



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:51 PM GMT

PDB ID : 1HJV  
Title : Crystal structure of hcgp-39 in complex with chitin tetramer  
Authors : Houston, D.R.; Recklies, A.D.; Krupa, J.C.; Van Aalten, D.M.F.  
Deposited on : 2003-02-28  
Resolution : 2.75 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

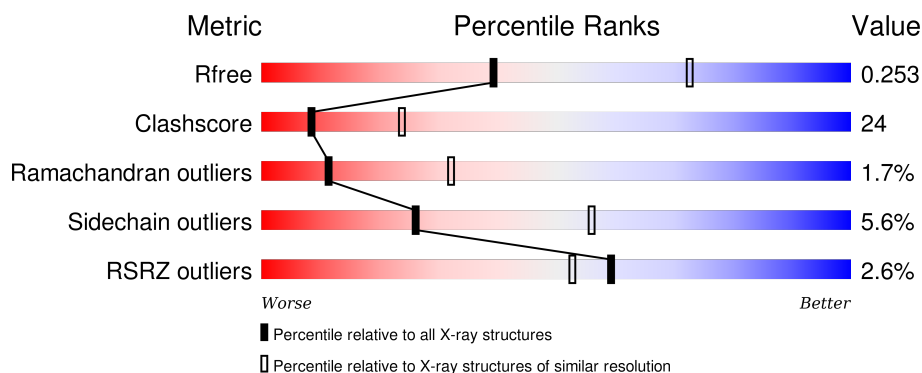
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	362	<div> <div>0%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div>•</div> </div> </div>
1	B	362	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>•</div> </div> </div>
1	C	362	<div> <div>4%</div> <div> <div></div> <div>46%</div> <div>48%</div> <div>6%</div> </div> </div>
1	D	362	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>41%</div> <div>•</div> </div> </div>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	2	-	-	-	X
3	NAG	B	2	-	-	-	X
3	NAG	C	-1	-	-	X	-
3	NAG	C	2	-	-	-	X
3	NAG	D	-1	-	-	X	-
3	NAG	D	2	-	-	-	X
5	SO4	B	1385	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12296 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 CHITINASE-3 LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	2	0
			2871	1833	495	532	11			
1	B	362	Total	C	N	O	S	0	1	0
			2868	1831	496	530	11			
1	C	362	Total	C	N	O	S	0	2	0
			2873	1834	496	532	11			
1	D	362	Total	C	N	O	S	0	1	0
			2866	1830	494	531	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	ILE	THR	CONFLICT	UNP P36222
B	311	ILE	THR	CONFLICT	UNP P36222
A	311	ILE	THR	CONFLICT	UNP P36222
B	311	ILE	THR	CONFLICT	UNP P36222

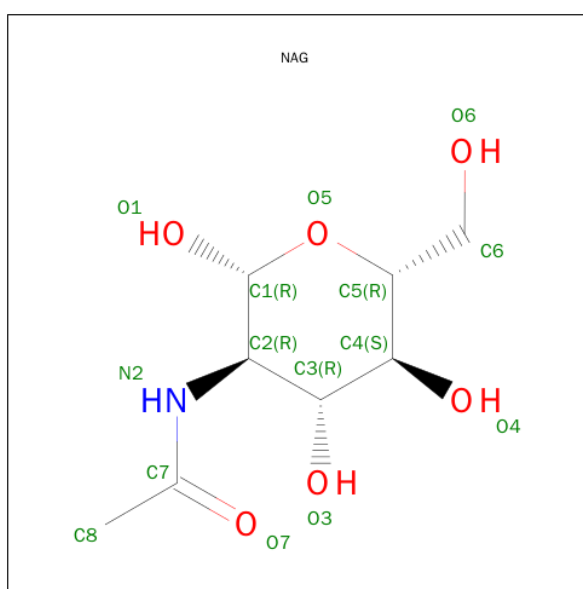
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			43	24	3	16		
2	B	3	Total	C	N	O	0	0
			43	24	3	16		
2	C	3	Total	C	N	O	0	0
			43	24	3	16		
2	D	3	Total	C	N	O	0	0
			43	24	3	16		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			57	32	4	21		
3	B	4	Total	C	N	O	0	0
			57	32	4	21		
3	C	4	Total	C	N	O	0	0
			57	32	4	21		
3	D	4	Total	C	N	O	0	0
			57	32	4	21		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

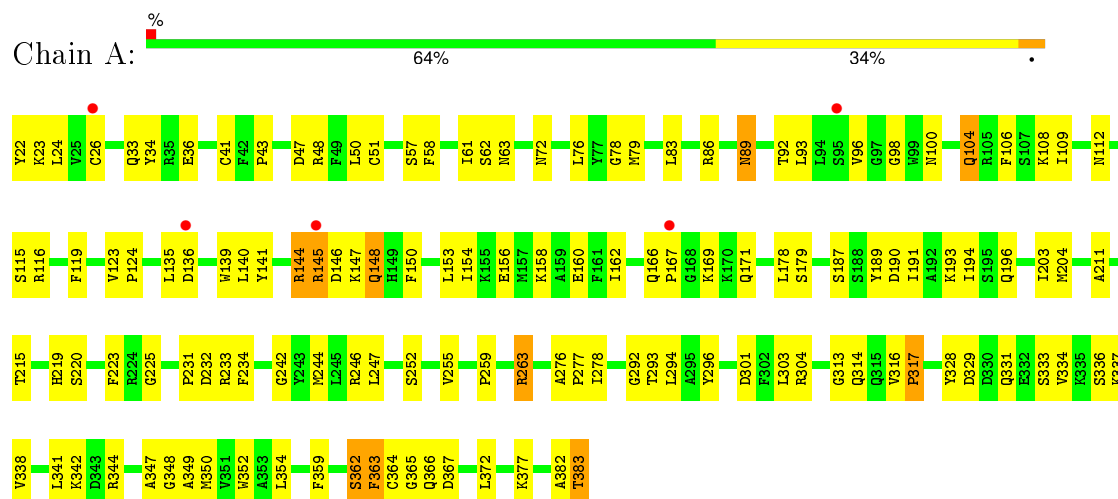
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	101	Total 101	O 101	0	0
6	B	80	Total 80	O 80	0	0
6	C	53	Total 53	O 53	0	0
6	D	68	Total 68	O 68	0	0

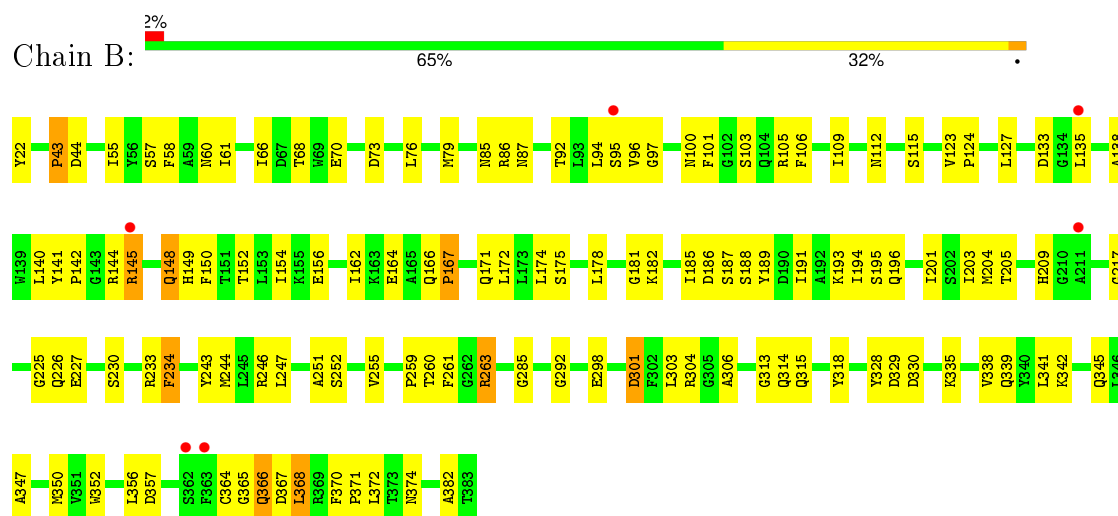
### 3 Residue-property plots

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: CHITINASE-3 LIKE PROTEIN 1



