE:HB2	1:C:1254:THR:HG23	1.85	0.57
1:A:385:PHE:HB2	1:A:422:ARG:HB2	1.86	0.57
1:C:667:TYR:HB2	1:C:684:ARG:HA	1.87	0.56
1:B:600:VAL:HG12	1:B:738:THR:HA	1.87	0.56
1:C:1391:PRO:HG2	1:C:1410:VAL:HG11	1.87	0.56
1:B:1242:GLN:HB2	1:B:1246:GLY:HA2	1.87	0.56
1:D:1242:GLN:HB2	1:D:1246:GLY:HA2	1.88	0.56
1:D:385:PHE:HB2	1:D:422:ARG:HB2	1.85	0.56
1:B:138:TYR:HB2	1:B:221:VAL:HG22	1.87	0.56
1:B:1038:ASN:HD22	1:B:1041:LEU:H	1.54	0.56
1:D:138:TYR:HB2	1:D:221:VAL:HG22	1.86	0.56
1:A:1242:GLN:HB2	1:A:1246:GLY:HA2	1.87	0.56
1:C:1038:ASN:HD22	1:C:1041:LEU:H	1.53	0.56
1:C:1367:VAL:HG21	1:C:1449:VAL:HG21	1.87	0.56
1:C:1391:PRO:HA	1:C:1433:VAL:HG12	1.86	0.56
1:C:1242:GLN:HB2	1:C:1246:GLY:HA2	1.88	0.56
1:A:389:ASN:HB2	1:A:418:SER:HB2	1.87	0.56
1:A:1038:ASN:HD22	1:A:1041:LEU:H	1.54	0.56
1:C:389:ASN:HB2	1:C:418:SER:HB2	1.88	0.56
1:D:389:ASN:HB2	1:D:418:SER:HB2	1.88	0.55
1:C:814:VAL:HG11	1:C:824:VAL:HG11	1.89	0.55
1:A:600:VAL:HG12	1:A:738:THR:HA	1.86	0.55
1:D:958:ALA:HA	1:D:961:ASN:HD21	1.70	0.55
1:B:273:SER:HB2	1:B:314:LYS:HA	1.87	0.55
1:A:667:TYR:HB2	1:A:684:ARG:HA	1.89	0.55
1:B:1248:PHE:HB2	1:B:1254:THR:HG23	1.88	0.55
1:C:958:ALA:HA	1:C:961:ASN:HD21	1.70	0.55
1:B:389:ASN:HB2	1:B:418:SER:HB2	1.87	0.55
1:B:667:TYR:HB2	1:B:684:ARG:HA	1.89	0.55
1:D:616:SER:HA	1:D:619:TYR:CD2	2.42	0.55
1:B:616:SER:HA	1:B:619:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:PHE:HB2	1:A:1254:THR:HG23	1.89	0.55
1:D:1038:ASN:HD22	1:D:1041:LEU:H	1.54	0.55
1:A:794:VAL:HG12	1:A:814:VAL:HA	1.89	0.54
1:D:208:GLN:HG3	1:D:214:ARG:HG2	1.90	0.54
1:C:794:VAL:HG12	1:C:814:VAL:HA	1.89	0.54
1:D:667:TYR:HB2	1:D:684:ARG:HA	1.89	0.54
1:C:1038:ASN:HA	1:C:1084:GLY:HA3	1.89	0.54
1:B:814:VAL:HG11	1:B:824:VAL:HG11	1.90	0.54
1:C:1369:TYR:HE2	1:C:1372:SER:HA	1.73	0.54
1:A:813:THR:HB	1:A:855:THR:HG23	1.89	0.54
1:A:261:PRO:O	1:A:326:ILE:HG23	2.08	0.54
1:C:1369:TYR:CD2	1:C:1422:VAL:HB	2.43	0.54
1:C:498:LEU:HD23	1:C:508:THR:HA	1.88	0.54
1:B:498:LEU:HD23	1:B:508:THR:HA	1.89	0.54
1:C:1365:LEU:HD22	1:C:1447:VAL:HG11	1.89	0.54
1:A:958:ALA:HA	1:A:961:ASN:HD21	1.73	0.54
1:D:803:ILE:HB	1:D:806:GLU:HB2	1.90	0.54
1:B:500:MET:HG2	1:B:505:ILE:HA	1.90	0.54
1:A:498:LEU:HD23	1:A:508:THR:HA	1.90	0.54
1:A:1038:ASN:HA	1:A:1084:GLY:HA3	1.90	0.53
1:A:177:GLN:HB2	1:A:1299:LEU:HD13	1.90	0.53
1:B:1038:ASN:HA	1:B:1084:GLY:HA3	1.90	0.53
1:A:814:VAL:HG11	1:A:824:VAL:HG11	1.89	0.53
1:D:148:VAL:HG23	1:D:183:LEU:HD21	1.91	0.53
1:C:803:ILE:HB	1:C:806:GLU:HB2	1.90	0.53
1:D:500:MET:HG2	1:D:505:ILE:HA	1.89	0.53
1:C:813:THR:HB	1:C:855:THR:HG23	1.90	0.53
1:D:794:VAL:HG12	1:D:814:VAL:HA	1.89	0.53
1:C:500:MET:HG2	1:C:505:ILE:HA	1.91	0.53
1:C:208:GLN:HG3	1:C:214:ARG:HG2	1.90	0.53
1:C:993:THR:HB	1:C:995:GLN:HE21	1.74	0.53
1:C:273:SER:HB3	1:C:314:LYS:HG3	1.91	0.53
1:B:256:TYR:HA	1:B:787:ARG:HG2	1.90	0.53
1:A:273:SER:HB3	1:A:314:LYS:HG3	1.91	0.53
1:C:261:PRO:O	1:C:326:ILE:HG23	2.08	0.53
1:A:803:ILE:HB	1:A:806:GLU:HB2	1.90	0.53
1:D:813:THR:HB	1:D:855:THR:HG23	1.89	0.53
1:B:177:GLN:HB2	1:B:1299:LEU:HD13	1.91	0.53
1:D:1038:ASN:HA	1:D:1084:GLY:HA3	1.90	0.53
1:D:814:VAL:HG11	1:D:824:VAL:HG11	1.90	0.53
1:D:1160:GLN:HA	1:D:1163:ARG:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:PHE:HE2	1:D:309:PHE:HA	1.74	0.53
1:B:135:LYS:HE2	1:B:142:GLN:HE22	1.73	0.53
1:B:813:THR:HB	1:B:855:THR:HG23	1.90	0.53
1:B:1160:GLN:HA	1:B:1163:ARG:HG2	1.91	0.52
1:C:1392:LEU:HG	1:C:1394:PRO:HD2	1.92	0.52
1:C:256:TYR:HA	1:C:787:ARG:HG2	1.91	0.52
1:C:589:ALA:HB3	1:C:746:VAL:HG21	1.91	0.52
1:C:1182:HIS:CD2	1:C:1237:TRP:HB3	2.44	0.52
1:C:1363:ILE:HD11	1:C:1433:VAL:HG22	1.92	0.52
1:D:261:PRO:O	1:D:326:ILE:HG23	2.09	0.52
1:C:286:PHE:HE2	1:C:309:PHE:HA	1.74	0.52
1:B:261:PRO:O	1:B:326:ILE:HG23	2.09	0.52
1:D:256:TYR:HA	1:D:787:ARG:HG2	1.91	0.52
1:B:794:VAL:HG12	1:B:814:VAL:HA	1.91	0.52
1:B:371:LEU:HD11	1:B:423:VAL:HG21	1.91	0.52
1:C:177:GLN:HB2	1:C:1299:LEU:HD13	1.92	0.52
1:C:1160:GLN:HA	1:C:1163:ARG:HG2	1.91	0.52
1:B:208:GLN:HG3	1:B:214:ARG:HG2	1.92	0.52
1:A:500:MET:HG2	1:A:505:ILE:HA	1.92	0.52
1:B:133:THR:HG22	1:B:146:PHE:HB3	1.91	0.52
1:C:148:VAL:HG23	1:C:183:LEU:HD21	1.92	0.52
1:A:1182:HIS:CD2	1:A:1237:TRP:HB3	2.45	0.52
1:D:498:LEU:HD23	1:D:508:THR:HA	1.92	0.52
1:D:993:THR:HB	1:D:995:GLN:HE21	1.73	0.52
1:D:273:SER:HB3	1:D:314:LYS:HG3	1.92	0.51
1:D:1242:GLN:HB3	1:D:1248:PHE:CE1	2.45	0.51
1:A:135:LYS:HE2	1:A:142:GLN:HE22	1.74	0.51
1:C:345:ARG:HD3	1:C:438:SER:HA	1.92	0.51
1:B:589:ALA:HB3	1:B:746:VAL:HG21	1.93	0.51
1:B:148:VAL:HG23	1:B:183:LEU:HD21	1.93	0.51
1:A:1160:GLN:HA	1:A:1163:ARG:HG2	1.91	0.51
1:B:826:VAL:HG13	1:B:874:ALA:HB2	1.93	0.51
1:D:265:THR:HG23	1:D:323:GLU:HB2	1.93	0.51
1:A:1022:ASP:OD1	1:A:1024:SER:HB2	2.10	0.51
1:B:1182:HIS:CD2	1:B:1237:TRP:HB3	2.45	0.51
1:B:350:LEU:HD13	1:B:421:VAL:HB	1.93	0.51
1:C:1125:LEU:HA	1:C:1128:LEU:HD12	1.92	0.51
1:B:345:ARG:HD3	1:B:438:SER:HA	1.93	0.51
1:A:286:PHE:HE2	1:A:309:PHE:HA	1.76	0.51
1:D:135:LYS:HE2	1:D:142:GLN:HE22	1.76	0.51
1:A:826:VAL:HG13	1:A:874:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:PHE:HE2	1:B:309:PHE:HA	1.76	0.51
1:B:273:SER:HB3	1:B:314:LYS:HG3	1.93	0.51
1:C:1022:ASP:OD1	1:C:1024:SER:HB2	2.11	0.51
1:A:208:GLN:HG3	1:A:214:ARG:HG2	1.92	0.51
1:B:1242:GLN:HB3	1:B:1248:PHE:CE1	2.46	0.51
1:A:371:LEU:HD11	1:A:423:VAL:HG21	1.91	0.51
1:B:1022:ASP:OD1	1:B:1024:SER:HB2	2.11	0.51
1:B:820:LYS:HD2	1:B:891:PRO:HB3	1.93	0.50
1:D:1125:LEU:HA	1:D:1128:LEU:HD12	1.93	0.50
1:D:133:THR:HG22	1:D:146:PHE:HB3	1.93	0.50
1:A:256:TYR:HA	1:A:787:ARG:HG2	1.92	0.50
1:A:589:ALA:HB3	1:A:746:VAL:HG21	1.93	0.50
1:B:1125:LEU:HA	1:B:1128:LEU:HD12	1.93	0.50
1:A:148:VAL:HG23	1:A:183:LEU:HD21	1.93	0.50
1:B:803:ILE:HB	1:B:806:GLU:HB2	1.91	0.50
1:D:1182:HIS:CD2	1:D:1237:TRP:HB3	2.46	0.50
1:C:1242:GLN:HB3	1:C:1248:PHE:CE1	2.46	0.50
1:B:1053:ARG:HH12	1:B:1113:PRO:HD2	1.77	0.50
1:D:345:ARG:HD3	1:D:438:SER:HA	1.92	0.50
1:A:345:ARG:HD3	1:A:438:SER:HA	1.94	0.50
1:A:993:THR:HB	1:A:995:GLN:HE21	1.75	0.50
1:A:1242:GLN:HB3	1:A:1248:PHE:CE1	2.46	0.50
1:B:993:THR:HB	1:B:995:GLN:HE21	1.76	0.50
1:A:387:ARG:HB2	1:A:420:THR:HB	1.94	0.50
1:A:390:GLU:HG3	1:A:417:THR:HA	1.94	0.50
1:D:589:ALA:HB3	1:D:746:VAL:HG21	1.93	0.50
1:C:1053:ARG:HH12	1:C:1113:PRO:HD2	1.77	0.50
1:C:1385:MET:HB2	1:C:1413:ASN:HB3	1.93	0.50
1:A:1080:PHE:CE1	1:A:1105:ILE:HD11	2.47	0.50
1:C:1383:VAL:HG13	1:C:1447:VAL:HG22	1.94	0.49
1:A:1125:LEU:HA	1:A:1128:LEU:HD12	1.93	0.49
1:D:371:LEU:HD11	1:D:423:VAL:HG21	1.94	0.49
1:C:1175:VAL:HG22	1:C:1453:TYR:HA	1.93	0.49
1:B:828:LEU:HD21	1:B:834:PHE:HE1	1.77	0.49
1:C:498:LEU:HB3	1:C:505:ILE:HD11	1.94	0.49
1:D:1053:ARG:HH12	1:D:1113:PRO:HD2	1.77	0.49
1:D:177:GLN:HB2	1:D:1299:LEU:HD13	1.93	0.49
1:D:1022:ASP:OD1	1:D:1024:SER:HB2	2.11	0.49
1:C:133:THR:HG22	1:C:146:PHE:HB3	1.94	0.49
1:C:135:LYS:HE2	1:C:142:GLN:HE22	1.76	0.49
1:A:828:LEU:HD21	1:A:834:PHE:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LYS:HB3	1:B:678:PHE:HD2	1.78	0.49
1:C:826:VAL:HG13	1:C:874:ALA:HB2	1.94	0.49
1:C:1408:THR:HG22	1:C:1417:ILE:HG12	1.93	0.49
1:C:371:LEU:HD11	1:C:423:VAL:HG21	1.93	0.49
1:B:265:THR:HG23	1:B:323:GLU:HB2	1.94	0.49
1:A:1206:VAL:HG11	1:A:1241:GLN:HG3	1.94	0.49
1:A:1183:TRP:HE3	1:A:1209:THR:HG22	1.77	0.49
1:D:826:VAL:HG13	1:D:874:ALA:HB2	1.94	0.49
1:B:1106:THR:HG21	1:B:1128:LEU:HD11	1.94	0.49
1:B:230:GLU:HB2	1:B:606:LEU:HD22	1.95	0.49
1:D:350:LEU:HD13	1:D:421:VAL:HB	1.93	0.49
1:A:920:LEU:HD12	1:A:1324:LEU:HD13	1.95	0.49
1:B:913:GLU:HG3	1:B:1329:LYS:HG3	1.94	0.49
1:C:820:LYS:HD2	1:C:891:PRO:HB3	1.94	0.49
1:B:1206:VAL:HG11	1:B:1241:GLN:HG3	1.95	0.49
1:A:133:THR:HG22	1:A:146:PHE:HB3	1.95	0.49
1:A:1053:ARG:HH12	1:A:1113:PRO:HD2	1.78	0.49
1:C:828:LEU:HD21	1:C:834:PHE:HE1	1.78	0.49
1:C:1399:LEU:HB3	1:C:1405:VAL:HG21	1.94	0.49
1:B:321:HIS:CD2	1:B:337:GLY:HA3	2.48	0.49
1:A:1075:LYS:C	1:A:1077:ASN:H	2.16	0.49
1:D:116:LYS:HB3	1:D:678:PHE:HD2	1.77	0.49
1:C:390:GLU:HG3	1:C:417:THR:HA	1.95	0.49
1:B:1119:PRO:HB2	1:C:117:ARG:HH22	1.77	0.49
1:B:498:LEU:HB3	1:B:505:ILE:HD11	1.96	0.48
1:C:265:THR:HG23	1:C:323:GLU:HB2	1.94	0.48
1:C:350:LEU:HD13	1:C:421:VAL:HB	1.94	0.48
1:D:391:ALA:HB2	1:D:413:ASN:HD21	1.78	0.48
1:D:230:GLU:HB2	1:D:606:LEU:HD22	1.95	0.48
1:D:1206:VAL:HG11	1:D:1241:GLN:HG3	1.95	0.48
1:C:1183:TRP:HE3	1:C:1209:THR:HG22	1.78	0.48
1:C:823:ARG:HG2	1:C:845:PRO:HB2	1.95	0.48
1:D:498:LEU:HB3	1:D:505:ILE:HD11	1.95	0.48
1:A:230:GLU:HB2	1:A:606:LEU:HD22	1.94	0.48
1:D:920:LEU:HD12	1:D:1324:LEU:HD13	1.96	0.48
1:B:390:GLU:HG3	1:B:417:THR:HA	1.95	0.48
1:B:387:ARG:HB2	1:B:420:THR:HB	1.95	0.48
1:A:265:THR:HG23	1:A:323:GLU:HB2	1.94	0.48
1:C:1075:LYS:C	1:C:1077:ASN:H	2.16	0.48
1:D:820:LYS:HD2	1:D:891:PRO:HB3	1.96	0.48
1:A:1119:PRO:HB2	1:D:117:ARG:HH12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:TYR:CZ	1:C:522:GLY:HA3	2.49	0.48
1:D:261:PRO:HD2	1:D:853:ARG:NH2	2.28	0.48
1:C:116:LYS:HB3	1:C:678:PHE:HD2	1.78	0.48
1:C:860:VAL:HG11	1:C:870:PHE:HE2	1.78	0.48
1:A:350:LEU:HD13	1:A:421:VAL:HB	1.95	0.48
1:B:1183:TRP:HE3	1:B:1209:THR:HG22	1.77	0.48
1:A:498:LEU:HB3	1:A:505:ILE:HD11	1.96	0.48
1:A:116:LYS:HB3	1:A:678:PHE:HD2	1.79	0.48
1:A:261:PRO:HD2	1:A:853:ARG:NH2	2.28	0.48
1:D:387:ARG:HB2	1:D:420:THR:HB	1.96	0.48
1:C:321:HIS:CD2	1:C:337:GLY:HA3	2.49	0.48
1:C:1206:VAL:HG11	1:C:1241:GLN:HG3	1.96	0.48
1:C:1379:ALA:HB2	1:C:1422:VAL:HG13	1.96	0.48
1:D:321:HIS:CD2	1:D:337:GLY:HA3	2.48	0.48
1:C:538:ALA:HB3	1:C:558:TYR:HB2	1.96	0.47
1:C:1080:PHE:CE1	1:C:1105:ILE:HD11	2.49	0.47
1:B:920:LEU:HD12	1:B:1324:LEU:HD13	1.95	0.47
1:B:1306:PRO:O	1:B:1307:GLU:HB2	2.15	0.47
1:A:619:TYR:CD1	1:A:619:TYR:N	2.82	0.47
1:D:1232:THR:HG22	1:D:1264:TYR:OH	2.14	0.47
1:D:1080:PHE:CE1	1:D:1105:ILE:HD11	2.49	0.47
1:D:619:TYR:CD1	1:D:619:TYR:N	2.83	0.47
1:C:261:PRO:HD2	1:C:853:ARG:NH2	2.30	0.47
1:D:828:LEU:HD21	1:D:834:PHE:HE1	1.78	0.47
1:B:1075:LYS:C	1:B:1077:ASN:H	2.17	0.47
1:B:823:ARG:HG2	1:B:845:PRO:HB2	1.97	0.47
1:C:1343:LEU:HD13	1:C:1449:VAL:HB	1.97	0.47
1:D:1145:TYR:HB3	1:D:1185:ARG:HH21	1.79	0.47
1:B:619:TYR:N	1:B:619:TYR:CD1	2.83	0.47
1:A:820:LYS:HD2	1:A:891:PRO:HB3	1.95	0.47
1:A:823:ARG:HG2	1:A:845:PRO:HB2	1.96	0.47
1:B:1118:HIS:CD2	1:B:1120:VAL:H	2.33	0.47
1:A:1106:THR:HG21	1:A:1128:LEU:HD11	1.95	0.47
1:C:1232:THR:HG22	1:C:1264:TYR:OH	2.15	0.47
1:A:581:SER:HA	1:A:756:VAL:HG13	1.97	0.47
1:A:321:HIS:CD2	1:A:337:GLY:HA3	2.49	0.47
1:C:1399:LEU:HD22	1:C:1429:LEU:HD23	1.97	0.47
1:D:1183:TRP:HE3	1:D:1209:THR:HG22	1.80	0.47
1:D:390:GLU:HG3	1:D:417:THR:HA	1.96	0.47
1:B:238:ILE:HG12	1:B:375:LYS:HG2	1.97	0.47
1:B:538:ALA:HB3	1:B:558:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:984:ILE:HB	1:D:1008:LEU:HD11	1.97	0.47
1:B:1080:PHE:CE1	1:B:1105:ILE:HD11	2.50	0.47
1:D:480:TYR:CZ	1:D:522:GLY:HA3	2.50	0.47
1:D:823:ARG:HG2	1:D:845:PRO:HB2	1.97	0.47
1:C:1118:HIS:CD2	1:C:1120:VAL:H	2.34	0.46
1:B:860:VAL:HG11	1:B:870:PHE:HE2	1.80	0.46
1:B:480:TYR:CZ	1:B:522:GLY:HA3	2.50	0.46
1:A:480:TYR:CZ	1:A:522:GLY:HA3	2.50	0.46
1:D:1075:LYS:C	1:D:1077:ASN:H	2.17	0.46
1:A:615:ALA:O	1:A:619:TYR:CE1	2.69	0.46
1:C:387:ARG:HB2	1:C:420:THR:HB	1.96	0.46
1:C:1106:THR:HG21	1:C:1128:LEU:HD11	1.97	0.46
1:D:860:VAL:HG11	1:D:870:PHE:HE2	1.80	0.46
1:C:231:VAL:HB	1:C:336:THR:HG21	1.97	0.46
1:D:935:LEU:HB3	1:D:939:VAL:HG21	1.98	0.46
1:C:984:ILE:HB	1:C:1008:LEU:HD11	1.96	0.46
1:C:985:TYR:CE2	1:C:1259:HIS:HB2	2.50	0.46
1:A:913:GLU:HG3	1:A:1329:LYS:HG3	1.96	0.46
2:B:2501:NAG:C8	2:B:2502:NAG:H82	2.42	0.46
1:B:261:PRO:HD2	1:B:853:ARG:NH2	2.29	0.46
1:D:1118:HIS:CD2	1:D:1120:VAL:H	2.34	0.46
1:A:117:ARG:HH12	1:D:1119:PRO:HB2	1.80	0.46
1:B:391:ALA:HB2	1:B:413:ASN:HD21	1.81	0.46