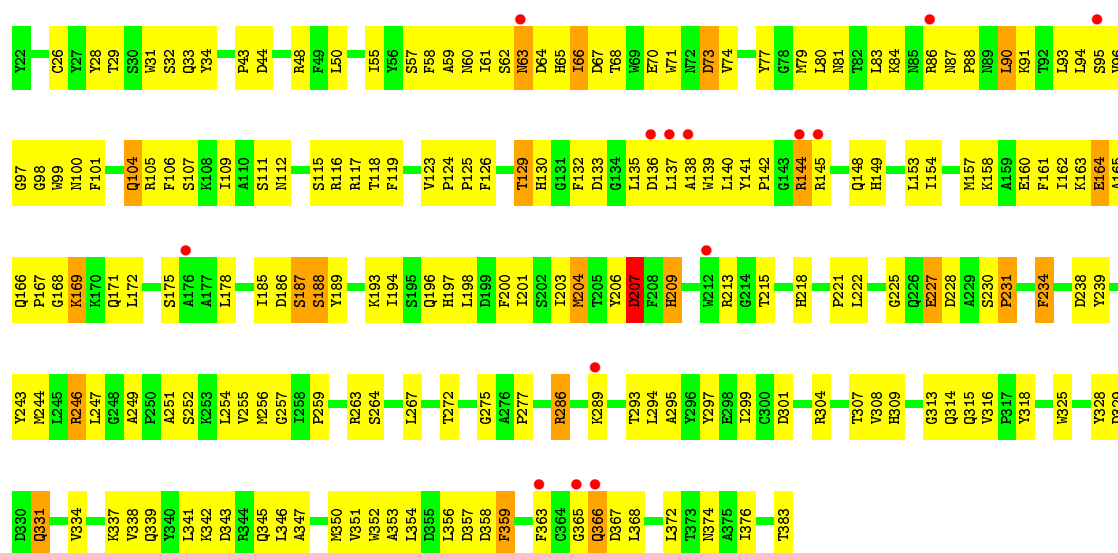
#### • Molecule 1: CHITINASE-3 LIKE PROTEIN 1



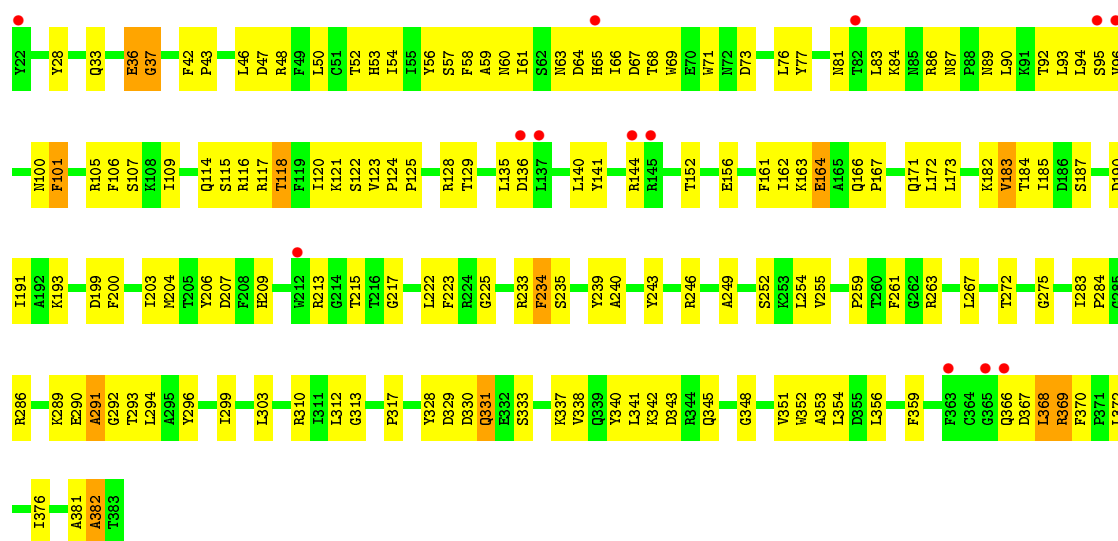
#### • Molecule 1: CHITINASE-3 LIKE PROTEIN 1







• Molecule 1: CHITINASE-3 LIKE PROTEIN 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.64Å 123.32Å 135.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.79 – 2.75 24.79 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.0 (24.79-2.75) 98.3 (24.79-2.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.212 , 0.253 0.227 , 0.253	Depositor DCC
$R_{free}$ test set	970 reflections (2.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 47935 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.69 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8110e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.47	0/2955	0.71	0/4002
1	B	0.48	0/2948	0.73	0/3992
1	C	0.42	0/2957	0.67	0/4004
1	D	0.45	0/2946	0.68	0/3990
All	All	0.46	0/11806	0.70	0/15988

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2871	0	2789	122	0
1	B	2868	0	2790	107	0
1	C	2873	0	2791	188	0
1	D	2866	0	2785	139	0
2	A	43	0	39	3	0
2	B	43	0	39	0	0
2	C	43	0	39	4	0
2	D	43	0	39	1	0
3	A	57	0	51	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	57	0	51	7	0
3	C	57	0	51	14	0
3	D	57	0	51	13	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	1	0
4	D	14	0	13	0	0
5	A	15	0	0	0	0
5	B	15	0	0	0	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
6	A	101	0	0	24	0
6	B	80	0	0	12	0
6	C	53	0	0	2	0
6	D	68	0	0	9	0
All	All	12296	0	11567	566	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 24.