1:A:1145:TYR:HB3	1:A:1185:ARG:HH21	1.80	0.46
1:A:1145:TYR:HD1	1:A:1208:MET:HB3	1.80	0.46
1:C:581:SER:HA	1:C:756:VAL:HG13	1.97	0.46
1:C:1145:TYR:HB3	1:C:1185:ARG:HH21	1.80	0.46
1:B:1232:THR:HG22	1:B:1264:TYR:OH	2.15	0.46
1:C:913:GLU:HG3	1:C:1329:LYS:HG3	1.98	0.46
1:C:230:GLU:HB2	1:C:606:LEU:HD22	1.97	0.46
1:A:538:ALA:HB3	1:A:558:TYR:HB2	1.98	0.46
1:A:860:VAL:HG11	1:A:870:PHE:HE2	1.81	0.46
1:C:391:ALA:HB2	1:C:413:ASN:HD21	1.80	0.46
1:C:1381:VAL:HG22	1:C:1449:VAL:HG23	1.98	0.46
1:D:1106:THR:HG21	1:D:1128:LEU:HD11	1.97	0.46
1:C:108:LYS:HA	1:C:113:GLU:HG3	1.98	0.46
1:C:1306:PRO:O	1:C:1307:GLU:HB2	2.16	0.46
1:C:920:LEU:HD12	1:C:1324:LEU:HD13	1.97	0.46
1:B:581:SER:HA	1:B:756:VAL:HG13	1.98	0.46
1:A:1306:PRO:O	1:A:1307:GLU:HB2	2.16	0.46
1:A:391:ALA:HB2	1:A:413:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:VAL:HG23	1:A:405:VAL:HG23	1.98	0.46
1:C:1145:TYR:HD1	1:C:1208:MET:HB3	1.81	0.46
1:C:1213:LEU:HD23	1:C:1260:ALA:HB1	1.98	0.46
1:D:1306:PRO:O	1:D:1307:GLU:HB2	2.16	0.46
1:D:913:GLU:HG3	1:D:1329:LYS:HG3	1.98	0.46
1:C:615:ALA:O	1:C:619:TYR:CE1	2.69	0.46
1:A:1118:HIS:CD2	1:A:1120:VAL:H	2.33	0.46
1:B:984:ILE:HB	1:B:1008:LEU:HD11	1.97	0.46
1:A:238:ILE:HG12	1:A:375:LYS:HG2	1.97	0.45
1:C:1417:ILE:HD13	1:C:1429:LEU:HD22	1.98	0.45
1:C:1250:SER:HB2	1:C:1253:ASP:OD1	2.15	0.45
1:B:1145:TYR:HB3	1:B:1185:ARG:HH21	1.80	0.45
1:A:984:ILE:HB	1:A:1008:LEU:HD11	1.97	0.45
1:D:31:TYR:H	1:D:680:ASN:CB	2.30	0.45
1:B:958:ALA:HB1	1:B:1248:PHE:HZ	1.81	0.45
1:D:958:ALA:HB1	1:D:1248:PHE:HZ	1.80	0.45
1:D:581:SER:HA	1:D:756:VAL:HG13	1.97	0.45
1:D:369:VAL:HG23	1:D:405:VAL:HG23	1.98	0.45
1:D:1278:VAL:HB	1:D:1290:PHE:HB2	1.99	0.45
1:D:238:ILE:HG12	1:D:375:LYS:HG2	1.98	0.45
1:C:1038:ASN:ND2	1:C:1041:LEU:H	2.15	0.45
1:D:1145:TYR:HD1	1:D:1208:MET:HB3	1.81	0.45
1:C:61:SER:HB3	1:C:74:PHE:CE1	2.52	0.45
1:D:538:ALA:HB3	1:D:558:TYR:HB2	1.98	0.45
1:C:958:ALA:HB1	1:C:1248:PHE:HZ	1.81	0.45
1:D:1250:SER:HB2	1:D:1253:ASP:OD1	2.17	0.45
1:B:985:TYR:CE2	1:B:1259:HIS:HB2	2.52	0.45
1:B:1250:SER:HB2	1:B:1253:ASP:OD1	2.16	0.45
1:A:1152:TYR:O	1:A:1156:LEU:HB2	2.17	0.45
1:D:1092:LYS:HB3	1:D:1093:GLY:H	1.63	0.45
1:C:619:TYR:CD1	1:C:619:TYR:N	2.84	0.44
1:A:1232:THR:HG22	1:A:1264:TYR:OH	2.16	0.44
1:C:369:VAL:HG23	1:C:405:VAL:HG23	1.99	0.44
1:B:1213:LEU:HD23	1:B:1260:ALA:HB1	1.99	0.44
1:C:387:ARG:HG3	1:C:422:ARG:HD2	2.00	0.44
1:D:387:ARG:HG3	1:D:422:ARG:HD2	1.99	0.44
1:A:985:TYR:CE2	1:A:1259:HIS:HB2	2.52	0.44
1:D:108:LYS:HA	1:D:113:GLU:HG3	1.99	0.44
1:A:935:LEU:HB3	1:A:939:VAL:HG21	1.99	0.44
1:D:128:LEU:HD23	1:D:621:LEU:HB3	2.00	0.44
2:A:2501:NAG:C8	2:A:2502:NAG:H82	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:ALA:O	1:B:619:TYR:CE1	2.69	0.44
1:D:615:ALA:O	1:D:619:TYR:CE1	2.70	0.44
1:D:1038:ASN:ND2	1:D:1041:LEU:H	2.15	0.44
1:A:31:TYR:H	1:A:680:ASN:CB	2.31	0.44
2:C:2501:NAG:C8	2:C:2502:NAG:H82	2.43	0.44
1:B:1038:ASN:ND2	1:B:1041:LEU:H	2.16	0.44
1:A:1193:VAL:HB	1:B:387:ARG:NH1	2.33	0.44
1:C:388:GLY:HA3	1:C:393:TYR:H	1.83	0.44
1:B:231:VAL:HB	1:B:336:THR:HG21	2.00	0.44
1:C:599:ALA:HB3	1:C:740:ILE:H	1.82	0.44
1:B:259:PRO:HG2	1:B:297:HIS:HA	2.00	0.44
1:A:380:PRO:HB3	1:A:401:GLU:HA	2.00	0.44
1:B:581:SER:O	1:B:756:VAL:HA	2.18	0.44
1:D:388:GLY:HA3	1:D:393:TYR:H	1.82	0.44
1:C:238:ILE:HG12	1:C:375:LYS:HG2	1.99	0.44
1:D:1281:GLN:HA	1:D:1287:SER:HB3	2.00	0.44
1:A:958:ALA:HB1	1:A:1248:PHE:HZ	1.82	0.44
1:B:1145:TYR:HD1	1:B:1208:MET:HB3	1.81	0.44
1:A:1110:LEU:HD22	1:A:1156:LEU:HG	1.99	0.44
1:B:369:VAL:HG23	1:B:405:VAL:HG23	1.99	0.44
1:B:108:LYS:HA	1:B:113:GLU:HG3	1.99	0.44
1:D:985:TYR:CE2	1:D:1259:HIS:HB2	2.53	0.44
1:B:935:LEU:HB3	1:B:939:VAL:HG21	1.99	0.44
1:D:380:PRO:HB3	1:D:401:GLU:HA	1.99	0.44
1:C:1177:LYS:HG3	1:C:1455:THR:HG21	1.98	0.44
1:C:31:TYR:H	1:C:680:ASN:CB	2.31	0.44
1:A:599:ALA:HB3	1:A:740:ILE:H	1.83	0.44
4:A:2601:NAG:C8	4:A:2602:NAG:H83	2.48	0.44
1:A:1250:SER:HB2	1:A:1253:ASP:OD1	2.18	0.44
1:D:581:SER:O	1:D:756:VAL:HA	2.18	0.44
1:C:1152:TYR:O	1:C:1156:LEU:HB2	2.17	0.44
1:B:128:LEU:HD23	1:B:621:LEU:HB3	1.99	0.44
1:B:797:THR:HB	1:B:811:LYS:HB2	2.00	0.44
1:B:380:PRO:HB3	1:B:401:GLU:HA	2.00	0.44
1:B:602:GLN:HB3	1:B:763:THR:HG23	2.00	0.44
1:A:1101:LEU:O	1:A:1105:ILE:HG23	2.18	0.43
1:D:61:SER:HB3	1:D:74:PHE:CE1	2.53	0.43
1:A:1213:LEU:HD23	1:A:1260:ALA:HB1	2.00	0.43
1:A:108:LYS:HA	1:A:113:GLU:HG3	1.99	0.43
1:C:380:PRO:HB3	1:C:401:GLU:HA	2.00	0.43
1:A:984:ILE:HD12	1:A:1051:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1448:LYS:HA	1:C:1460:ILE:HG12	2.01	0.43
1:D:602:GLN:HB3	1:D:763:THR:HG23	2.00	0.43
1:C:156:HIS:HB3	1:C:777:GLY:HA2	2.00	0.43
1:D:231:VAL:HB	1:D:336:THR:HG21	1.99	0.43
1:B:31:TYR:H	1:B:680:ASN:CB	2.30	0.43
1:B:388:GLY:HA3	1:B:393:TYR:H	1.82	0.43
1:B:1279:THR:HG22	1:B:1289:LYS:HG3	2.01	0.43
1:A:1038:ASN:ND2	1:A:1041:LEU:H	2.15	0.43
1:A:231:VAL:HB	1:A:336:THR:HG21	2.00	0.43
1:B:822:ILE:HG22	1:B:889:SER:HA	2.01	0.43
1:C:1278:VAL:HB	1:C:1290:PHE:HB2	2.01	0.43
1:D:1101:LEU:O	1:D:1105:ILE:HG23	2.18	0.43
1:A:1279:THR:HG22	1:A:1289:LYS:HG3	2.01	0.43
1:B:599:ALA:HB3	1:B:740:ILE:H	1.84	0.43
1:B:100:VAL:HG22	1:B:121:MET:HG2	2.00	0.43
4:D:2601:NAG:C8	4:D:2602:NAG:H83	2.48	0.43
1:D:903:LEU:HD23	1:D:904:LEU:H	1.84	0.43
1:C:1182:HIS:ND1	1:C:1237:TRP:HE3	2.17	0.43
4:C:2601:NAG:C8	4:C:2602:NAG:H83	2.48	0.43
1:D:1152:TYR:O	1:D:1156:LEU:HB2	2.18	0.43
1:C:970:TYR:HA	1:C:1014:ARG:HH21	1.84	0.43
1:D:822:ILE:HG22	1:D:889:SER:HA	2.00	0.43
1:A:1305:LEU:HA	1:A:1306:PRO:HD3	1.95	0.43
1:B:970:TYR:HA	1:B:1014:ARG:HH21	1.84	0.43
1:C:797:THR:HB	1:C:811:LYS:HB2	2.00	0.43
4:B:2601:NAG:C8	4:B:2602:NAG:H83	2.49	0.43
1:B:1278:VAL:HB	1:B:1290:PHE:HB2	2.00	0.43
1:A:1182:HIS:ND1	1:A:1237:TRP:HE3	2.16	0.43
1:A:581:SER:O	1:A:756:VAL:HA	2.19	0.43
1:C:935:LEU:HB3	1:C:939:VAL:HG21	2.01	0.43
1:B:933:LEU:H	1:B:1310:GLY:HA2	1.84	0.42
1:D:933:LEU:H	1:D:1310:GLY:HA2	1.84	0.42
1:C:46:LYS:HA	1:C:88:ALA:HA	2.01	0.42
1:D:167:ILE:HG22	1:D:175:ILE:HD12	2.01	0.42
1:A:259:PRO:HG2	1:A:297:HIS:HA	2.01	0.42
1:D:599:ALA:HB3	1:D:740:ILE:H	1.83	0.42
1:A:797:THR:HB	1:A:811:LYS:HB2	2.01	0.42
1:A:822:ILE:HG22	1:A:889:SER:HA	2.00	0.42
1:C:933:LEU:H	1:C:1310:GLY:HA2	1.84	0.42
1:D:46:LYS:HA	1:D:88:ALA:HA	2.01	0.42
1:A:1278:VAL:HB	1:A:1290:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1182:HIS:ND1	1:D:1237:TRP:HE3	2.16	0.42
1:A:61:SER:HB3	1:A:74:PHE:CE1	2.54	0.42
1:B:156:HIS:HB3	1:B:777:GLY:HA2	2.01	0.42
1:D:970:TYR:HA	1:D:1014:ARG:HH21	1.84	0.42
1:A:388:GLY:HA3	1:A:393:TYR:H	1.83	0.42
1:B:1281:GLN:HA	1:B:1287:SER:HB3	2.00	0.42
1:D:360:ARG:HH11	1:D:458:PHE:HB2	1.85	0.42
1:B:1152:TYR:O	1:B:1156:LEU:HB2	2.18	0.42
1:A:1092:LYS:HB3	1:A:1093:GLY:H	1.63	0.42
1:B:61:SER:HB3	1:B:74:PHE:CE1	2.54	0.42
1:A:903:LEU:HD23	1:A:904:LEU:H	1.85	0.42
1:C:1376:SER:HB3	1:C:1422:VAL:HG21	2.01	0.42
1:B:820:LYS:HD3	1:B:888:PRO:HB2	2.01	0.42
1:D:820:LYS:HD3	1:D:888:PRO:HB2	2.01	0.42
1:B:1101:LEU:O	1:B:1105:ILE:HG23	2.20	0.42
1:C:1281:GLN:HA	1:C:1287:SER:HB3	2.02	0.42
1:D:797:THR:HB	1:D:811:LYS:HB2	2.01	0.42
1:B:1206:VAL:HG23	1:B:1253:ASP:OD2	2.19	0.42
1:D:734:TYR:H	1:D:759:PRO:HB2	1.85	0.42
1:A:46:LYS:HA	1:A:88:ALA:HA	2.02	0.42
1:B:360:ARG:HH11	1:B:458:PHE:HB2	1.85	0.42
1:C:360:ARG:HH11	1:C:458:PHE:HB2	1.83	0.42
1:D:100:VAL:HG22	1:D:121:MET:HG2	2.02	0.42
1:C:1377:ASN:O	1:C:1421:LYS:HG3	2.19	0.42
1:A:970:TYR:HA	1:A:1014:ARG:HH21	1.84	0.42
1:A:1050:ALA:O	1:A:1053:ARG:HD3	2.20	0.42
1:B:1182:HIS:ND1	1:B:1237:TRP:HE3	2.17	0.42
1:C:422:ARG:NE	1:D:1193:VAL:HG21	2.35	0.42
1:C:820:LYS:HD3	1:C:888:PRO:HB2	2.02	0.42
1:D:1206:VAL:HG23	1:D:1253:ASP:OD2	2.20	0.42
1:C:1101:LEU:O	1:C:1105:ILE:HG23	2.19	0.42
1:D:61:SER:HB3	1:D:74:PHE:HE1	1.85	0.42
1:D:49:VAL:HG21	1:D:60:VAL:HG21	2.02	0.42
1:C:1206:VAL:HG23	1:C:1253:ASP:OD2	2.20	0.41
1:B:984:ILE:HD12	1:B:1051:GLN:HG3	2.02	0.41
1:C:1039:THR:HG21	1:C:1081:ARG:O	2.20	0.41
1:B:1094:GLY:HA2	1:B:1145:TYR:HE2	1.86	0.41
1:B:330:GLY:C	1:B:332:VAL:H	2.24	0.41
1:A:128:LEU:HD23	1:A:621:LEU:HB3	2.01	0.41
1:D:1039:THR:HG21	1:D:1081:ARG:O	2.20	0.41
1:A:360:ARG:HH11	1:A:458:PHE:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:TYR:H	1:B:759:PRO:HB2	1.86	0.41
1:B:1331:ASN:HD22	1:B:1331:ASN:N	2.18	0.41
1:C:802:VAL:HG21	1:C:808:PHE:CD1	2.55	0.41
1:A:602:GLN:HB3	1:A:763:THR:HG23	2.02	0.41
1:B:260:VAL:HA	1:B:261:PRO:HD3	1.94	0.41
1:A:820:LYS:HD3	1:A:888:PRO:HB2	2.01	0.41
1:D:156:HIS:HB3	1:D:777:GLY:HA2	2.03	0.41
1:C:167:ILE:HG22	1:C:175:ILE:HD12	2.03	0.41
1:A:387:ARG:HG3	1:A:422:ARG:HD2	2.02	0.41
1:C:822:ILE:HG22	1:C:889:SER:HA	2.01	0.41
1:A:734:TYR:H	1:A:759:PRO:HB2	1.85	0.41
1:A:933:LEU:H	1:A:1310:GLY:HA2	1.84	0.41
1:A:388:GLY:O	1:A:392:ASN:HA	2.21	0.41
1:D:259:PRO:HG2	1:D:297:HIS:HA	2.02	0.41
1:B:137:ILE:H	1:B:137:ILE:HG13	1.76	0.41
1:A:1333:LEU:H	1:A:1334:PRO:HD2	1.86	0.41
1:A:542:ILE:O	1:A:553:GLY:HA3	2.21	0.41
1:C:602:GLN:HB3	1:C:763:THR:HG23	2.02	0.41
1:C:330:GLY:C	1:C:332:VAL:H	2.24	0.41
1:D:330:GLY:C	1:D:332:VAL:H	2.24	0.41
1:C:1279:THR:HG22	1:C:1289:LYS:HG3	2.03	0.41
1:D:802:VAL:HG21	1:D:808:PHE:CD1	2.55	0.41
1:C:734:TYR:H	1:C:759:PRO:HB2	1.85	0.41
1:C:581:SER:O	1:C:756:VAL:HA	2.20	0.41
1:A:758:VAL:HA	1:A:759:PRO:HD3	1.88	0.41
1:C:259:PRO:HG2	1:C:297:HIS:HA	2.02	0.41
1:C:1333:LEU:H	1:C:1334:PRO:HD2	1.85	0.41
1:C:903:LEU:HD23	1:C:904:LEU:H	1.85	0.41
1:B:903:LEU:HD23	1:B:904:LEU:H	1.86	0.41
1:B:961:ASN:HB2	1:B:1246:GLY:HA3	2.03	0.41
1:C:961:ASN:HB2	1:C:1246:GLY:HA3	2.03	0.41
1:D:388:GLY:O	1:D:392:ASN:HA	2.21	0.41
1:B:991:ASN:O	4:B:2601:NAG:H61	2.21	0.41
1:C:137:ILE:H	1:C:137:ILE:HG13	1.75	0.41
1:D:192:PHE:HA	1:D:193:PRO:HD3	1.99	0.41
1:C:1118:HIS:HD2	1:C:1120:VAL:HG22	1.84	0.41
1:B:1050:ALA:O	1:B:1053:ARG:HD3	2.21	0.41
1:C:1050:ALA:HA	1:C:1053:ARG:HD3	2.02	0.41
1:B:1183:TRP:H	1:B:1209:THR:CG2	2.34	0.41
1:C:1094:GLY:HA2	1:C:1145:TYR:HE2	1.86	0.41
1:A:1039:THR:HG21	1:A:1081:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1297:ARG:HH22	1:B:1320:GLY:HA3	1.86	0.41
1:A:1331:ASN:HD22	1:A:1331:ASN:N	2.19	0.41
1:D:468:LEU:HA	1:D:469:PRO:HD3	2.00	0.41
1:A:1206:VAL:HG23	1:A:1253:ASP:OD2	2.22	0.40
1:C:758:VAL:HA	1:C:759:PRO:HD3	1.87	0.40
1:A:330:GLY:C	1:A:332:VAL:H	2.24	0.40
1:C:542:ILE:O	1:C:553:GLY:HA3	2.21	0.40
1:A:802:VAL:HG21	1:A:808:PHE:CD1	2.56	0.40
1:C:1106:THR:HG22	1:C:1124:ALA:HB1	2.03	0.40
1:D:984:ILE:HD12	1:D:1051:GLN:HG3	2.03	0.40
1:B:388:GLY:O	1:B:392:ASN:HA	2.21	0.40
1:D:1110:LEU:HD22	1:D:1156:LEU:HG	2.03	0.40
1:D:758:VAL:HA	1:D:759:PRO:HD3	1.88	0.40
1:B:1039:THR:HG21	1:B:1081:ARG:O	2.21	0.40
1:A:100:VAL:HG22	1:A:121:MET:HG2	2.02	0.40
1:D:1050:ALA:O	1:D:1053:ARG:HD3	2.21	0.40
1:C:388:GLY:O	1:C:392:ASN:HA	2.21	0.40
1:C:204:LYS:HD2	1:C:216:GLU:HG2	2.03	0.40
1:D:593:SER:HB3	1:D:773:SER:HB2	2.03	0.40
1:B:542:ILE:O	1:B:553:GLY:HA3	2.21	0.40
1:D:1279:THR:HG22	1:D:1289:LYS:HG3	2.03	0.40
1:A:961:ASN:HB2	1:A:1246:GLY:HA3	2.03	0.40
1:A:1305:LEU:HD13	1:A:1312:TYR:CD1	2.57	0.40
1:A:61:SER:HB3	1:A:74:PHE:HE1	1.87	0.40
1:B:61:SER:HB3	1:B:74:PHE:HE1	1.86	0.40
1:B:593:SER:HB3	1:B:773:SER:HB2	2.02	0.40
1:B:1118:HIS:HD2	1:B:1120:VAL:HG22	1.84	0.40
1:C:1183:TRP:H	1:C:1209:THR:CG2	2.34	0.40
1:A:984:ILE:HG13	1:A:1052:ALA:HA	2.04	0.40
1:C:468:LEU:HD22	1:C:474:GLN:HG3	2.03	0.40
1:B:802:VAL:HG21	1:B:808:PHE:CD1	2.57	0.40
1:C:1331:ASN:N	1:C:1331:ASN:HD22	2.19	0.40
1:D:542:ILE:O	1:D:553:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1265/1451 (87%)	1061 (84%)	147 (12%)	57 (4%)	3	34
1	B	1265/1451 (87%)	1058 (84%)	149 (12%)	58 (5%)	3	33
1	C	1398/1451 (96%)	1162 (83%)	177 (13%)	59 (4%)	3	35
1	D	1265/1451 (87%)	1059 (84%)	149 (12%)	57 (4%)	3	34
All	All	5193/5804 (90%)	4340 (84%)	622 (12%)	231 (4%)	3	34