All (566) 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)
1:D:162:ILE:HG12	1:D:171:GLN:HE22	1.31	0.95
1:A:145:ARG:HG3	6:A:2041:HOH:O	1.64	0.94
1:C:193:LYS:O	1:C:196:GLN:HG2	1.69	0.93
1:C:144:ARG:HH11	1:C:144:ARG:HB2	1.34	0.92
1:D:352:TRP:HB3	6:D:2061:HOH:O	1.69	0.91
1:A:112:ASN:HB3	1:A:115:SER:HB2	1.52	0.91
1:D:166:GLN:HG3	1:D:167:PRO:HD3	1.52	0.91
1:D:47:ASP:HB3	1:D:50:LEU:HB2	1.54	0.90
1:B:94:LEU:O	1:B:135:LEU:HD12	1.72	0.90
1:A:162:ILE:HG12	1:A:171:GLN:OE1	1.76	0.85
1:C:154:ILE:HD13	1:C:198:LEU:HD21	1.58	0.85
1:B:204:MET:HE1	3:B:-1:NAG:C1	2.07	0.85
1:D:48:ARG:HE	1:D:86:ARG:HB2	1.43	0.84
1:B:261:PHE:HD1	6:B:2072:HOH:O	1.60	0.84
1:A:57:SER:HB2	1:A:58:PHE:CD1	2.12	0.83
1:C:209:HIS:CE1	1:C:213:ARG:HH11	1.98	0.81
3:C:-2:NAG:H82	3:C:-1:NAG:H61	1.60	0.81
1:A:61:ILE:HG21	1:A:109:ILE:HD13	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:PHE:CD1	6:B:2072:HOH:O	2.33	0.80
1:D:163:LYS:HA	1:D:166:GLN:HE21	1.48	0.79
1:A:48:ARG:HB3	1:A:83:LEU:HD22	1.63	0.79
1:A:204:MET:HE2	3:A:1:NAG:H62	1.65	0.79
1:C:62:SER:O	1:C:63:ASN:HB2	1.82	0.79
1:D:123:VAL:HB	1:D:124:PRO:HD3	1.65	0.79
1:C:352:TRP:CZ3	3:C:-1:NAG:H83	2.18	0.78
1:C:93:LEU:HD23	1:C:135:LEU:O	1.85	0.77
1:A:334:VAL:O	1:A:338:VAL:HG23	1.84	0.77
1:C:203:ILE:HD12	1:C:244:MET:SD	2.25	0.77
1:C:144:ARG:NH1	1:C:144:ARG:HB2	1.99	0.76
1:B:44:ASP:HB3	1:B:79:MET:HE3	1.66	0.76
1:A:89:ASN:N	1:A:89:ASN:HD22	1.84	0.76
1:B:352:TRP:O	6:B:2072:HOH:O	2.04	0.76
1:D:54:ILE:HG13	1:D:90:LEU:HD11	1.68	0.75
1:D:204:MET:HE1	3:D:-1:NAG:C1	2.16	0.75
1:C:198:LEU:HD12	1:C:201:ILE:HG12	1.69	0.74
1:D:164:GLU:O	1:D:167:PRO:HD2	1.87	0.74
1:C:104:GLN:HA	1:C:104:GLN:HE21	1.51	0.74
1:C:185:ILE:HA	1:C:189:TYR:HD2	1.53	0.73
1:A:193:LYS:O	1:A:196:GLN:HG2	1.87	0.73
1:A:144:ARG:N	1:A:144:ARG:HD3	2.03	0.73
1:D:162:ILE:HG12	1:D:171:GLN:NE2	2.05	0.72
1:D:331:GLN:HE21	1:D:331:GLN:H	1.38	0.72
1:D:166:GLN:CG	1:D:167:PRO:HD3	2.20	0.71
1:A:204:MET:CE	3:A:1:NAG:H62	2.20	0.71
1:B:328:TYR:HA	6:B:2068:HOH:O	1.91	0.71
1:A:204:MET:HE1	3:A:-1:NAG:C1	2.21	0.71
1:C:198:LEU:HD12	1:C:201:ILE:CG1	2.20	0.70
1:C:74:VAL:HG13	1:C:130:HIS:CE1	2.26	0.70
1:C:33:GLN:HG3	1:C:34:TYR:CD1	2.26	0.70
1:C:111:SER:HA	1:C:149:HIS:HD2	1.56	0.70
1:C:209:HIS:CE1	1:C:213:ARG:NH1	2.59	0.70
1:C:158:LYS:HD2	1:C:197:HIS:O	1.92	0.70
1:C:185:ILE:HA	1:C:189:TYR:CD2	2.27	0.69
1:B:162:ILE:HD11	6:B:2032:HOH:O	1.91	0.69
1:A:277:PRO:HB2	1:C:144:ARG:NH2	2.08	0.69
1:C:87:ASN:ND2	1:C:90:LEU:HB3	2.07	0.69
1:C:123:VAL:HB	1:C:124:PRO:HD3	1.75	0.69
1:C:70:GLU:O	1:C:73:ASP:HB2	1.93	0.68
1:C:206:TYR:O	1:C:207:ASP:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLN:HB2	1:B:368:LEU:HD12	1.74	0.68
1:A:169:LYS:NZ	6:A:2050:HOH:O	2.25	0.68
1:A:150:PHE:O	6:A:2047:HOH:O	2.12	0.67
1:C:341:LEU:HD12	1:C:342:LYS:N	2.09	0.67
1:C:295:ALA:O	1:C:299:ILE:HG13	1.94	0.67
1:C:161:PHE:CD2	1:C:172:LEU:HB2	2.30	0.66
1:B:127:LEU:HD12	1:B:172:LEU:HD13	1.76	0.66
1:C:64:ASP:OD1	1:C:115:SER:HB3	1.95	0.66
1:C:141:TYR:HH	3:C:1:NAG:HO6	1.39	0.66
1:C:198:LEU:CD1	1:C:201:ILE:HG12	2.25	0.65
1:C:112:ASN:HB3	1:C:115:SER:HB2	1.77	0.65
1:C:366:GLN:HB3	1:C:368:LEU:HG	1.78	0.65
1:C:163:LYS:O	1:C:166:GLN:HG2	1.97	0.65
1:A:225:GLY:HA2	1:A:313:GLY:HA3	1.77	0.65
1:B:105:ARG:HH21	1:B:105:ARG:HG2	1.61	0.64
1:D:105:ARG:HH21	1:D:105:ARG:HG2	1.62	0.64
1:C:334:VAL:O	1:C:338:VAL:HG23	1.98	0.64
1:A:158:LYS:O	1:A:162:ILE:HG13	1.98	0.64
1:A:61:ILE:HG21	1:A:109:ILE:CD1	2.26	0.63
1:D:66:ILE:HG23	1:D:66:ILE:O	1.97	0.63
1:B:203:ILE:HD12	1:B:244:MET:SD	2.39	0.63
1:C:160:GLU:OE1	1:C:163:LYS:HD3	1.98	0.63
1:C:29:THR:OG1	1:C:32:SER:HB3	1.98	0.63
3:C:-2:NAG:H82	3:C:-1:NAG:C6	2.29	0.63
1:A:76:LEU:HD13	6:A:2022:HOH:O	1.98	0.63
1:D:65:HIS:CE1	1:D:118:THR:HG22	2.33	0.63
1:B:246:ARG:HD2	6:B:2047:HOH:O	1.99	0.62
1:D:48:ARG:NE	1:D:86:ARG:HB2	2.12	0.62
1:B:44:ASP:H	1:B:79:MET:HE2	1.65	0.62
1:C:352:TRP:CZ2	3:C:-1:NAG:H3	2.35	0.62
1:A:144:ARG:CD	1:A:144:ARG:H	2.13	0.62
1:A:43:PRO:HB2	1:A:79:MET:HB2	1.81	0.62
1:C:50:LEU:HD13	1:C:374:ASN:OD1	2.00	0.62
1:A:41:CYS:HB2	1:A:359:PHE:CZ	2.36	0.61
1:C:55:ILE:CG2	1:C:95:SER:HB2	2.30	0.61
1:B:135:LEU:HD23	6:B:2025:HOH:O	2.00	0.61
1:C:209:HIS:HE1	1:C:213:ARG:HH11	1.49	0.61
1:C:87:ASN:HD22	1:C:90:LEU:HB3	1.64	0.61
1:A:112:ASN:HB3	1:A:115:SER:CB	2.29	0.61
1:B:186:ASP:HA	6:B:2035:HOH:O	2.01	0.61
1:C:100:ASN:ND2	3:C:-2:NAG:H62	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASP:OD1	1:B:79:MET:HE1	2.00	0.61
1:B:368:LEU:O	1:B:368:LEU:HD13	2.01	0.61
1:A:301:ASP:HA	1:A:304:ARG:NH1	2.16	0.61
1:B:338:VAL:HA	1:B:341:LEU:CD2	2.31	0.61
1:A:365:GLY:C	1:A:367:ASP:H	2.03	0.61
1:B:182:LYS:NZ	1:B:186:ASP:OD2	2.34	0.60
1:C:162:ILE:HG12	1:C:171:GLN:HE22	1.66	0.60
1:D:144:ARG:HA	1:D:187:SER:O	2.01	0.60
1:D:368:LEU:HD12	1:D:368:LEU:C	2.22	0.60
1:A:252:SER:O	1:A:347:ALA:HB2	2.01	0.60
2:C:-7:NAG:HN2	2:C:-6:NAG:H62	1.65	0.60
1:B:96:VAL:HG13	1:B:96:VAL:O	2.01	0.59
2:A:-7:NAG:H82	2:A:-6:NAG:H61	1.83	0.59
1:B:61:ILE:HG21	1:B:109:ILE:HD13	1.84	0.59
1:D:261:PHE:HB3	1:D:356:LEU:HD13	1.84	0.59
1:D:331:GLN:H	1:D:331:GLN:NE2	2.00	0.59
1:B:260:THR:N	6:B:2072:HOH:O	2.36	0.59
1:A:147:LYS:HE3	1:A:189:TYR:O	2.02	0.59
2:A:-7:NAG:C8	2:A:-6:NAG:H61	2.32	0.59
1:B:112:ASN:HB3	1:B:115:SER:HB2	1.85	0.59
1:B:100:ASN:ND2	3:B:-2:NAG:H62	2.17	0.58
1:D:381:ALA:O	1:D:382:ALA:HB2	2.03	0.58
1:D:73:ASP:HB2	6:D:2014:HOH:O	2.03	0.58
3:D:1:NAG:H83	6:D:2003:HOH:O	2.03	0.58
1:B:162:ILE:O	1:B:166:GLN:HG2	2.04	0.58
1:A:72:ASN:ND2	1:A:76:LEU:HD13	2.19	0.58
1:B:204:MET:HE3	3:B:-1:NAG:H82	1.86	0.58
1:C:162:ILE:HG12	1:C:171:GLN:NE2	2.18	0.58
1:C:331:GLN:H	1:C:331:GLN:NE2	2.01	0.58
1:D:144:ARG:NH1	1:D:187:SER:CB	2.67	0.58
1:D:234:PHE:HB3	1:D:239:TYR:CD1	2.38	0.58
1:A:162:ILE:O	1:A:166:GLN:HG2	2.04	0.58
2:C:-7:NAG:N2	2:C:-6:NAG:H62	2.19	0.58
1:B:100:ASN:CG	3:B:-2:NAG:H62	2.24	0.58
1:A:296:TYR:CG	1:A:372:LEU:HD11	2.38	0.57
1:D:372:LEU:O	1:D:376:ILE:HG13	2.04	0.57
1:C:104:GLN:HA	1:C:104:GLN:NE2	2.18	0.57
1:D:352:TRP:O	6:D:2061:HOH:O	2.17	0.57
1:B:86[A]:ARG:HH11	1:B:86[A]:ARG:HG2	1.70	0.57
1:D:60:ASN:HB2	1:D:69:TRP:CE3	2.40	0.57