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	PRO
1	A	425	TYR
1	A	429	SER
1	A	580	ALA
1	A	736	PRO
1	A	761	THR
1	A	953	ASP
1	A	1095	VAL
1	A	1199	PRO
1	A	1307	GLU
1	B	425	TYR
1	B	429	SER
1	B	580	ALA
1	B	736	PRO
1	B	761	THR
1	B	953	ASP
1	B	1095	VAL
1	B	1199	PRO
1	B	1307	GLU
1	C	429	SER
1	C	580	ALA
1	C	736	PRO

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Mol	Chain	Res	Type
1	C	761	THR
1	C	953	ASP
1	C	1095	VAL
1	C	1199	PRO
1	C	1307	GLU
1	D	429	SER
1	D	580	ALA
1	D	736	PRO
1	D	761	THR
1	D	953	ASP
1	D	1095	VAL
1	D	1199	PRO
1	D	1307	GLU
1	A	81	ASN
1	A	255	THR
1	A	296	SER
1	A	309	PHE
1	A	331	THR
1	A	581	SER
1	A	739	TRP
1	A	748	SER
1	A	1076	ASP
1	A	1096	GLU
1	B	81	ASN
1	B	198	PRO
1	B	255	THR
1	B	296	SER
1	B	581	SER
1	B	739	TRP
1	B	748	SER
1	B	1076	ASP
1	B	1096	GLU
1	C	81	ASN
1	C	198	PRO
1	C	255	THR
1	C	296	SER
1	C	330	GLY
1	C	425	TYR
1	C	581	SER
1	C	739	TRP
1	C	1076	ASP
1	C	1096	GLU

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Mol	Chain	Res	Type
1	D	81	ASN
1	D	198	PRO
1	D	255	THR
1	D	296	SER
1	D	309	PHE
1	D	425	TYR
1	D	581	SER
1	D	739	TRP
1	D	1076	ASP
1	D	1096	GLU
1	A	311	LEU
1	A	330	GLY
1	A	734	TYR
1	A	762	ILE
1	A	883	CYS
1	A	1060	GLU
1	A	1116	VAL
1	A	1142	SER
1	A	1191	ALA
1	A	1236	LYS
1	B	309	PHE
1	B	311	LEU
1	B	330	GLY
1	B	331	THR
1	B	734	TYR
1	B	762	ILE
1	B	1060	GLU
1	B	1116	VAL
1	B	1142	SER
1	B	1191	ALA
1	B	1236	LYS
1	C	309	PHE
1	C	311	LEU
1	C	331	THR
1	C	630	PHE
1	C	734	TYR
1	C	748	SER
1	C	762	ILE
1	C	883	CYS
1	C	1060	GLU
1	C	1116	VAL
1	C	1142	SER

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Mol	Chain	Res	Type
1	C	1187	GLN
1	C	1387	SER
1	C	1460	ILE
1	D	311	LEU
1	D	330	GLY
1	D	331	THR
1	D	734	TYR
1	D	748	SER
1	D	762	ILE
1	D	883	CYS
1	D	1060	GLU
1	D	1116	VAL
1	D	1142	SER
1	D	1187	GLN
1	D	1236	LYS
1	A	180	SER
1	A	241	ILE
1	A	254	TYR
1	A	630	PHE
1	A	1092	LYS
1	A	1144	VAL
1	A	1187	GLN
1	A	1222	ALA
1	A	1283	SER
1	A	1333	LEU
1	B	180	SER
1	B	241	ILE
1	B	254	TYR
1	B	454	PRO
1	B	630	PHE
1	B	883	CYS
1	B	1092	LYS
1	B	1144	VAL
1	B	1222	ALA
1	B	1283	SER
1	B	1333	LEU
1	C	180	SER
1	C	241	ILE
1	C	254	TYR
1	C	737	GLU
1	C	749	ALA
1	C	1092	LYS

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Mol	Chain	Res	Type
1	C	1144	VAL
1	C	1191	ALA
1	C	1222	ALA
1	C	1236	LYS
1	C	1333	LEU
1	C	1338	GLU
1	D	180	SER
1	D	241	ILE
1	D	254	TYR
1	D	454	PRO
1	D	630	PHE
1	D	642	CYS
1	D	1092	LYS
1	D	1144	VAL
1	D	1191	ALA
1	D	1222	ALA
1	D	1333	LEU
1	A	454	PRO
1	A	642	CYS
1	A	648	VAL
1	A	737	GLU
1	A	749	ALA
1	A	1113	PRO
1	A	1242	GLN
1	B	281	GLU
1	B	521	LYS
1	B	642	CYS
1	B	737	GLU
1	B	749	ALA
1	B	1113	PRO
1	B	1242	GLN
1	B	1273	GLY
1	C	281	GLU
1	C	339	GLN
1	C	454	PRO
1	C	632	GLY
1	C	648	VAL
1	C	1113	PRO
1	C	1242	GLN
1	D	281	GLU
1	D	339	GLN
1	D	632	GLY

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Mol	Chain	Res	Type
1	D	737	GLU
1	D	749	ALA
1	D	1113	PRO
1	D	1242	GLN
1	A	339	GLN
1	A	521	LYS
1	A	632	GLY
1	B	339	GLN
1	B	632	GLY
1	B	648	VAL
1	B	1179	ASN
1	C	521	LYS
1	C	683	ILE
1	C	1273	GLY
1	C	1283	SER
1	D	521	LYS
1	D	648	VAL
1	D	1283	SER
1	A	683	ILE
1	A	1273	GLY
1	B	683	ILE
1	D	683	ILE
1	D	1273	GLY
1	A	257	GLY
1	B	213	GLY
1	B	257	GLY
1	C	213	GLY
1	C	257	GLY
1	D	257	GLY
1	A	213	GLY
1	A	652	GLY
1	B	652	GLY
1	B	1188	LYS
1	C	652	GLY
1	D	652	GLY
1	C	437	VAL
1	D	213	GLY
1	D	437	VAL
1	A	437	VAL
1	A	1188	LYS
1	B	437	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1013/1268 (80%)	868 (86%)	145 (14%)	4	27
1	B	1013/1268 (80%)	869 (86%)	144 (14%)	4	28
1	C	1132/1268 (89%)	970 (86%)	162 (14%)	4	27
1	D	1013/1268 (80%)	868 (86%)	145 (14%)	4	27
All	All	4171/5072 (82%)	3575 (86%)	596 (14%)	4	27

All (596) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	34	LEU
1	A	42	GLU
1	A	56	GLU
1	A	60	VAL
1	A	82	ASP
1	A	114	PHE
1	A	121	MET
1	A	126	ASP
1	A	129	VAL
1	A	153	GLU
1	A	154	ASN
1	A	161	LEU
1	A	173	ASN
1	A	175	ILE
1	A	194	LEU
1	A	198	PRO
1	A	199	PHE
1	A	200	GLN
1	A	238	ILE
1	A	251	CYS
1	A	265	THR
1	A	268	ILE
1	A	294	LEU

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Mol	Chain	Res	Type
1	A	321	HIS
1	A	326	ILE
1	A	331	THR
1	A	333	VAL
1	A	334	GLU
1	A	335	LEU
1	A	336	THR
1	A	341	SER
1	A	347	ILE
1	A	353	VAL
1	A	357	SER
1	A	360	ARG
1	A	361	GLN
1	A	371	LEU
1	A	405	VAL
1	A	406	GLN
1	A	409	ILE
1	A	420	THR
1	A	421	VAL
1	A	432	TYR
1	A	458	PHE
1	A	474	GLN
1	A	505	ILE
1	A	511	HIS
1	A	520	MET
1	A	524	PHE
1	A	541	LEU
1	A	542	ILE
1	A	563	CYS
1	A	585	LEU
1	A	587	VAL
1	A	598	ARG
1	A	600	VAL
1	A	610	ASP
1	A	619	TYR
1	A	622	LEU
1	A	675	LEU
1	A	679	THR
1	A	683	ILE
1	A	740	ILE
1	A	742	ASP
1	A	754	VAL

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Mol	Chain	Res	Type
1	A	761	THR
1	A	764	GLU
1	A	778	LEU
1	A	780	ILE
1	A	786	LEU
1	A	793	PHE
1	A	818	LEU
1	A	821	CYS
1	A	826	VAL
1	A	828	LEU
1	A	842	GLU
1	A	843	GLN
1	A	848	ILE
1	A	849	CYS
1	A	855	THR
1	A	856	VAL
1	A	857	SER
1	A	865	LEU
1	A	872	VAL
1	A	875	GLU
1	A	893	HIS
1	A	897	ASP
1	A	903	LEU
1	A	908	GLU
1	A	916	PHE
1	A	919	LEU
1	A	929	GLU
1	A	931	LEU
1	A	938	ASN
1	A	942	GLU
1	A	949	SER
1	A	959	MET
1	A	961	ASN
1	A	968	MET
1	A	983	ASN
1	A	984	ILE
1	A	992	GLU
1	A	1000	ILE
1	A	1005	ILE
1	A	1008	LEU
1	A	1024	SER
1	A	1039	THR