1:C:58:PHE:CZ	1:C:98:GLY:HA2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:SER:HB2	1:C:200:PHE:CE1	2.39	0.57
1:C:178:LEU:O	1:C:204:MET:HG3	2.04	0.57
1:C:43:PRO:HB2	1:C:79:MET:HB2	1.85	0.57
1:D:61:ILE:HA	1:D:65:HIS:O	2.05	0.56
1:C:164:GLU:O	1:C:169:LYS:HD2	2.05	0.56
1:D:56:TYR:HB3	1:D:94:LEU:HD12	1.87	0.56
1:A:86:ARG:CZ	1:A:86:ARG:HB2	2.35	0.56
1:C:28:TYR:OH	1:C:43:PRO:HD3	2.06	0.56
1:C:194:ILE:O	1:C:198:LEU:HG	2.06	0.56
1:D:191:ILE:CG2	1:D:249:ALA:HB2	2.36	0.56
1:C:329:ASP:OD2	1:C:337:LYS:HE3	2.06	0.55
1:B:43:PRO:HB2	1:B:79:MET:HB3	1.88	0.55
1:B:142:PRO:HB2	1:B:188:SER:HB3	1.89	0.55
1:A:144:ARG:HG2	6:A:2041:HOH:O	2.06	0.55
1:A:148:GLN:NE2	6:A:2044:HOH:O	2.40	0.55
1:C:142:PRO:O	1:C:188:SER:HB3	2.06	0.55
1:A:154:ILE:N	6:A:2047:HOH:O	2.11	0.55
1:C:221:PRO:HB2	1:C:314:GLN:HB3	1.89	0.55
1:A:36:GLU:HB3	6:A:2012:HOH:O	2.05	0.55
1:B:203:ILE:HG23	1:B:205:THR:HG23	1.88	0.55
1:A:61:ILE:HD11	1:A:119:PHE:CZ	2.42	0.55
1:B:55:ILE:CG2	1:B:95:SER:HB2	2.37	0.55
1:C:60:ASN:CG	1:C:61:ILE:H	2.11	0.54
1:A:144:ARG:N	6:A:2041:HOH:O	2.41	0.54
1:A:89:ASN:N	1:A:89:ASN:ND2	2.51	0.54
1:A:22:TYR:CE2	1:A:342:LYS:HE3	2.42	0.54
1:A:92:THR:C	1:A:93:LEU:HD12	2.27	0.54
1:C:153:LEU:O	1:C:157:MET:HB2	2.07	0.54
3:A:-1:NAG:C1	3:A:1:NAG:H62	2.37	0.54
1:C:277:PRO:HG2	6:C:2039:HOH:O	2.07	0.54
1:C:90:LEU:HD12	1:C:90:LEU:C	2.27	0.54
1:C:341:LEU:HB2	1:C:346:LEU:HD12	1.90	0.54
1:C:301:ASP:O	1:C:304:ARG:HG3	2.08	0.54
1:A:57:SER:N	6:A:2010:HOH:O	2.41	0.54
1:C:126:PHE:O	1:C:129:THR:HG22	2.07	0.54
1:C:185:ILE:HD13	1:C:244:MET:CE	2.37	0.54
1:C:365:GLY:C	1:C:367:ASP:H	2.11	0.54
1:C:29:THR:HB	1:C:31:TRP:CE2	2.42	0.54
1:D:343:ASP:O	1:D:345:GLN:HG3	2.07	0.54
1:C:105:ARG:HH21	1:C:105:ARG:HG2	1.73	0.54
1:B:230:SER:HB2	6:B:2042:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH2	6:A:2090:HOH:O	2.40	0.54
1:D:59:ALA:O	1:D:96:VAL:HG23	2.08	0.54
1:C:97:GLY:HA3	1:C:138:ALA:O	2.08	0.54
1:D:48:ARG:HH21	1:D:86:ARG:H	1.55	0.53
1:C:74:VAL:HG13	1:C:130:HIS:HE1	1.72	0.53
1:C:341:LEU:CB	1:C:346:LEU:HD12	2.39	0.53
1:A:352:TRP:CZ3	3:A:-1:NAG:H83	2.44	0.53
1:A:341:LEU:HD21	1:A:349:ALA:HB2	1.89	0.53
1:D:343:ASP:C	1:D:345:GLN:H	2.12	0.53
1:B:124:PRO:HB3	1:B:164:GLU:HG3	1.90	0.53
1:D:352:TRP:CE2	3:D:-1:NAG:H5	2.43	0.53
1:C:165:ALA:HA	1:C:169:LYS:HG3	1.91	0.53
1:B:225:GLY:HA2	1:B:313:GLY:HA3	1.90	0.53
1:D:87:ASN:ND2	1:D:90:LEU:HB2	2.24	0.53
1:C:119:PHE:O	1:C:123:VAL:HG23	2.08	0.53
1:D:141:TYR:HH	3:D:1:NAG:HO6	1.52	0.53
1:A:116:ARG:NE	1:A:156:GLU:OE1	2.41	0.53
1:D:290:GLU:O	1:D:291:ALA:C	2.46	0.53
1:A:242:GLY:O	1:A:246:ARG:HB2	2.09	0.53
1:D:259:PRO:HA	6:D:2061:HOH:O	2.08	0.53
1:B:203:ILE:O	1:B:203:ILE:HG23	2.07	0.53
1:B:148:GLN:HB2	6:B:2030:HOH:O	2.07	0.53
1:A:204:MET:CE	3:A:-1:NAG:C1	2.87	0.53
1:A:96:VAL:CG1	1:A:135:LEU:HD11	2.39	0.53
1:A:96:VAL:HG12	1:A:135:LEU:HD11	1.91	0.53
1:D:352:TRP:CZ2	3:D:-1:NAG:H3	2.45	0.52
1:B:204:MET:HE2	3:B:1:NAG:H61	1.91	0.52
1:A:48:ARG:HB3	1:A:83:LEU:CD2	2.38	0.52
1:D:215:THR:HB	1:D:275:GLY:HA2	1.91	0.52
1:B:44:ASP:H	1:B:79:MET:CE	2.23	0.52
1:C:33:GLN:HG3	1:C:34:TYR:CE1	2.44	0.52
1:C:96:VAL:O	1:C:96:VAL:HG13	2.09	0.52
1:D:296:TYR:HA	1:D:299:ILE:HD12	1.92	0.52
1:D:116:ARG:O	1:D:120:ILE:HG13	2.09	0.52
1:A:24:LEU:O	1:A:51:CYS:HB3	2.08	0.52
1:B:101:PHE:C	1:B:101:PHE:CD1	2.83	0.52
1:C:111:SER:HA	1:C:149:HIS:CD2	2.41	0.52
1:B:301:ASP:O	1:B:304:ARG:HG3	2.09	0.52
1:C:97:GLY:O	1:C:101:PHE:HB2	2.09	0.52
1:D:95:SER:HA	1:D:136:ASP:HB3	1.92	0.52
1:B:338:VAL:HA	1:B:341:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ARG:O	1:D:121:LYS:HB2	2.09	0.51
1:C:251:ALA:HB1	1:C:345:GLN:O	2.09	0.51
1:C:55:ILE:HG21	1:C:95:SER:HB2	1.91	0.51
1:D:352:TRP:CZ3	3:D:-1:NAG:H83	2.46	0.51
1:C:99:TRP:HB2	3:C:-1:NAG:O3	2.10	0.51
1:A:328:TYR:N	1:A:328:TYR:CD1	2.79	0.51
1:C:90:LEU:HD12	1:C:91:LYS:N	2.25	0.51
1:C:368:LEU:C	1:C:368:LEU:HD12	2.30	0.51
1:C:80:LEU:HD12	1:C:83:LEU:HD12	1.93	0.51
1:A:263:ARG:NH1	1:A:293:THR:OG1	2.43	0.51
1:B:191:ILE:O	1:B:195:SER:HB2	2.11	0.51
1:C:359:PHE:H	1:C:359:PHE:HD1	1.59	0.51
1:C:59:ALA:O	1:C:96:VAL:HG23	2.11	0.51
1:D:338:VAL:O	1:D:341:LEU:HG	2.11	0.51
1:D:341:LEU:HD12	1:D:342:LYS:N	2.25	0.50
1:D:225:GLY:HA2	1:D:313:GLY:HA3	1.93	0.50
1:B:368:LEU:HD12	1:B:368:LEU:H	1.76	0.50
1:A:255:VAL:CG1	1:A:350:MET:HB2	2.41	0.50
1:C:357:ASP:OD1	1:C:358:ASP:N	2.45	0.50
1:D:144:ARG:NH1	1:D:187:SER:HB2	2.26	0.50
1:C:297:TYR:HB2	1:C:363:PHE:CG	2.45	0.50
1:D:144:ARG:HH11	1:D:187:SER:HB2	1.75	0.50
1:D:96:VAL:HG13	1:D:96:VAL:O	2.12	0.50
3:C:-1:NAG:C1	3:C:1:NAG:H62	2.41	0.50
1:A:76:LEU:HD22	6:A:2022:HOH:O	2.12	0.50
1:B:338:VAL:O	1:B:341:LEU:HG	2.11	0.50
1:D:267:LEU:HD13	1:D:272:THR:HG22	1.92	0.50
1:B:233:ARG:HG2	1:B:233:ARG:HH11	1.77	0.50
1:C:77:TYR:O	1:C:81:ASN:ND2	2.45	0.50
1:D:100:ASN:O	1:D:101:PHE:C	2.50	0.50
1:A:341:LEU:HD12	1:A:342:LYS:N	2.27	0.50
1:D:293:THR:CG2	1:D:294:LEU:N	2.75	0.50
1:B:370:PHE:O	1:B:374:ASN:HB2	2.12	0.49
1:C:166:GLN:N	1:C:167:PRO:CD	2.74	0.49
1:B:150:PHE:CZ	1:B:154:ILE:HD11	2.47	0.49
1:D:100:ASN:ND2	3:D:-2:NAG:H62	2.27	0.49
1:C:124:PRO:HB2	1:C:125:PRO:CD	2.42	0.49
1:C:246[A]:ARG:HG3	1:C:246[A]:ARG:HH11	1.76	0.49
1:B:204:MET:CE	3:B:-1:NAG:C1	2.85	0.49
1:B:145:ARG:HH21	1:B:149:HIS:CE1	2.30	0.49
1:B:178:LEU:HG	1:B:201:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD13	6:B:2025:HOH:O	2.11	0.49
1:B:182:LYS:HD2	1:B:234:PHE:CD2	2.48	0.49
1:C:162:ILE:HA	1:C:171:GLN:HE21	1.78	0.49
1:C:239:TYR:CD1	1:C:239:TYR:C	2.86	0.49
1:B:185:ILE:HA	1:B:189:TYR:CD2	2.48	0.49
1:D:213:ARG:HD3	6:D:2027:HOH:O	2.12	0.49
1:C:215:THR:HB	1:C:275:GLY:HA2	1.95	0.48
1:C:100:ASN:ND2	3:C:-2:NAG:C6	2.77	0.48
1:A:43:PRO:HB2	1:A:79:MET:CB	2.44	0.48
1:D:234:PHE:HB3	1:D:239:TYR:CE1	2.48	0.48
1:B:303:LEU:HA	1:B:306:ALA:HB3	1.94	0.48
1:D:368:LEU:HD12	1:D:369:ARG:N	2.28	0.48
1:D:234:PHE:CB	1:D:239:TYR:CD1	2.97	0.48
1:B:144:ARG:HG2	1:B:187:SER:HB2	1.94	0.48
1:B:22:TYR:CE2	1:B:342:LYS:HE3	2.48	0.48
1:A:57:SER:HB2	1:A:58:PHE:CG	2.48	0.48
1:A:135:LEU:HG	1:A:136:ASP:N	2.29	0.48
1:A:100:ASN:ND2	3:A:-2:NAG:H62	2.28	0.48
1:B:261:PHE:HB3	1:B:356:LEU:HD13	1.96	0.48
1:C:352:TRP:CH2	3:C:-1:NAG:H3	2.49	0.48
1:C:341:LEU:HD12	1:C:342:LYS:HG3	1.94	0.48
1:A:47:ASP:OD1	1:A:50:LEU:N	2.46	0.48
1:A:220:SER:O	1:A:316:VAL:HG11	2.14	0.48
1:D:48:ARG:NH1	1:D:83:LEU:HD23	2.29	0.47
1:A:352:TRP:CE2	3:A:-1:NAG:H5	2.49	0.47
1:A:263:ARG:HG3	6:A:2057:HOH:O	2.13	0.47
1:C:141:TYR:OH	3:C:1:NAG:O6	2.20	0.47
1:B:185:ILE:HA	1:B:189:TYR:HD2	1.78	0.47
1:C:227:GLU:HG3	1:C:228:ASP:N	2.27	0.47
1:D:84:LYS:HE2	1:D:92:THR:HG23	1.96	0.47
1:A:211:ALA:O	1:A:278:ILE:HD11	2.15	0.47
1:D:92:THR:C	1:D:93:LEU:HD12	2.34	0.47
1:B:365:GLY:C	1:B:367:ASP:H	2.16	0.47
1:D:286:ARG:HD3	6:D:2045:HOH:O	2.14	0.47
1:C:256:MET:CE	1:C:337:LYS:HB3	2.43	0.47
1:C:225:GLY:HA2	1:C:313:GLY:HA3	1.95	0.47
1:D:352:TRP:CH2	3:D:-1:NAG:H3	2.49	0.47
1:C:351:VAL:HG12	1:C:352:TRP:N	2.30	0.47
1:A:104:GLN:HG2	6:A:2032:HOH:O	2.13	0.47
1:D:190:ASP:OD1	1:D:193:LYS:HB2	2.15	0.47
1:B:92:THR:O	1:B:133:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:GLN:N	1:D:167:PRO:CD	2.78	0.47
1:C:204:MET:HE1	3:C:-1:NAG:C7	2.45	0.47
1:A:204:MET:HE2	3:A:1:NAG:C6	2.40	0.47
1:A:139:TRP:CE3	1:A:150:PHE:HD1	2.32	0.47
1:A:153:LEU:N	6:A:2047:HOH:O	2.47	0.47
1:A:178:LEU:HD22	1:A:189:TYR:CE1	2.50	0.47
1:B:285:GLY:HA3	1:B:298:GLU:OE2	2.15	0.47
1:D:359:PHE:HB2	1:D:370:PHE:CZ	2.50	0.47
1:D:47:ASP:HB3	1:D:50:LEU:CB	2.37	0.47
1:B:174:LEU:HD12	1:B:175:SER:N	2.30	0.47
1:C:55:ILE:HG12	1:C:93:LEU:HB2	1.97	0.47
1:C:66:ILE:HG23	1:C:66:ILE:O	2.14	0.47
1:C:70:GLU:HB2	1:C:73:ASP:OD1	2.15	0.47
1:A:76:LEU:HB2	6:A:2022:HOH:O	2.14	0.47
1:B:330:ASP:HA	1:B:372:LEU:HD21	1.97	0.47
1:A:215:THR:HA	1:A:276:ALA:O	2.15	0.47
1:C:48:ARG:CD	1:C:86:ARG:HB3	2.44	0.47
1:C:372:LEU:O	1:C:376:ILE:HG13	2.15	0.47
1:C:64:ASP:OD1	1:C:115:SER:CB	2.63	0.47
1:D:203:ILE:HD11	1:D:240:ALA:HB1	1.97	0.47
1:C:293:THR:O	1:C:294:LEU:HD23	2.15	0.47
1:D:135:LEU:N	1:D:173:LEU:O	2.44	0.47
1:A:141:TYR:CE1	1:A:179:SER:HB2	2.49	0.46
1:A:48:ARG:CD	1:A:86:ARG:HB3	2.46	0.46
1:C:62:SER:O	1:C:65:HIS:CE1	2.67	0.46
1:C:104:GLN:CA	1:C:104:GLN:HE21	2.16	0.46
1:A:140:LEU:HA	1:A:141:TYR:HA	1.64	0.46
1:C:57:SER:HB2	1:C:58:PHE:CD1	2.50	0.46
1:D:206:TYR:O	1:D:207:ASP:HB2	2.14	0.46
1:D:366:GLN:O	1:D:367:ASP:HB2	2.15	0.46
1:B:68:THR:HB	1:B:73:ASP:HB2	1.97	0.46
1:D:351:VAL:HG12	1:D:352:TRP:N	2.31	0.46
1:D:299:ILE:O	1:D:303:LEU:HG	2.15	0.46
1:D:353:ALA:O	1:D:354:LEU:C	2.54	0.46
1:C:247:LEU:HA	1:C:247:LEU:HD23	1.74	0.46
1:B:209:HIS:CD2	1:B:217:GLY:HA3	2.51	0.46
1:C:209:HIS:NE2	1:C:213:ARG:NH1	2.64	0.46
1:C:139:TRP:O	1:C:141:TYR:HA	2.14	0.46
1:C:60:ASN:CG	1:C:61:ILE:N	2.69	0.46
1:C:186:ASP:OD1	1:C:243:TYR:OH	2.30	0.46
1:A:203:ILE:HG23	1:A:203:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:PHE:HE1	6:D:2061:HOH:O	1.99	0.46
1:C:135:LEU:HD21	1:C:137:LEU:HD21	1.98	0.46
1:D:343:ASP:C	1:D:345:GLN:N	2.69	0.46
1:D:162:ILE:HA	1:D:171:GLN:HE21	1.79	0.46
1:B:251:ALA:HB1	1:B:345:GLN:O	2.16	0.46
1:D:310:ARG:NH2	1:D:330:ASP:OD2	2.45	0.46
1:D:252:SER:HA	6:D:2037:HOH:O	2.15	0.46
1:A:72:ASN:ND2	6:A:2022:HOH:O	2.49	0.46
1:C:55:ILE:HA	1:C:93:LEU:O	2.15	0.46
1:A:153:LEU:HB3	6:A:2047:HOH:O	2.15	0.46
1:A:365:GLY:O	1:A:366:GLN:HB2	2.16	0.46
1:A:293:THR:HG22	1:A:294:LEU:N	2.30	0.46
1:C:84:LYS:HZ3	1:C:133:ASP:CG	2.20	0.46
1:D:89:ASN:N	1:D:89:ASN:HD22	2.12	0.46
1:C:185:ILE:CD1	1:C:244:MET:HE1	2.46	0.46
1:C:95:SER:HA	1:C:136:ASP:HB3	1.98	0.46
1:B:55:ILE:HG22	1:B:95:SER:HB2	1.97	0.46
1:D:340:TYR:O	1:D:343:ASP:HB2	2.16	0.46
1:D:57:SER:HB2	1:D:58:PHE:CD1	2.51	0.46
3:A:2:NAG:H2	6:A:2008:HOH:O	2.16	0.45
1:D:123:VAL:CB	1:D:124:PRO:HD3	2.41	0.45
1:D:57:SER:HA	1:D:58:PHE:HA	1.52	0.45
1:B:263:ARG:HA	1:B:292:GLY:O	2.16	0.45
1:B:66:ILE:O	1:B:66:ILE:HG23	2.17	0.45
1:D:283:ILE:HA	1:D:284:PRO:HD3	1.76	0.45
1:A:76:LEU:C	1:A:78:GLY:N	2.66	0.45
1:C:200:PHE:CD1	1:C:200:PHE:C	2.90	0.45
1:A:263:ARG:HD2	1:A:292:GLY:O	2.16	0.45
1:C:328:TYR:CD1	1:C:328:TYR:N	2.84	0.45
1:D:28:TYR:OH	1:D:43:PRO:HD3	2.17	0.45
1:A:72:ASN:HD22	1:A:76:LEU:HD13	1.81	0.45
1:A:377:LYS:HD3	6:A:2096:HOH:O	2.15	0.45
3:A:-2:NAG:H3	6:A:2001:HOH:O	2.17	0.45
1:D:243:TYR:O	1:D:246:ARG:HB3	2.17	0.45
1:B:181:GLY:O	1:B:185:ILE:HG13	2.17	0.45
1:A:23:LYS:O	1:A:348:GLY:HA3	2.16	0.45
1:C:62:SER:HA	4:C:1384:NAG:H82	1.98	0.45
1:B:252:SER:O	1:B:347:ALA:HB2	2.15	0.45
1:B:85:ASN:C	1:B:87:ASN:H	2.20	0.45
1:C:124:PRO:HD2	1:C:125:PRO:HD2	1.97	0.45
2:A:-7:NAG:H82	2:A:-6:NAG:C6	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:TYR:CD1	1:D:372:LEU:HD11	2.52	0.45
1:A:203:ILE:HD12	1:A:244:MET:SD	2.56	0.45
1:C:57:SER:HA	1:C:58:PHE:HA	1.65	0.45
1:A:362:SER:O	1:A:364:CYS:N	2.50	0.45
1:D:71:TRP:CE2	2:D:-6:NAG:H2	2.52	0.44
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.17	0.44
1:A:98:GLY:HA3	6:A:2030:HOH:O	2.16	0.44
1:C:249:ALA:HB1	1:C:254:LEU:HD13	2.00	0.44
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.68	0.44
1:A:26:CYS:HB3	1:A:354:LEU:HG	1.99	0.44
1:C:352:TRP:CE2	3:C:-1:NAG:H5	2.53	0.44
1:C:112:ASN:HB3	1:C:115:SER:CB	2.46	0.44
1:C:308:VAL:HG12	1:C:309:HIS:N	2.32	0.44
1:C:339:GLN:O	1:C:343:ASP:OD1	2.35	0.44
1:D:263:ARG:HA	1:D:292:GLY:O	2.18	0.44
1:B:315:GLN:HE22	1:C:315:GLN:NE2	2.16	0.44
1:C:178:LEU:HD22	1:C:189:TYR:CE1	2.52	0.44
1:A:144:ARG:HA	1:A:187:SER:O	2.17	0.44
1:C:204:MET:CE	3:C:-1:NAG:C7	2.95	0.44
1:C:368:LEU:O	1:C:368:LEU:HD12	2.18	0.44
1:C:142:PRO:O	1:C:188:SER:CB	2.66	0.44
1:B:57:SER:HB2	1:B:58:PHE:CD1	2.53	0.44
1:A:341:LEU:HD12	1:A:341:LEU:C	2.38	0.44
1:C:309:HIS:HB2	1:C:318:TYR:CE2	2.53	0.44
1:B:203:ILE:O	1:B:203:ILE:CG2	2.66	0.44
1:C:203:ILE:O	1:C:203:ILE:HG23	2.18	0.44
1:D:68:THR:HB	1:D:73:ASP:HB2	1.98	0.44
1:B:57:SER:HA	1:B:58:PHE:HA	1.61	0.44
1:C:234:PHE:HB3	1:C:239:TYR:CD1	2.52	0.44
1:C:86:ARG:C	1:C:88:PRO:HD3	2.38	0.44
1:D:77:TYR:O	1:D:81:ASN:ND2	2.51	0.44
1:C:255:VAL:HG12	1:C:350:MET:HB2	1.99	0.44
1:C:109:ILE:HG12	6:C:2010:HOH:O	2.18	0.44
1:A:225:GLY:HA2	1:A:313:GLY:CA	2.45	0.43
1:C:48:ARG:HD3	1:C:86:ARG:HB3	2.00	0.43
1:C:267:LEU:CD1	1:C:272:THR:HG22	2.48	0.43
1:C:213:ARG:NH1	1:C:231:PRO:HD3	2.33	0.43
1:B:43:PRO:HB2	1:B:79:MET:CB	2.47	0.43
1:D:369:ARG:H	1:D:369:ARG:HG3	1.68	0.43
1:A:341:LEU:CD2	1:A:349:ALA:HB2	2.48	0.43
1:C:257:GLY:HA2	1:C:350:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:O	1:A:314:GLN:HG2	2.18	0.43