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Mol	Chain	Res	Type
1	A	1046	LEU
1	A	1067	LEU
1	A	1073	ARG
1	A	1077	ASN
1	A	1086	LEU
1	A	1087	LEU
1	A	1089	ASN
1	A	1091	ILE
1	A	1100	THR
1	A	1101	LEU
1	A	1105	ILE
1	A	1107	ILE
1	A	1110	LEU
1	A	1112	ILE
1	A	1114	LEU
1	A	1125	LEU
1	A	1150	LEU
1	A	1163	ARG
1	A	1184	GLU
1	A	1206	VAL
1	A	1236	LYS
1	A	1242	GLN
1	A	1245	GLN
1	A	1252	GLN
1	A	1277	GLN
1	A	1280	ILE
1	A	1281	GLN
1	A	1289	LYS
1	A	1291	GLN
1	A	1292	VAL
1	A	1294	ASN
1	A	1295	ASN
1	A	1298	LEU
1	A	1315	LYS
1	A	1328	LEU
1	A	1331	ASN
1	A	1333	LEU
1	B	32	MET
1	B	34	LEU
1	B	42	GLU
1	B	56	GLU
1	B	60	VAL

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Mol	Chain	Res	Type
1	B	82	ASP
1	B	114	PHE
1	B	121	MET
1	B	126	ASP
1	B	129	VAL
1	B	153	GLU
1	B	154	ASN
1	B	161	LEU
1	B	173	ASN
1	B	175	ILE
1	B	194	LEU
1	B	195	SER
1	B	199	PHE
1	B	200	GLN
1	B	238	ILE
1	B	251	CYS
1	B	265	THR
1	B	268	ILE
1	B	294	LEU
1	B	321	HIS
1	B	326	ILE
1	B	331	THR
1	B	333	VAL
1	B	334	GLU
1	B	335	LEU
1	B	336	THR
1	B	341	SER
1	B	347	ILE
1	B	353	VAL
1	B	360	ARG
1	B	361	GLN
1	B	371	LEU
1	B	405	VAL
1	B	406	GLN
1	B	409	ILE
1	B	420	THR
1	B	421	VAL
1	B	432	TYR
1	B	458	PHE
1	B	474	GLN
1	B	505	ILE
1	B	511	HIS

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Mol	Chain	Res	Type
1	B	520	MET
1	B	524	PHE
1	B	541	LEU
1	B	542	ILE
1	B	563	CYS
1	B	585	LEU
1	B	587	VAL
1	B	598	ARG
1	B	600	VAL
1	B	610	ASP
1	B	619	TYR
1	B	622	LEU
1	B	675	LEU
1	B	679	THR
1	B	683	ILE
1	B	740	ILE
1	B	742	ASP
1	B	754	VAL
1	B	761	THR
1	B	764	GLU
1	B	778	LEU
1	B	780	ILE
1	B	786	LEU
1	B	793	PHE
1	B	818	LEU
1	B	821	CYS
1	B	826	VAL
1	B	828	LEU
1	B	842	GLU
1	B	843	GLN
1	B	848	ILE
1	B	849	CYS
1	B	855	THR
1	B	856	VAL
1	B	857	SER
1	B	865	LEU
1	B	872	VAL
1	B	875	GLU
1	B	893	HIS
1	B	897	ASP
1	B	902	PRO
1	B	903	LEU

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Mol	Chain	Res	Type
1	B	908	GLU
1	B	916	PHE
1	B	919	LEU
1	B	929	GLU
1	B	931	LEU
1	B	938	ASN
1	B	942	GLU
1	B	949	SER
1	B	959	MET
1	B	961	ASN
1	B	968	MET
1	B	983	ASN
1	B	984	ILE
1	B	992	GLU
1	B	1000	ILE
1	B	1005	ILE
1	B	1008	LEU
1	B	1024	SER
1	B	1039	THR
1	B	1046	LEU
1	B	1073	ARG
1	B	1077	ASN
1	B	1086	LEU
1	B	1087	LEU
1	B	1089	ASN
1	B	1091	ILE
1	B	1100	THR
1	B	1101	LEU
1	B	1105	ILE
1	B	1107	ILE
1	B	1110	LEU
1	B	1112	ILE
1	B	1114	LEU
1	B	1125	LEU
1	B	1150	LEU
1	B	1163	ARG
1	B	1184	GLU
1	B	1188	LYS
1	B	1206	VAL
1	B	1236	LYS
1	B	1242	GLN
1	B	1245	GLN

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Mol	Chain	Res	Type
1	B	1252	GLN
1	B	1277	GLN
1	B	1280	ILE
1	B	1281	GLN
1	B	1289	LYS
1	B	1291	GLN
1	B	1292	VAL
1	B	1294	ASN
1	B	1295	ASN
1	B	1298	LEU
1	B	1315	LYS
1	B	1328	LEU
1	B	1331	ASN
1	C	32	MET
1	C	34	LEU
1	C	42	GLU
1	C	56	GLU
1	C	60	VAL
1	C	82	ASP
1	C	114	PHE
1	C	121	MET
1	C	126	ASP
1	C	129	VAL
1	C	154	ASN
1	C	161	LEU
1	C	173	ASN
1	C	175	ILE
1	C	194	LEU
1	C	199	PHE
1	C	200	GLN
1	C	238	ILE
1	C	251	CYS
1	C	265	THR
1	C	268	ILE
1	C	294	LEU
1	C	321	HIS
1	C	326	ILE
1	C	331	THR
1	C	333	VAL
1	C	334	GLU
1	C	335	LEU
1	C	336	THR

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Mol	Chain	Res	Type
1	C	341	SER
1	C	347	ILE
1	C	353	VAL
1	C	357	SER
1	C	360	ARG
1	C	361	GLN
1	C	371	LEU
1	C	405	VAL
1	C	406	GLN
1	C	408	SER
1	C	409	ILE
1	C	420	THR
1	C	421	VAL
1	C	432	TYR
1	C	458	PHE
1	C	474	GLN
1	C	505	ILE
1	C	511	HIS
1	C	520	MET
1	C	524	PHE
1	C	541	LEU
1	C	542	ILE
1	C	563	CYS
1	C	585	LEU
1	C	587	VAL
1	C	598	ARG
1	C	600	VAL
1	C	610	ASP
1	C	619	TYR
1	C	622	LEU
1	C	675	LEU
1	C	679	THR
1	C	683	ILE
1	C	740	ILE
1	C	742	ASP
1	C	754	VAL
1	C	761	THR
1	C	764	GLU
1	C	778	LEU
1	C	780	ILE
1	C	786	LEU
1	C	793	PHE

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Mol	Chain	Res	Type
1	C	818	LEU
1	C	821	CYS
1	C	826	VAL
1	C	828	LEU
1	C	842	GLU
1	C	843	GLN
1	C	848	ILE
1	C	849	CYS
1	C	855	THR
1	C	856	VAL
1	C	857	SER
1	C	865	LEU
1	C	872	VAL
1	C	875	GLU
1	C	893	HIS
1	C	897	ASP
1	C	903	LEU
1	C	908	GLU
1	C	916	PHE
1	C	919	LEU
1	C	929	GLU
1	C	931	LEU
1	C	938	ASN
1	C	942	GLU
1	C	949	SER
1	C	959	MET
1	C	961	ASN
1	C	968	MET
1	C	983	ASN
1	C	984	ILE
1	C	992	GLU
1	C	1000	ILE
1	C	1005	ILE
1	C	1008	LEU
1	C	1024	SER
1	C	1039	THR
1	C	1046	LEU
1	C	1073	ARG
1	C	1077	ASN
1	C	1086	LEU
1	C	1087	LEU
1	C	1089	ASN

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Mol	Chain	Res	Type
1	C	1091	ILE
1	C	1100	THR
1	C	1101	LEU
1	C	1105	ILE
1	C	1107	ILE
1	C	1110	LEU
1	C	1112	ILE
1	C	1114	LEU
1	C	1125	LEU
1	C	1150	LEU
1	C	1163	ARG
1	C	1184	GLU
1	C	1188	LYS
1	C	1206	VAL
1	C	1236	LYS
1	C	1242	GLN
1	C	1245	GLN
1	C	1252	GLN
1	C	1277	GLN
1	C	1280	ILE
1	C	1281	GLN
1	C	1289	LYS
1	C	1291	GLN
1	C	1292	VAL
1	C	1294	ASN
1	C	1295	ASN
1	C	1298	LEU
1	C	1315	LYS
1	C	1328	LEU
1	C	1331	ASN
1	C	1333	LEU
1	C	1356	LYS
1	C	1362	GLN
1	C	1363	ILE
1	C	1365	LEU
1	C	1384	LYS
1	C	1401	ARG
1	C	1402	SER
1	C	1408	THR
1	C	1422	VAL
1	C	1425	GLN
1	C	1426	THR

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Mol	Chain	Res	Type
1	C	1430	PHE
1	C	1434	LEU
1	C	1442	LEU
1	C	1446	ILE
1	C	1451	ASP
1	C	1457	GLU
1	C	1467	CYS
1	D	32	MET
1	D	34	LEU
1	D	42	GLU
1	D	56	GLU
1	D	60	VAL
1	D	82	ASP
1	D	114	PHE
1	D	121	MET
1	D	126	ASP
1	D	129	VAL
1	D	153	GLU
1	D	154	ASN
1	D	161	LEU
1	D	173	ASN
1	D	175	ILE
1	D	194	LEU
1	D	199	PHE
1	D	200	GLN
1	D	238	ILE
1	D	251	CYS
1	D	265	THR
1	D	268	ILE
1	D	294	LEU
1	D	321	HIS
1	D	326	ILE
1	D	331	THR
1	D	333	VAL
1	D	334	GLU
1	D	335	LEU
1	D	336	THR
1	D	341	SER
1	D	347	ILE
1	D	353	VAL
1	D	360	ARG
1	D	361	GLN

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Mol	Chain	Res	Type
1	D	371	LEU
1	D	382	LYS
1	D	405	VAL
1	D	406	GLN
1	D	409	ILE
1	D	420	THR
1	D	421	VAL
1	D	432	TYR
1	D	458	PHE
1	D	474	GLN
1	D	505	ILE
1	D	511	HIS
1	D	520	MET
1	D	524	PHE
1	D	541	LEU
1	D	542	ILE
1	D	563	CYS
1	D	585	LEU
1	D	587	VAL
1	D	598	ARG
1	D	600	VAL
1	D	610	ASP
1	D	619	TYR
1	D	622	LEU
1	D	675	LEU
1	D	679	THR
1	D	683	ILE
1	D	740	ILE
1	D	742	ASP
1	D	754	VAL
1	D	761	THR
1	D	764	GLU
1	D	778	LEU
1	D	780	ILE
1	D	786	LEU
1	D	793	PHE
1	D	818	LEU
1	D	821	CYS
1	D	826	VAL
1	D	828	LEU
1	D	829	GLU
1	D	842	GLU

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Mol	Chain	Res	Type
1	D	843	GLN
1	D	848	ILE
1	D	849	CYS
1	D	855	THR
1	D	856	VAL
1	D	857	SER
1	D	865	LEU
1	D	872	VAL
1	D	875	GLU
1	D	893	HIS
1	D	897	ASP
1	D	903	LEU
1	D	908	GLU
1	D	916	PHE
1	D	919	LEU
1	D	929	GLU
1	D	931	LEU
1	D	938	ASN
1	D	942	GLU
1	D	949	SER
1	D	959	MET
1	D	961	ASN
1	D	968	MET
1	D	983	ASN
1	D	984	ILE
1	D	992	GLU
1	D	999	GLU
1	D	1000	ILE
1	D	1005	ILE
1	D	1008	LEU
1	D	1024	SER
1	D	1039	THR
1	D	1046	LEU
1	D	1073	ARG
1	D	1077	ASN
1	D	1086	LEU
1	D	1087	LEU
1	D	1089	ASN
1	D	1091	ILE
1	D	1100	THR
1	D	1101	LEU
1	D	1105	ILE

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Mol	Chain	Res	Type
1	D	1107	ILE
1	D	1110	LEU
1	D	1112	ILE
1	D	1114	LEU
1	D	1125	LEU
1	D	1150	LEU
1	D	1163	ARG
1	D	1184	GLU
1	D	1188	LYS
1	D	1206	VAL
1	D	1236	LYS
1	D	1242	GLN
1	D	1245	GLN
1	D	1252	GLN
1	D	1277	GLN
1	D	1280	ILE
1	D	1281	GLN
1	D	1289	LYS
1	D	1291	GLN
1	D	1292	VAL
1	D	1294	ASN
1	D	1295	ASN
1	D	1298	LEU
1	D	1315	LYS
1	D	1328	LEU
1	D	1331	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	208	GLN
1	A	368	GLN
1	A	406	GLN
1	A	413	ASN
1	A	460	HIS
1	A	995	GLN
1	A	1038	ASN
1	A	1065	GLN
1	A	1118	HIS
1	A	1179	ASN
1	A	1233	ASN

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Mol	Chain	Res	Type
1	A	1242	GLN
1	A	1325	GLN
1	A	1331	ASN
1	B	112	GLN
1	B	208	GLN
1	B	368	GLN
1	B	406	GLN
1	B	413	ASN
1	B	460	HIS
1	B	995	GLN
1	B	1038	ASN
1	B	1065	GLN
1	B	1118	HIS
1	B	1179	ASN
1	B	1233	ASN
1	B	1242	GLN
1	B	1325	GLN
1	B	1331	ASN
1	C	106	GLN
1	C	112	GLN
1	C	208	GLN
1	C	368	GLN
1	C	406	GLN
1	C	413	ASN
1	C	995	GLN
1	C	1038	ASN
1	C	1065	GLN
1	C	1118	HIS
1	C	1179	ASN
1	C	1242	GLN
1	C	1325	GLN
1	C	1331	ASN
1	C	1435	GLN
1	D	112	GLN
1	D	208	GLN
1	D	368	GLN
1	D	406	GLN
1	D	413	ASN
1	D	917	ASN
1	D	995	GLN
1	D	1013	GLN
1	D	1038	ASN

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Mol	Chain	Res	Type
1	D	1065	GLN
1	D	1072	GLN
1	D	1118	HIS
1	D	1179	ASN
1	D	1242	GLN
1	D	1291	GLN
1	D	1331	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MEQ	A	975	1	8,9,10	0.56	0	7,10,12	1.09	1 (14%)
1	MEQ	B	975	1	8,9,10	0.60	0	7,10,12	1.07	1 (14%)
1	MEQ	C	975	1	8,9,10	0.64	0	7,10,12	1.10	1 (14%)
1	MEQ	D	975	1	8,9,10	0.54	0	7,10,12	1.11	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MEQ	A	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	B	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	C	975	1	-	0/7/9/11	0/0/0/0
1	MEQ	D	975	1	-	0/7/9/11	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	975	MEQ	O-C-CA	-2.79	118.21	125.49
1	C	975	MEQ	O-C-CA	-2.77	118.28	125.49
1	A	975	MEQ	O-C-CA	-2.74	118.34	125.49
1	B	975	MEQ	O-C-CA	-2.72	118.41	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

36 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	2001	1,2	14,14,15	1.61	2 (14%)	15,19,21	1.16	1 (6%)
2	NAG	A	2002	2	14,14,15	1.51	1 (7%)	15,19,21	1.00	1 (6%)
2	NAG	A	2401	1,2	14,14,15	1.54	1 (7%)	15,19,21	2.01	2 (13%)
2	NAG	A	2402	2	14,14,15	1.68	1 (7%)	15,19,21	1.24	2 (13%)
2	NAG	A	2501	1,2	14,14,15	1.86	1 (7%)	15,19,21	1.85	4 (26%)
2	NAG	A	2502	2	14,14,15	1.37	1 (7%)	15,19,21	1.86	3 (20%)
4	NAG	A	2601	1,4	14,14,15	2.04	6 (42%)	15,19,21	3.07	8 (53%)
4	NAG	A	2602	4	14,14,15	2.58	5 (35%)	15,19,21	2.26	3 (20%)
4	MAN	A	2603	4	11,11,12	3.88	10 (90%)	14,15,17	3.12	7 (50%)
2	NAG	B	2001	1,2	14,14,15	1.64	2 (14%)	15,19,21	1.17	1 (6%)
2	NAG	B	2002	2	14,14,15	1.53	1 (7%)	15,19,21	1.03	0
2	NAG	B	2401	1,2	14,14,15	1.53	1 (7%)	15,19,21	1.88	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	2402	2	14,14,15	1.73	2 (14%)	15,19,21	1.36	2 (13%)
2	NAG	B	2501	1,2	14,14,15	1.89	3 (21%)	15,19,21	1.78	4 (26%)
2	NAG	B	2502	2	14,14,15	1.67	2 (14%)	15,19,21	1.78	2 (13%)
4	NAG	B	2601	1,4	14,14,15	2.01	7 (50%)	15,19,21	3.16	8 (53%)
4	NAG	B	2602	4	14,14,15	2.52	5 (35%)	15,19,21	2.31	4 (26%)
4	MAN	B	2603	4	11,11,12	4.35	10 (90%)	14,15,17	3.14	10 (71%)
2	NAG	C	2001	1,2	14,14,15	1.82	2 (14%)	15,19,21	1.15	1 (6%)
2	NAG	C	2002	2	14,14,15	1.54	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	C	2401	1,2	14,14,15	1.63	1 (7%)	15,19,21	1.95	3 (20%)
2	NAG	C	2402	2	14,14,15	1.76	3 (21%)	15,19,21	1.14	2 (13%)
2	NAG	C	2501	1,2	14,14,15	1.92	2 (14%)	15,19,21	1.76	3 (20%)
2	NAG	C	2502	2	14,14,15	1.38	1 (7%)	15,19,21	1.87	3 (20%)
4	NAG	C	2601	1	14,14,15	2.23	8 (57%)	15,19,21	3.01	9 (60%)
4	NAG	C	2602	4	14,14,15	33.60	6 (42%)	12,19,21	9.26	7 (58%)
4	MAN	C	2603	4	11,11,12	2.84	9 (81%)	14,15,17	3.29	10 (71%)
2	NAG	D	2001	1,2	14,14,15	1.68	2 (14%)	15,19,21	1.14	1 (6%)
2	NAG	D	2002	2	14,14,15	1.50	1 (7%)	15,19,21	1.00	0
2	NAG	D	2401	1,2	14,14,15	1.56	1 (7%)	15,19,21	1.87	3 (20%)
2	NAG	D	2402	2	14,14,15	1.76	2 (14%)	15,19,21	1.15	2 (13%)
2	NAG	D	2501	1,2	14,14,15	2.01	2 (14%)	15,19,21	1.81	4 (26%)
2	NAG	D	2502	2	14,14,15	1.40	1 (7%)	15,19,21	1.87	2 (13%)
4	NAG	D	2601	1,4	14,14,15	1.89	5 (35%)	15,19,21	3.06	9 (60%)
4	NAG	D	2602	4	14,14,15	2.37	5 (35%)	15,19,21	2.32	4 (26%)
4	MAN	D	2603	4	11,11,12	2.72	8 (72%)	14,15,17	3.30	7 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2502	2	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	A	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	B	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	B	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	C	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	2601	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2602	4	4/4/5/7	0/6/22/26	1/1/1/1
4	MAN	C	2603	4	-	0/2/19/22	0/1/1/1
2	NAG	D	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2002	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2402	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2502	2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	2601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2602	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	D	2603	4	-	0/2/19/22	0/1/1/1

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2402	NAG	C3-C2	2.00	1.57	1.52
4	C	2603	MAN	C6-C5	2.01	1.59	1.51
2	B	2501	NAG	C2-N2	2.01	1.49	1.46
4	D	2602	NAG	O4-C4	2.01	1.47	1.43
2	C	2402	NAG	C2-N2	2.04	1.49	1.46
2	B	2501	NAG	C4-C5	2.06	1.57	1.53
4	B	2601	NAG	O5-C1	2.06	1.47	1.43
2	D	2402	NAG	C4-C5	2.06	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2601	NAG	O4-C4	2.09	1.48	1.43
2	C	2501	NAG	C4-C3	2.09	1.57	1.52
4	D	2602	NAG	C4-C3	2.11	1.57	1.52
2	C	2001	NAG	C3-C2	2.12	1.57	1.52
4	B	2601	NAG	C3-C2	2.14	1.57	1.52
4	B	2602	NAG	C2-N2	2.15	1.50	1.46
4	B	2601	NAG	O4-C4	2.15	1.48	1.43
2	B	2502	NAG	C4-C3	2.17	1.58	1.52
2	A	2001	NAG	C3-C2	2.17	1.57	1.52
2	C	2402	NAG	C4-C5	2.17	1.57	1.53
4	A	2601	NAG	O5-C1	2.21	1.47	1.43
4	B	2601	NAG	C7-N2	2.22	1.42	1.34
4	A	2602	NAG	C2-N2	2.23	1.50	1.46
4	C	2601	NAG	O4-C4	2.24	1.48	1.43
4	D	2603	MAN	O5-C5	2.26	1.48	1.43
4	D	2603	MAN	O5-C1	2.26	1.47	1.43
4	C	2601	NAG	C7-N2	2.27	1.43	1.34
4	A	2601	NAG	C7-N2	2.27	1.43	1.34
4	C	2601	NAG	C3-C2	2.28	1.57	1.52
4	C	2603	MAN	O4-C4	2.30	1.48	1.43
2	D	2001	NAG	C3-C2	2.34	1.57	1.52
4	B	2601	NAG	C4-C5	2.39	1.58	1.53
4	D	2603	MAN	C4-C3	2.39	1.58	1.52
4	C	2601	NAG	O5-C1	2.39	1.47	1.43
4	C	2603	MAN	O2-C2	2.41	1.48	1.43
4	C	2603	MAN	C4-C3	2.42	1.58	1.52
4	D	2603	MAN	O4-C4	2.43	1.48	1.43
4	B	2602	NAG	C4-C3	2.43	1.58	1.52
2	B	2001	NAG	C3-C2	2.43	1.58	1.52
4	C	2602	NAG	C2-N2	2.44	1.50	1.46
2	D	2501	NAG	O5-C5	2.46	1.48	1.43
4	D	2603	MAN	O2-C2	2.47	1.48	1.43
4	D	2601	NAG	C4-C5	2.50	1.58	1.53
4	C	2603	MAN	O5-C5	2.52	1.49	1.43
4	D	2601	NAG	C2-N2	2.52	1.50	1.46
4	D	2602	NAG	C4-C5	2.56	1.58	1.53
4	A	2603	MAN	O3-C3	2.57	1.49	1.43
4	A	2601	NAG	C3-C2	2.58	1.58	1.52
4	D	2601	NAG	C3-C2	2.58	1.58	1.52
4	A	2601	NAG	C4-C5	2.59	1.58	1.53
4	A	2603	MAN	C6-C5	2.60	1.61	1.51
4	C	2601	NAG	C1-C2	2.62	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2602	NAG	C3-C2	2.62	1.58	1.52
4	C	2603	MAN	O5-C1	2.66	1.48	1.43
4	C	2601	NAG	C4-C5	2.66	1.58	1.53
4	A	2602	NAG	C4-C3	2.67	1.59	1.52
4	B	2603	MAN	C6-C5	2.73	1.61	1.51
4	B	2602	NAG	C4-C5	2.79	1.59	1.53
4	A	2601	NAG	C2-N2	2.79	1.51	1.46
4	A	2602	NAG	C3-C2	2.79	1.58	1.52
4	A	2602	NAG	C4-C5	2.84	1.59	1.53
4	B	2602	NAG	C3-C2	2.84	1.59	1.52
4	A	2603	MAN	O2-C2	2.89	1.49	1.43
4	B	2601	NAG	C2-N2	2.92	1.51	1.46
4	D	2603	MAN	C4-C5	2.98	1.59	1.53
4	B	2603	MAN	O4-C4	3.00	1.50	1.43
2	A	2502	NAG	C1-C2	3.05	1.56	1.52
4	C	2603	MAN	C4-C5	3.08	1.59	1.53
4	D	2601	NAG	C4-C3	3.10	1.60	1.52
4	C	2601	NAG	C2-N2	3.18	1.52	1.46
4	B	2603	MAN	O3-C3	3.19	1.50	1.43
2	C	2502	NAG	C1-C2	3.25	1.57	1.52
4	A	2603	MAN	O4-C4	3.29	1.50	1.43
4	D	2603	MAN	C1-C2	3.31	1.60	1.52
4	A	2601	NAG	C4-C3	3.34	1.61	1.52
4	B	2601	NAG	C4-C3	3.35	1.61	1.52
4	C	2603	MAN	C1-C2	3.42	1.60	1.52
4	C	2602	NAG	C4-C5	3.47	1.58	1.52
2	D	2502	NAG	C1-C2	3.47	1.57	1.52
4	B	2603	MAN	O5-C1	3.57	1.49	1.43
2	B	2502	NAG	C1-C2	3.58	1.57	1.52
4	B	2603	MAN	C4-C3	3.59	1.61	1.52
4	A	2603	MAN	O5-C5	3.66	1.51	1.43
4	C	2601	NAG	C4-C3	3.74	1.62	1.52
2	B	2001	NAG	C1-C2	3.83	1.57	1.52
4	B	2603	MAN	O5-C5	3.84	1.51	1.43
4	B	2603	MAN	O2-C2	3.86	1.52	1.43
2	A	2001	NAG	C1-C2	3.86	1.57	1.52
2	A	2401	NAG	C1-C2	3.87	1.57	1.52
2	D	2401	NAG	C1-C2	3.96	1.58	1.52
2	B	2401	NAG	C1-C2	3.98	1.58	1.52
2	D	2001	NAG	C1-C2	4.11	1.58	1.52
2	D	2002	NAG	C1-C2	4.33	1.58	1.52
4	A	2603	MAN	C4-C3	4.35	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2002	NAG	C1-C2	4.36	1.58	1.52
2	A	2002	NAG	C1-C2	4.37	1.58	1.52
4	A	2603	MAN	C1-C2	4.40	1.62	1.52
2	B	2002	NAG	C1-C2	4.42	1.58	1.52
2	C	2401	NAG	C1-C2	4.45	1.58	1.52
2	B	2501	NAG	C1-C2	4.57	1.58	1.52
2	C	2402	NAG	C1-C2	4.59	1.58	1.52
4	C	2602	NAG	C1-C2	4.63	1.58	1.53
2	A	2402	NAG	C1-C2	4.63	1.58	1.52
4	A	2603	MAN	C4-C5	4.65	1.63	1.53
2	A	2501	NAG	C1-C2	4.67	1.58	1.52
4	A	2603	MAN	O5-C1	4.73	1.51	1.43
2	B	2402	NAG	C1-C2	4.81	1.59	1.52
4	C	2602	NAG	C3-C2	4.84	1.61	1.53
4	B	2603	MAN	C1-C2	4.85	1.63	1.52
2	C	2001	NAG	C1-C2	4.87	1.59	1.52
2	D	2402	NAG	C1-C2	4.87	1.59	1.52
2	C	2501	NAG	C1-C2	4.91	1.59	1.52
4	B	2603	MAN	C4-C5	4.99	1.63	1.53
4	D	2603	MAN	C2-C3	5.03	1.59	1.52
4	C	2603	MAN	C2-C3	5.31	1.59	1.52
2	D	2501	NAG	C1-C2	5.48	1.60	1.52
4	A	2603	MAN	C2-C3	6.05	1.60	1.52
4	D	2602	NAG	C1-C2	6.57	1.61	1.52
4	B	2602	NAG	C1-C2	6.91	1.62	1.52
4	A	2602	NAG	C1-C2	7.03	1.62	1.52
4	B	2603	MAN	C2-C3	8.83	1.64	1.52
4	C	2602	NAG	O5-C1	80.57	2.95	1.43
4	C	2602	NAG	C3-C4	96.12	3.08	1.52