1:C:185:ILE:HD13	1:C:244:MET:HE1	2.01	0.43
1:B:70:GLU:N	1:B:73:ASP:OD2	2.51	0.43
1:D:161:PHE:HD2	1:D:172:LEU:O	2.01	0.43
1:D:204:MET:HE1	3:D:-1:NAG:N2	2.32	0.43
1:D:204:MET:HE1	3:D:-1:NAG:C7	2.48	0.43
1:C:140:LEU:HA	1:C:141:TYR:HA	1.77	0.43
1:B:342:LYS:NZ	1:B:382:ALA:O	2.51	0.43
1:C:140:LEU:HA	1:C:141:TYR:CD1	2.53	0.43
1:B:44:ASP:OD1	1:B:79:MET:CE	2.65	0.43
1:B:166:GLN:HB2	1:B:167:PRO:HD3	2.00	0.43
1:C:153:LEU:O	1:C:157:MET:CB	2.66	0.43
1:C:107:SER:OG	1:C:145:ARG:NH2	2.51	0.43
1:B:123:VAL:HG11	1:B:135:LEU:HD22	2.01	0.43
1:C:116:ARG:O	1:C:119:PHE:N	2.52	0.43
1:D:43:PRO:O	1:D:83:LEU:HD11	2.19	0.43
1:D:66:ILE:O	1:D:66:ILE:CG2	2.67	0.43
1:D:122:SER:O	1:D:125:PRO:HG2	2.18	0.43
1:B:366:GLN:HB2	1:B:368:LEU:CD1	2.46	0.43
1:C:64:ASP:HB3	1:C:118:THR:HB	2.00	0.43
1:A:26:CYS:CB	1:A:354:LEU:HD11	2.49	0.43
1:B:357:ASP:OD1	1:B:371:PRO:HD2	2.19	0.43
1:C:148:GLN:O	1:C:149:HIS:C	2.56	0.43
1:B:338:VAL:O	1:B:342:LYS:HG3	2.19	0.43
1:D:56:TYR:OH	1:D:76:LEU:HD23	2.19	0.43
1:D:183:VAL:HG12	1:D:184:THR:N	2.33	0.43
1:A:333:SER:O	1:A:337:LYS:HG3	2.19	0.43
1:A:139:TRP:C	1:A:140:LEU:HD23	2.39	0.43
1:C:366:GLN:O	1:C:367:ASP:HB2	2.18	0.43
1:B:57:SER:HB3	1:B:95:SER:HB3	1.99	0.43
1:A:219:HIS:CD2	1:A:263:ARG:HB2	2.54	0.43
1:C:187:SER:O	1:C:188:SER:HB3	2.19	0.42
1:C:252:SER:O	1:C:347:ALA:HB2	2.19	0.42
1:A:166:GLN:OE1	1:A:166:GLN:HA	2.19	0.42
1:C:234:PHE:HB3	1:C:239:TYR:CG	2.54	0.42
1:D:28:TYR:OH	1:D:42:PHE:HA	2.19	0.42
1:C:352:TRP:HA	1:C:353:ALA:HA	1.63	0.42
1:A:255:VAL:HG11	1:A:350:MET:HB2	2.02	0.42
1:D:222:LEU:HG	1:D:223:PHE:CE2	2.54	0.42
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.71	0.42
1:D:52:THR:C	1:D:53:HIS:ND1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:MET:HE2	3:B:1:NAG:C6	2.49	0.42
1:A:57:SER:HB2	1:A:58:PHE:CE1	2.53	0.42
1:D:116:ARG:NE	1:D:156:GLU:OE1	2.53	0.42
1:A:255:VAL:HG12	1:A:350:MET:HB2	2.00	0.42
1:B:97:GLY:HA3	1:B:138:ALA:O	2.19	0.42
1:A:57:SER:HA	1:A:58:PHE:HA	1.64	0.42
1:D:182:LYS:O	1:D:183:VAL:C	2.58	0.42
1:D:54:ILE:CG1	1:D:90:LEU:HD11	2.46	0.42
1:C:164:GLU:OE2	1:C:172:LEU:HD11	2.20	0.42
1:D:105:ARG:O	1:D:109:ILE:HG13	2.19	0.42
1:D:57:SER:HB2	1:D:58:PHE:CG	2.54	0.42
1:C:94:LEU:HD22	1:C:132:PHE:CD2	2.54	0.42
1:C:264:SER:HA	1:C:325:TRP:O	2.18	0.42
1:A:303:LEU:HA	1:A:303:LEU:HD23	1.86	0.42
1:D:36:GLU:O	1:D:37:GLY:C	2.58	0.42
1:D:140:LEU:HA	1:D:141:TYR:CD1	2.54	0.42
1:A:86:ARG:NH2	6:A:2025:HOH:O	2.52	0.42
1:A:193:LYS:O	1:A:194:ILE:C	2.56	0.42
1:D:191:ILE:HG21	1:D:249:ALA:HB2	2.01	0.42
1:B:194:ILE:HG13	1:B:195:SER:N	2.34	0.42
1:C:26:CYS:HB2	1:C:354:LEU:HD11	2.02	0.42
1:C:230:SER:HA	1:C:231:PRO:HD3	1.88	0.42
1:D:124:PRO:O	1:D:128:ARG:HG2	2.19	0.42
1:C:66:ILE:HG21	1:C:123:VAL:HA	2.02	0.42
1:C:43:PRO:HB2	1:C:79:MET:CB	2.49	0.42
1:D:254:LEU:HD12	1:D:254:LEU:HA	1.80	0.42
1:D:163:LYS:HA	1:D:166:GLN:NE2	2.26	0.41
1:C:135:LEU:HG	1:C:136:ASP:N	2.35	0.41
1:B:44:ASP:CB	1:B:79:MET:HE3	2.45	0.41
1:B:96:VAL:CG1	1:B:96:VAL:O	2.66	0.41
1:D:381:ALA:O	1:D:382:ALA:CB	2.68	0.41
1:A:104:GLN:H	1:A:104:GLN:HG2	1.49	0.41
1:D:352:TRP:HZ3	3:D:-1:NAG:H83	1.86	0.41
1:D:204:MET:CE	3:D:-1:NAG:C1	2.93	0.41
1:D:121:LYS:O	1:D:124:PRO:HD2	2.20	0.41
1:B:366:GLN:CB	1:B:368:LEU:HD12	2.48	0.41
1:B:60:ASN:CG	1:B:61:ILE:H	2.22	0.41
1:C:126:PHE:CD1	1:C:126:PHE:C	2.94	0.41
1:C:293:THR:HG22	1:C:294:LEU:N	2.35	0.41
1:A:362:SER:OG	1:A:363:PHE:CD1	2.72	0.41
1:D:71:TRP:CD1	1:D:71:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LEU:HD12	1:D:222:LEU:O	2.21	0.41
1:A:263:ARG:HA	1:A:263:ARG:HD2	1.96	0.41
1:B:314:GLN:O	1:B:315:GLN:HB2	2.20	0.41
1:A:150:PHE:C	6:A:2047:HOH:O	2.55	0.41
1:B:243:TYR:CE2	1:B:247:LEU:HD11	2.56	0.41
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.87	0.41
1:C:116:ARG:O	1:C:117:ARG:C	2.59	0.41
1:C:267:LEU:HD13	1:C:272:THR:HG22	2.03	0.41
1:B:243:TYR:CZ	1:B:247:LEU:HD11	2.56	0.41
1:C:218:HIS:NE2	1:C:316:VAL:HB	2.36	0.41
1:A:33:GLN:HG3	1:A:34:TYR:CD1	2.54	0.41
1:D:328:TYR:HD2	1:D:329:ASP:O	2.03	0.41
1:A:232:ASP:HB2	1:A:233:ARG:H	1.69	0.41
1:B:193:LYS:HA	1:B:196:GLN:OE1	2.20	0.41
1:C:71:TRP:CZ2	2:C:-6:NAG:H2	2.55	0.41
1:C:58:PHE:CD2	1:C:98:GLY:HA3	2.56	0.41
1:C:175:SER:CB	1:C:200:PHE:CE1	3.02	0.41
1:D:184:THR:O	1:D:185:ILE:C	2.58	0.41
1:A:150:PHE:CZ	1:A:154:ILE:HD11	2.56	0.41
1:C:254:LEU:HD23	1:C:346:LEU:HD22	2.02	0.41
1:A:372:LEU:HD23	1:A:372:LEU:HA	1.82	0.41
1:C:94:LEU:HD22	1:C:132:PHE:CE2	2.56	0.41
1:D:36:GLU:O	1:D:37:GLY:O	2.39	0.41
1:D:333:SER:O	1:D:337:LYS:HG3	2.21	0.41
1:D:199:ASP:O	1:D:200:PHE:HB3	2.20	0.41
1:D:209:HIS:CD2	1:D:217:GLY:HA3	2.56	0.41
1:B:335:LYS:HG2	1:B:339:GLN:NE2	2.35	0.41
1:D:140:LEU:HA	1:D:141:TYR:HA	1.80	0.41
1:D:33:GLN:NE2	1:D:76:LEU:HD21	2.35	0.41
1:C:286:ARG:O	1:C:289:LYS:HG3	2.21	0.40
1:B:140:LEU:HA	1:B:141:TYR:HA	1.78	0.40
1:B:255:VAL:HG12	1:B:350:MET:HB2	2.03	0.40
1:B:318:TYR:CD1	1:B:318:TYR:C	2.95	0.40
1:D:64:ASP:OD1	1:D:115:SER:HB3	2.21	0.40
3:D:-2:NAG:C7	3:D:-1:NAG:H61	2.50	0.40
1:C:204:MET:HE2	1:C:204:MET:HB3	1.93	0.40
1:C:66:ILE:HB	1:C:119:PHE:HE1	1.86	0.40
1:A:146:ASP:O	1:A:147:LYS:C	2.60	0.40
1:D:296:TYR:CG	1:D:372:LEU:HD11	2.57	0.40
1:B:350:MET:SD	1:B:350:MET:C	3.00	0.40
1:A:123:VAL:HB	1:A:124:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HA	1:D:348:GLY:O	2.22	0.40
1:C:297:TYR:HB2	1:C:363:PHE:CD1	2.56	0.40
1:D:293:THR:HG22	1:D:294:LEU:N	2.37	0.40
1:C:293:THR:CG2	1:C:294:LEU:N	2.85	0.40
1:B:226:GLN:HG3	1:C:238:ASP:OD1	2.20	0.40
1:A:382:ALA:O	1:A:383:THR:HG23	2.21	0.40
1:A:62:SER:O	1:A:63:ASN:CB	2.70	0.40
1:C:34:TYR:CZ	2:C:-5:NAG:H3	2.57	0.40
1:C:44:ASP:OD1	1:C:79:MET:HE2	2.21	0.40
1:C:234:PHE:HB3	1:C:239:TYR:CE1	2.57	0.40
1:B:152:THR:O	1:B:156:GLU:HG3	2.21	0.40
1:A:190:ASP:O	1:A:191:ILE:C	2.59	0.40
1:D:46:LEU:HD23	1:D:46:LEU:N	2.36	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	362/362 (100%)	329 (91%)	29 (8%)	4 (1%)	17	46
1	B	361/362 (100%)	336 (93%)	24 (7%)	1 (0%)	46	77
1	C	362/362 (100%)	309 (85%)	44 (12%)	9 (2%)	7	21
1	D	361/362 (100%)	304 (84%)	47 (13%)	10 (3%)	6	18
All	All	1446/1448 (100%)	1278 (88%)	144 (10%)	24 (2%)	11	32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	SER
1	A	363	PHE