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2602	NAG	C1-O5-C5	-26.28	64.87	113.47
4	C	2602	NAG	O4-C4-C3	-11.08	82.91	110.06
2	C	2401	NAG	C8-C7-N2	-2.48	111.35	116.11
4	C	2601	NAG	C8-C7-N2	-2.40	111.52	116.11
4	D	2601	NAG	C8-C7-N2	-2.06	112.17	116.11
2	D	2401	NAG	C8-C7-N2	-2.04	112.21	116.11
2	A	2502	NAG	C4-C3-C2	2.00	114.34	111.23
2	A	2002	NAG	C2-N2-C7	2.01	125.63	123.04
2	C	2502	NAG	C4-C3-C2	2.02	114.36	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2603	MAN	O3-C3-C2	2.02	113.65	110.00
2	B	2501	NAG	O3-C3-C4	2.03	114.90	110.34
4	C	2603	MAN	O4-C4-C5	2.04	114.64	109.24
4	C	2603	MAN	C3-C4-C5	2.04	113.76	110.20
2	C	2002	NAG	C2-N2-C7	2.05	125.68	123.04
4	C	2603	MAN	O6-C6-C5	2.06	118.14	111.33
2	A	2501	NAG	O3-C3-C4	2.09	115.04	110.34
4	C	2603	MAN	O5-C5-C6	2.11	111.91	107.35
4	D	2603	MAN	O5-C5-C6	2.14	111.97	107.35
2	A	2401	NAG	C4-C3-C2	2.14	114.55	111.23
2	B	2401	NAG	C4-C3-C2	2.15	114.56	111.23
2	D	2501	NAG	C2-N2-C7	2.17	125.83	123.04
4	B	2603	MAN	O2-C2-C3	2.19	114.52	110.12
4	C	2601	NAG	C3-C2-N2	2.19	115.80	110.56
4	D	2602	NAG	O5-C5-C6	2.21	112.13	107.35
4	C	2603	MAN	O3-C3-C2	2.23	114.03	110.00
4	A	2601	NAG	C3-C2-N2	2.24	115.93	110.56
4	B	2603	MAN	O3-C3-C2	2.25	114.07	110.00
2	D	2402	NAG	C1-O5-C5	2.27	115.13	112.25
4	A	2603	MAN	O3-C3-C4	2.27	115.46	110.34
2	C	2402	NAG	C1-O5-C5	2.29	115.15	112.25
4	B	2602	NAG	C3-C4-C5	2.30	114.21	110.20
4	B	2602	NAG	O5-C5-C6	2.31	112.35	107.35
4	B	2603	MAN	O5-C5-C6	2.34	112.42	107.35
2	C	2401	NAG	C4-C3-C2	2.35	114.88	111.23
4	B	2603	MAN	O2-C2-C1	2.37	113.96	109.21
4	D	2603	MAN	O2-C2-C1	2.38	113.98	109.21
4	B	2601	NAG	C3-C2-N2	2.40	116.30	110.56
4	B	2603	MAN	O6-C6-C5	2.42	119.33	111.33
2	A	2501	NAG	O5-C5-C6	2.42	112.59	107.35
2	C	2501	NAG	O5-C5-C6	2.48	112.72	107.35
4	C	2601	NAG	C4-C3-C2	2.48	115.09	111.23
4	D	2601	NAG	C4-C3-C2	2.49	115.10	111.23
2	D	2402	NAG	C2-N2-C7	2.49	126.24	123.04
2	D	2401	NAG	C4-C3-C2	2.51	115.12	111.23
2	C	2502	NAG	C3-C2-N2	2.53	116.62	110.56
4	C	2603	MAN	O2-C2-C1	2.59	114.39	109.21
2	D	2502	NAG	C3-C2-N2	2.60	116.79	110.56
4	C	2601	NAG	O5-C5-C6	2.60	112.98	107.35
2	A	2402	NAG	C2-N2-C7	2.60	126.38	123.04
2	C	2402	NAG	C2-N2-C7	2.61	126.39	123.04
2	B	2501	NAG	O5-C5-C6	2.62	113.03	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2502	NAG	C3-C2-N2	2.64	116.89	110.56
4	A	2601	NAG	C4-C3-C2	2.64	115.33	111.23
4	B	2603	MAN	O4-C4-C5	2.68	116.34	109.24
2	A	2501	NAG	C4-C3-C2	2.68	115.40	111.23
2	A	2502	NAG	C3-C2-N2	2.69	117.00	110.56
4	D	2601	NAG	O5-C5-C6	2.71	113.21	107.35
4	D	2601	NAG	C3-C2-N2	2.73	117.10	110.56
4	D	2602	NAG	C3-C4-C5	2.77	115.02	110.20
4	A	2601	NAG	O5-C5-C6	2.77	113.35	107.35
4	C	2602	NAG	O5-C5-C6	2.79	113.40	106.36
4	A	2603	MAN	O2-C2-C1	2.85	114.92	109.21
2	D	2001	NAG	C2-N2-C7	2.88	126.74	123.04
2	A	2402	NAG	C1-O5-C5	2.89	115.92	112.25
2	B	2402	NAG	C2-N2-C7	2.92	126.79	123.04
4	B	2601	NAG	C4-C3-C2	2.94	115.80	111.23
2	B	2001	NAG	C2-N2-C7	3.00	126.89	123.04
2	C	2501	NAG	C4-C3-C2	3.00	115.89	111.23
2	C	2001	NAG	C2-N2-C7	3.04	126.95	123.04
4	B	2601	NAG	O5-C5-C6	3.06	113.98	107.35
4	A	2603	MAN	O5-C5-C6	3.11	114.08	107.35
2	A	2001	NAG	C2-N2-C7	3.11	127.04	123.04
4	A	2603	MAN	C1-O5-C5	3.13	116.22	112.25
2	B	2501	NAG	C4-C3-C2	3.17	116.15	111.23
2	D	2501	NAG	O5-C5-C6	3.17	114.22	107.35
4	D	2601	NAG	O4-C4-C3	3.20	117.54	110.34
4	C	2601	NAG	O7-C7-N2	3.20	128.40	121.86
4	A	2602	NAG	C3-C4-C5	3.21	115.79	110.20
4	A	2601	NAG	O7-C7-N2	3.23	128.46	121.86
4	D	2601	NAG	O7-C7-N2	3.25	128.49	121.86
4	B	2601	NAG	O7-C7-N2	3.31	128.61	121.86
2	B	2402	NAG	C1-O5-C5	3.36	116.51	112.25
4	A	2601	NAG	O4-C4-C3	3.37	117.92	110.34
4	B	2601	NAG	O4-C4-C3	3.38	117.94	110.34
2	D	2501	NAG	C4-C3-C2	3.38	116.48	111.23
4	C	2601	NAG	O4-C4-C3	3.59	118.42	110.34
4	B	2603	MAN	C2-C3-C4	3.61	117.17	111.04
4	C	2601	NAG	C1-O5-C5	3.62	116.84	112.25
4	C	2602	NAG	O4-C4-C5	3.70	117.33	109.88
2	D	2501	NAG	C1-O5-C5	3.74	116.99	112.25
4	A	2603	MAN	C2-C3-C4	3.81	117.51	111.04
4	B	2603	MAN	C1-O5-C5	3.84	117.12	112.25
2	C	2501	NAG	C1-O5-C5	4.01	117.34	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2603	MAN	O5-C1-C2	4.04	117.42	110.86
4	C	2601	NAG	C3-C4-C5	4.05	117.25	110.20
4	D	2601	NAG	C1-O5-C5	4.09	117.43	112.25
4	D	2601	NAG	C3-C4-C5	4.10	117.34	110.20
4	B	2601	NAG	C3-C4-C5	4.10	117.35	110.20
4	A	2601	NAG	C1-O5-C5	4.11	117.46	112.25
4	C	2603	MAN	C2-C3-C4	4.13	118.05	111.04
2	B	2501	NAG	C1-O5-C5	4.16	117.53	112.25
4	A	2601	NAG	C3-C4-C5	4.18	117.49	110.20
4	C	2603	MAN	O5-C1-C2	4.19	117.65	110.86
4	D	2603	MAN	C2-C3-C4	4.19	118.16	111.04
4	B	2601	NAG	C1-O5-C5	4.29	117.70	112.25
2	A	2501	NAG	C1-O5-C5	4.71	118.23	112.25
4	A	2602	NAG	C2-N2-C7	4.87	129.29	123.04
4	C	2602	NAG	C3-C2-N2	4.95	119.24	110.59
4	D	2602	NAG	C2-N2-C7	4.98	129.44	123.04
4	B	2602	NAG	C2-N2-C7	5.05	129.53	123.04
4	C	2602	NAG	C2-N2-C7	5.09	129.58	123.04
4	A	2602	NAG	C4-C3-C2	5.19	119.30	111.23
4	B	2603	MAN	O5-C1-C2	5.28	119.43	110.86
2	B	2502	NAG	C1-O5-C5	5.33	119.02	112.25
4	C	2603	MAN	C1-O5-C5	5.34	119.02	112.25
4	A	2603	MAN	O5-C1-C2	5.46	119.72	110.86
4	D	2602	NAG	C4-C3-C2	5.62	119.96	111.23
4	D	2603	MAN	C1-O5-C5	5.68	119.45	112.25
2	A	2502	NAG	C1-O5-C5	5.72	119.51	112.25
4	B	2602	NAG	C4-C3-C2	5.75	120.17	111.23
2	C	2502	NAG	C1-O5-C5	5.76	119.55	112.25
2	D	2401	NAG	C1-O5-C5	5.77	119.57	112.25
2	D	2502	NAG	C1-O5-C5	5.78	119.59	112.25
2	C	2401	NAG	C1-O5-C5	5.91	119.75	112.25
2	B	2401	NAG	C1-O5-C5	6.04	119.91	112.25
4	A	2603	MAN	C1-C2-C3	6.32	117.01	109.54
4	B	2603	MAN	C1-C2-C3	6.43	117.14	109.54
2	A	2401	NAG	C1-O5-C5	6.53	120.53	112.25
4	D	2603	MAN	C1-C2-C3	7.19	118.05	109.54
4	C	2603	MAN	C1-C2-C3	7.25	118.12	109.54
4	C	2601	NAG	C2-N2-C7	7.26	132.37	123.04
4	A	2601	NAG	C2-N2-C7	7.35	132.49	123.04
4	D	2601	NAG	C2-N2-C7	7.48	132.65	123.04
4	B	2601	NAG	C2-N2-C7	7.51	132.68	123.04
4	C	2602	NAG	O1-C1-O5	11.76	142.41	110.25

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	2002	NAG	C1
2	B	2402	NAG	C1
2	A	2402	NAG	C1
2	A	2502	NAG	C1
2	D	2502	NAG	C1
2	C	2002	NAG	C1
2	D	2402	NAG	C1
2	C	2402	NAG	C1
2	A	2002	NAG	C1
2	C	2502	NAG	C1
4	C	2602	NAG	C2
4	C	2602	NAG	C5
4	C	2602	NAG	C1
4	C	2602	NAG	C4
4	B	2602	NAG	C1
4	D	2602	NAG	C1
2	B	2502	NAG	C1
4	A	2602	NAG	C1
2	D	2002	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2602	NAG	C1-C2-C3-C4-C5-O5

20 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2401	NAG	1	0
2	A	2501	NAG	2	0
2	A	2502	NAG	2	0
4	A	2601	NAG	1	0
4	A	2602	NAG	1	0
2	B	2401	NAG	1	0
2	B	2501	NAG	2	0
2	B	2502	NAG	2	0
4	B	2601	NAG	2	0
4	B	2602	NAG	1	0
2	C	2401	NAG	1	0
2	C	2501	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2502	NAG	2	0
4	C	2601	NAG	1	0
4	C	2602	NAG	1	0
2	D	2401	NAG	1	0
2	D	2501	NAG	1	0
2	D	2502	NAG	1	0
4	D	2601	NAG	1	0
4	D	2602	NAG	1	0

5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	2101	1	14,14,15	1.82	3 (21%)	15,19,21	2.18	3 (20%)
3	NAG	A	2201	1	14,14,15	1.78	2 (14%)	15,19,21	1.34	2 (13%)
3	NAG	A	2301	1	14,14,15	1.75	2 (14%)	15,19,21	2.45	4 (26%)
3	NAG	B	2101	1	14,14,15	1.95	3 (21%)	15,19,21	2.18	3 (20%)
3	NAG	B	2201	1	14,14,15	1.69	1 (7%)	15,19,21	1.46	1 (6%)
3	NAG	B	2301	1	14,14,15	1.80	2 (14%)	15,19,21	2.36	4 (26%)
3	NAG	C	2101	1	14,14,15	2.27	3 (21%)	15,19,21	2.12	4 (26%)
3	NAG	C	2201	1	14,14,15	1.82	1 (7%)	15,19,21	1.54	1 (6%)
3	NAG	C	2301	1	14,14,15	2.14	5 (35%)	15,19,21	2.42	5 (33%)
3	NAG	C	2701	1	14,14,15	1.53	2 (14%)	15,19,21	1.22	2 (13%)
3	NAG	D	2101	1	14,14,15	1.73	3 (21%)	15,19,21	2.26	3 (20%)
3	NAG	D	2201	1	14,14,15	1.68	1 (7%)	15,19,21	1.32	2 (13%)
3	NAG	D	2301	1	14,14,15	1.69	1 (7%)	15,19,21	2.38	6 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2101	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2201	1	-	0/6/23/26	0/1/1/1
3	NAG	D	2301	1	-	0/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2201	NAG	C3-C2	2.07	1.57	1.52
3	C	2301	NAG	C4-C3	2.11	1.57	1.52
3	C	2301	NAG	C2-N2	2.17	1.50	1.46
3	C	2701	NAG	C3-C2	2.18	1.57	1.52
3	D	2101	NAG	C3-C2	2.30	1.57	1.52
3	B	2101	NAG	C3-C2	2.31	1.57	1.52
3	B	2301	NAG	C2-N2	2.31	1.50	1.46
3	A	2301	NAG	C2-N2	2.36	1.50	1.46
3	A	2101	NAG	C3-C2	2.38	1.57	1.52
3	D	2101	NAG	C2-N2	2.41	1.50	1.46
3	C	2301	NAG	C3-C2	2.48	1.58	1.52
3	C	2101	NAG	C3-C2	2.55	1.58	1.52
3	A	2101	NAG	C2-N2	2.86	1.51	1.46
3	C	2301	NAG	O5-C1	3.00	1.48	1.43
3	C	2101	NAG	C2-N2	3.23	1.52	1.46
3	B	2101	NAG	C2-N2	3.41	1.52	1.46
3	C	2701	NAG	C1-C2	4.35	1.58	1.52
3	A	2301	NAG	C1-C2	4.41	1.58	1.52
3	D	2301	NAG	C1-C2	4.42	1.58	1.52
3	D	2101	NAG	C1-C2	4.47	1.58	1.52
3	B	2201	NAG	C1-C2	4.52	1.58	1.52
3	B	2301	NAG	C1-C2	4.53	1.58	1.52
3	A	2101	NAG	C1-C2	4.66	1.58	1.52
3	D	2201	NAG	C1-C2	4.72	1.59	1.52
3	A	2201	NAG	C1-C2	4.93	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2101	NAG	C1-C2	5.14	1.59	1.52
3	C	2201	NAG	C1-C2	5.24	1.59	1.52
3	C	2301	NAG	C1-C2	5.30	1.59	1.52
3	C	2101	NAG	C1-C2	6.20	1.61	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2301	NAG	C8-C7-N2	-2.40	111.51	116.11
3	C	2301	NAG	C8-C7-N2	-2.18	111.94	116.11
3	B	2301	NAG	C8-C7-N2	-2.04	112.20	116.11
3	C	2101	NAG	C6-C5-C4	-2.03	108.02	113.02
3	A	2201	NAG	C2-N2-C7	2.03	125.64	123.04
3	A	2301	NAG	O5-C5-C6	2.03	111.73	107.35
3	D	2301	NAG	C3-C2-N2	2.05	115.47	110.56
3	D	2201	NAG	C2-N2-C7	2.17	125.83	123.04
3	D	2301	NAG	O5-C5-C6	2.20	112.11	107.35
3	C	2301	NAG	O5-C5-C6	2.29	112.31	107.35
3	D	2301	NAG	O7-C7-N2	2.31	126.56	121.86
3	C	2701	NAG	C2-N2-C7	2.38	126.10	123.04
3	B	2301	NAG	O7-C7-N2	2.42	126.79	121.86
3	A	2301	NAG	O7-C7-N2	2.48	126.93	121.86
3	B	2101	NAG	C1-O5-C5	2.68	115.65	112.25
3	C	2301	NAG	O7-C7-N2	2.71	127.38	121.86
3	A	2101	NAG	C1-O5-C5	2.79	115.79	112.25
3	D	2101	NAG	C1-O5-C5	2.87	115.89	112.25
3	C	2701	NAG	C4-C3-C2	2.92	115.77	111.23
3	C	2101	NAG	C4-C3-C2	3.22	116.23	111.23
3	C	2101	NAG	C1-O5-C5	3.58	116.79	112.25
3	B	2101	NAG	C4-C3-C2	3.59	116.81	111.23
3	D	2101	NAG	C4-C3-C2	3.72	117.02	111.23
3	A	2101	NAG	C4-C3-C2	3.73	117.03	111.23
3	D	2201	NAG	C1-O5-C5	3.94	117.25	112.25
3	C	2201	NAG	C1-O5-C5	4.15	117.51	112.25
3	A	2201	NAG	C1-O5-C5	4.17	117.53	112.25
3	B	2301	NAG	C1-O5-C5	4.39	117.82	112.25
3	C	2301	NAG	C1-O5-C5	4.49	117.95	112.25
3	B	2201	NAG	C1-O5-C5	4.68	118.19	112.25
3	D	2301	NAG	C1-O5-C5	4.72	118.23	112.25
3	A	2301	NAG	C1-O5-C5	4.77	118.31	112.25
3	C	2101	NAG	C2-N2-C7	5.41	129.99	123.04
3	D	2301	NAG	C2-N2-C7	5.78	130.47	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2301	NAG	C2-N2-C7	6.10	130.88	123.04
3	B	2301	NAG	C2-N2-C7	6.18	130.98	123.04
3	A	2101	NAG	C2-N2-C7	6.30	131.14	123.04
3	A	2301	NAG	C2-N2-C7	6.43	131.30	123.04
3	B	2101	NAG	C2-N2-C7	6.44	131.31	123.04
3	D	2101	NAG	C2-N2-C7	6.74	131.70	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1269/1451 (87%)	-0.28	19 (1%)	76	67	81, 159, 293, 300	0
1	B	1269/1451 (87%)	-0.26	20 (1%)	74	65	65, 153, 297, 300	0
1	C	1402/1451 (96%)	-0.28	21 (1%)	76	67	60, 148, 292, 300	0
1	D	1269/1451 (87%)	-0.18	18 (1%)	78	69	91, 182, 300, 300	0
All	All	5209/5804 (89%)	-0.25	78 (1%)	76	67	60, 161, 299, 300	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1192	PRO	7.1
1	C	433	GLY	6.3
1	A	1191	ALA	5.1
1	B	277	ASP	4.6
1	D	633	PRO	4.6
1	C	435	GLN	4.2
1	A	1193	VAL	4.2
1	C	434	TYR	3.9
1	D	1192	PRO	3.7
1	C	1360	SER	3.6
1	A	1194	GLY	3.6
1	B	1193	VAL	3.5
1	B	729	GLU	3.5
1	B	276	SER	3.4
1	A	434	TYR	3.4
1	A	433	GLY	3.2
1	D	1189	PRO	3.2
1	D	1191	ALA	3.2
1	C	432	TYR	3.2
1	C	1191	ALA	3.2
1	B	433	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	435	GLN	3.1
1	A	281	GLU	3.1
1	B	1194	GLY	3.0
1	D	1081	ARG	2.9
1	A	436	TRP	2.9
1	D	71	ARG	2.8
1	A	1195	HIS	2.8
1	C	1192	PRO	2.7
1	D	1193	VAL	2.7
1	C	1035	ASN	2.7
1	B	284	GLN	2.7
1	B	434	TYR	2.7
1	B	279	HIS	2.6
1	D	1190	LYS	2.6
1	A	279	HIS	2.6
1	A	1190	LYS	2.6
1	C	1036	GLN	2.5
1	C	820	LYS	2.5
1	B	1192	PRO	2.5
1	D	1197	TYR	2.5
1	A	1334	PRO	2.5
1	D	1330	TYR	2.5
1	A	276	SER	2.4
1	C	1198	GLU	2.4
1	C	1375	ALA	2.4
1	D	889	SER	2.4
1	B	282	ASP	2.4
1	B	1195	HIS	2.4
1	A	644	ASN	2.4
1	D	553	GLY	2.3
1	C	889	SER	2.3
1	B	1188	LYS	2.3
1	A	787	ARG	2.3
1	C	1195	HIS	2.3
1	D	1332	ILE	2.3
1	B	1198	GLU	2.3
1	D	1335	GLU	2.3
1	C	1441	ASP	2.2
1	D	27	GLY	2.2
1	B	278	CYS	2.2
1	C	1377	ASN	2.2
1	C	436	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	888	PRO	2.2
1	D	276	SER	2.2
1	A	841	LYS	2.2
1	A	687	LYS	2.2
1	B	647	ASN	2.1
1	D	689	CYS	2.1
1	B	1197	TYR	2.1
1	B	256	TYR	2.1
1	C	1190	LYS	2.1
1	D	1196	PHE	2.1
1	B	1189	PRO	2.0
1	B	687	LYS	2.0
1	C	1358	HIS	2.0
1	A	878	GLU	2.0
1	C	270	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MEQ	B	975	10/11	0.90	0.20	-	164,187,254,273	0
1	MEQ	A	975	10/11	0.89	0.44	-	156,174,185,253	0
1	MEQ	D	975	10/11	0.85	0.35	-	190,274,288,289	0
1	MEQ	C	975	10/11	0.76	0.30	-	136,153,165,173	0

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	2401	14/15	0.72	0.32	2.84	208,291,293,294	0
2	NAG	C	2001	14/15	0.69	0.64	1.87	200,206,300,300	0
2	NAG	D	2001	14/15	0.78	0.68	1.59	287,288,290,291	0
2	NAG	B	2001	14/15	0.78	0.45	0.75	299,300,300,300	0
2	NAG	C	2401	14/15	0.76	0.26	0.54	156,171,244,254	0
2	NAG	A	2001	14/15	0.82	0.28	-0.17	292,292,294,295	0
4	MAN	C	2603	11/12	0.46	0.58	-	186,200,293,296	0
2	NAG	B	2002	14/15	0.77	0.65	-	296,298,300,300	0
2	NAG	D	2502	14/15	0.72	0.64	-	300,300,300,300	0
2	NAG	C	2002	14/15	0.72	0.68	-	194,299,300,300	0
2	NAG	D	2402	14/15	0.71	0.71	-	300,300,300,300	0
2	NAG	D	2501	14/15	0.78	0.57	-	193,295,300,300	0
2	NAG	C	2402	14/15	0.76	0.41	-	259,262,266,267	0
4	NAG	B	2601	14/15	0.96	0.24	-	143,166,224,228	0
4	MAN	D	2603	11/12	0.66	0.55	-	295,297,299,300	0
2	NAG	C	2501	14/15	0.90	0.42	-	186,209,298,300	0
2	NAG	B	2501	14/15	0.92	0.39	-	126,141,148,151	0
2	NAG	A	2002	14/15	0.73	0.42	-	292,293,295,295	0
2	NAG	C	2502	14/15	0.93	0.38	-	267,300,300,300	0
4	MAN	B	2603	11/12	0.83	0.47	-	100,100,100,100	0
4	NAG	C	2602	14/15	0.87	0.50	-	139,163,178,180	0
2	NAG	A	2501	14/15	0.90	0.51	-	180,196,251,259	0
4	NAG	B	2602	14/15	0.83	0.36	-	154,221,227,228	0
4	NAG	D	2601	14/15	0.77	0.38	-	167,210,263,270	0
2	NAG	D	2401	14/15	0.64	0.44	-	300,300,300,300	0
2	NAG	B	2401	14/15	0.57	0.40	-	300,300,300,300	0
4	NAG	D	2602	14/15	0.73	0.58	-	181,277,288,294	0
2	NAG	B	2402	14/15	0.80	0.79	-	300,300,300,300	0
2	NAG	B	2502	14/15	0.89	0.40	-	154,162,183,190	0
4	NAG	C	2601	14/15	0.90	0.36	-	119,140,154,161	0
4	NAG	A	2601	14/15	0.91	0.31	-	128,148,165,169	0
4	MAN	A	2603	11/12	0.60	0.62	-	100,100,100,100	0
4	NAG	A	2602	14/15	0.79	0.57	-	140,166,182,185	0
2	NAG	D	2002	14/15	0.64	0.51	-	286,288,291,291	0
2	NAG	A	2402	14/15	0.81	0.50	-	289,292,295,296	0
2	NAG	A	2502	14/15	0.77	0.56	-	211,286,300,300	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	2101	14/15	0.57	0.65	-	198,290,291,291	0
3	NAG	B	2201	14/15	0.74	0.59	-	190,197,262,265	0
3	NAG	D	2201	14/15	0.60	0.38	-	215,300,300,300	0
3	NAG	C	2201	14/15	0.33	0.65	-	202,298,300,300	0
3	NAG	C	2701	14/15	0.72	0.54	-	300,300,300,300	0
3	NAG	B	2101	14/15	0.80	0.41	-	180,203,294,295	0
3	NAG	C	2301	14/15	0.81	0.25	-	158,176,251,258	0
3	NAG	A	2201	14/15	0.69	0.30	-	183,192,270,280	0
3	NAG	D	2101	14/15	0.62	0.65	-	287,297,300,300	0
3	NAG	C	2101	14/15	0.70	0.49	-	129,154,175,189	0
3	NAG	B	2301	14/15	0.73	0.22	-	300,300,300,300	0
3	NAG	A	2301	14/15	0.87	0.15	-	278,290,292,292	0
3	NAG	D	2301	14/15	0.82	0.28	-	300,300,300,300	0

6.5 Other polymers

There are no such residues in this entry.