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Mol	Chain	Res	Type
1	C	66	ILE
1	C	68	THR
1	C	188	SER
1	D	36	GLU
1	D	37	GLY
1	A	231	PRO
1	C	63	ASN
1	D	101	PHE
1	D	114	GLN
1	D	291	ALA
1	D	312	LEU
1	D	382	ALA
1	B	366	GLN
1	C	204	MET
1	D	63	ASN
1	D	289	LYS
1	A	317	PRO
1	C	168	GLY
1	C	207	ASP
1	C	187	SER
1	C	231	PRO
1	D	183	VAL

### 5.3.2 Protein sidechains ⓘ

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	304/302 (101%)	288 (95%)	16 (5%)	28	58
1	B	303/302 (100%)	287 (95%)	16 (5%)	28	58
1	C	304/302 (101%)	280 (92%)	24 (8%)	15	37
1	D	303/302 (100%)	290 (96%)	13 (4%)	35	68
All	All	1214/1208 (100%)	1145 (94%)	69 (6%)	26	55

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	104	GLN
1	A	106	PHE
1	A	108	LYS
1	A	144	ARG
1	A	145	ARG
1	A	148	GLN
1	A	167	PRO
1	A	234	PHE
1	A	259	PRO
1	A	263	ARG
1	A	317	PRO
1	A	329	ASP
1	A	331	GLN
1	A	336	SER
1	A	383	THR
1	B	43	PRO
1	B	76	LEU
1	B	103	SER
1	B	106	PHE
1	B	145	ARG
1	B	148	GLN
1	B	167	PRO
1	B	171	GLN
1	B	227	GLU
1	B	234	PHE
1	B	259	PRO
1	B	263	ARG
1	B	301	ASP
1	B	329	ASP
1	B	364	CYS
1	B	368	LEU
1	C	67	ASP
1	C	73	ASP
1	C	90	LEU
1	C	104	GLN
1	C	106	PHE
1	C	129	THR
1	C	144	ARG
1	C	164	GLU
1	C	169	LYS
1	C	207	ASP
1	C	209	HIS

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Mol	Chain	Res	Type
1	C	222	LEU
1	C	227	GLU
1	C	234	PHE
1	C	246[A]	ARG
1	C	246[B]	ARG
1	C	259	PRO
1	C	263	ARG
1	C	286	ARG
1	C	307	THR
1	C	331	GLN
1	C	359	PHE
1	C	366	GLN
1	C	383	THR
1	D	67	ASP
1	D	106	PHE
1	D	118	THR
1	D	129	THR
1	D	152	THR
1	D	164	GLU
1	D	233	ARG
1	D	234	PHE
1	D	235	SER
1	D	317	PRO
1	D	331	GLN
1	D	368	LEU
1	D	369	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	72	ASN
1	A	85	ASN
1	A	89	ASN
1	A	100	ASN
1	A	315	GLN
1	A	331	GLN
1	B	85	ASN
1	B	89	ASN
1	B	148	GLN
1	B	149	HIS
1	B	339	GLN

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Mol	Chain	Res	Type
1	C	65	HIS
1	C	85	ASN
1	C	87	ASN
1	C	89	ASN
1	C	100	ASN
1	C	104	GLN
1	C	130	HIS
1	C	149	HIS
1	C	171	GLN
1	C	209	HIS
1	C	309	HIS
1	C	315	GLN
1	C	331	GLN
1	D	85	ASN
1	D	89	ASN
1	D	130	HIS
1	D	166	GLN
1	D	171	GLN
1	D	196	GLN
1	D	197	HIS
1	D	315	GLN
1	D	331	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

28 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
3	NAG	A	-1	3	14,14,15	0.76	0	15,19,21	0.81	0
3	NAG	A	-2	3	14,14,15	0.60	0	15,19,21	0.71	0
2	NAG	A	-5	2	15,15,15	0.52	0	17,21,21	0.77	0
2	NAG	A	-6	2	14,14,15	0.55	0	15,19,21	0.82	1 (6%)
2	NAG	A	-7	2	14,14,15	0.58	0	15,19,21	0.68	0
3	NAG	A	1	3	14,14,15	0.67	0	15,19,21	0.86	1 (6%)
3	NAG	A	2	3	15,15,15	0.64	0	17,21,21	0.96	1 (5%)
3	NAG	B	-1	3	14,14,15	0.87	0	15,19,21	1.03	2 (13%)
3	NAG	B	-2	3	14,14,15	0.53	0	15,19,21	0.66	0
2	NAG	B	-5	2	15,15,15	0.50	0	17,21,21	0.63	0
2	NAG	B	-6	2	14,14,15	0.71	0	15,19,21	0.83	1 (6%)
2	NAG	B	-7	2	14,14,15	0.67	0	15,19,21	0.71	0
3	NAG	B	1	3	14,14,15	0.55	0	15,19,21	0.94	1 (6%)
3	NAG	B	2	3	15,15,15	0.47	0	17,21,21	0.64	0
3	NAG	C	-1	3	14,14,15	0.73	0	15,19,21	1.13	2 (13%)
3	NAG	C	-2	3	14,14,15	0.63	0	15,19,21	0.87	1 (6%)
2	NAG	C	-5	2	15,15,15	0.58	0	17,21,21	0.60	0
2	NAG	C	-6	2	14,14,15	0.68	0	15,19,21	0.83	1 (6%)
2	NAG	C	-7	2	14,14,15	0.60	0	15,19,21	0.71	1 (6%)
3	NAG	C	1	3	14,14,15	0.73	0	15,19,21	0.99	1 (6%)
3	NAG	C	2	3	15,15,15	0.55	0	17,21,21	0.99	1 (5%)
3	NAG	D	-1	3	14,14,15	0.82	0	15,19,21	1.08	2 (13%)
3	NAG	D	-2	3	14,14,15	0.65	0	15,19,21	0.59	0
2	NAG	D	-5	2	15,15,15	0.67	0	17,21,21	0.75	0
2	NAG	D	-6	2	14,14,15	0.64	0	15,19,21	0.72	1 (6%)
2	NAG	D	-7	2	14,14,15	0.63	0	15,19,21	0.69	0
3	NAG	D	1	3	14,14,15	0.56	0	15,19,21	0.82	1 (6%)
3	NAG	D	2	3	15,15,15	0.57	0	17,21,21	0.69	0

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	-1	3	-	0/6/23/26	0/1/1/1
3	NAG	A	-2	3	-	0/6/23/26	0/1/1/1
2	NAG	A	-5	2	-	0/6/26/26	0/1/1/1
2	NAG	A	-6	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	-7	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/26/26	0/1/1/1
3	NAG	B	-1	3	-	0/6/23/26	0/1/1/1
3	NAG	B	-2	3	-	0/6/23/26	0/1/1/1
2	NAG	B	-5	2	-	2/6/26/26	0/1/1/1
2	NAG	B	-6	2	-	0/6/23/26	0/1/1/1
2	NAG	B	-7	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/26/26	0/1/1/1
3	NAG	C	-1	3	-	0/6/23/26	0/1/1/1
3	NAG	C	-2	3	-	0/6/23/26	0/1/1/1
2	NAG	C	-5	2	-	1/6/26/26	0/1/1/1
2	NAG	C	-6	2	-	0/6/23/26	0/1/1/1
2	NAG	C	-7	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/26/26	0/1/1/1
3	NAG	D	-1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	-2	3	-	0/6/23/26	0/1/1/1
2	NAG	D	-5	2	-	0/6/26/26	0/1/1/1
2	NAG	D	-6	2	-	0/6/23/26	0/1/1/1
2	NAG	D	-7	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	NAG	C2-N2-C7	-2.95	119.25	123.04
3	B	-1	NAG	C2-N2-C7	-2.82	119.42	123.04
3	C	-2	NAG	C2-N2-C7	-2.81	119.42	123.04
3	D	-1	NAG	C2-N2-C7	-2.79	119.46	123.04
3	C	1	NAG	C2-N2-C7	-2.73	119.53	123.04
2	A	-6	NAG	C2-N2-C7	-2.69	119.58	123.04
3	B	1	NAG	C2-N2-C7	-2.66	119.62	123.04
2	C	-6	NAG	C2-N2-C7	-2.55	119.76	123.04
3	D	1	NAG	C2-N2-C7	-2.39	119.97	123.04
2	D	-6	NAG	C2-N2-C7	-2.30	120.09	123.04
3	C	-1	NAG	C2-N2-C7	-2.18	120.23	123.04
2	B	-6	NAG	C2-N2-C7	-2.17	120.25	123.04
2	C	-7	NAG	C2-N2-C7	-2.11	120.32	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	NAG	C3-C4-C5	2.28	114.18	110.20
3	B	-1	NAG	C1-O5-C5	2.30	115.17	112.25
3	C	2	NAG	C4-C3-C2	2.33	113.66	110.43
3	D	-1	NAG	C1-O5-C5	2.34	115.22	112.25
3	C	-1	NAG	C1-O5-C5	2.87	115.89	112.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	-5	NAG	C8-C7-N2-C2
2	C	-5	NAG	O7-C7-N2-C2
2	B	-5	NAG	O7-C7-N2-C2

There are no ring outliers.

19 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	-1	NAG	5	0
3	A	-2	NAG	2	0
2	A	-6	NAG	3	0
2	A	-7	NAG	3	0
3	A	1	NAG	4	0
3	A	2	NAG	1	0
3	B	-1	NAG	3	0
3	B	-2	NAG	2	0
3	B	1	NAG	2	0
3	C	-1	NAG	10	0
3	C	-2	NAG	4	0
2	C	-5	NAG	1	0
2	C	-6	NAG	3	0
2	C	-7	NAG	2	0
3	C	1	NAG	3	0
3	D	-1	NAG	10	0
3	D	-2	NAG	2	0
2	D	-6	NAG	1	0
3	D	1	NAG	2	0

## 5.6 Ligand geometry

16 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	$\# Z  > 2$
4	NAG	A	1384	1	14,14,15	0.70	0	15,19,21	1.13	1 (6%)
5	SO4	A	1385	-	4,4,4	0.22	0	6,6,6	0.13	0
5	SO4	A	1386	-	4,4,4	0.30	0	6,6,6	0.27	0
5	SO4	A	1387	-	4,4,4	0.29	0	6,6,6	0.12	0
4	NAG	B	1384	1	14,14,15	0.75	0	15,19,21	0.78	1 (6%)
5	SO4	B	1385	-	4,4,4	0.25	0	6,6,6	0.07	0
5	SO4	B	1386	-	4,4,4	0.22	0	6,6,6	0.21	0
5	SO4	B	1387	-	4,4,4	0.32	0	6,6,6	0.14	0
4	NAG	C	1384	1	14,14,15	0.81	1 (7%)	15,19,21	0.75	0
5	SO4	C	1385	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	C	1386	-	4,4,4	0.20	0	6,6,6	0.11	0
5	SO4	C	1387	-	4,4,4	0.25	0	6,6,6	0.10	0
4	NAG	D	1384	1	14,14,15	0.64	0	15,19,21	0.65	0
5	SO4	D	1385	-	4,4,4	0.23	0	6,6,6	0.23	0
5	SO4	D	1386	-	4,4,4	0.23	0	6,6,6	0.15	0
5	SO4	D	1387	-	4,4,4	0.25	0	6,6,6	0.18	0

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
4	NAG	A	1384	1	-	0/6/23/26	0/1/1/1
5	SO4	A	1385	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1386	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1387	-	-	0/0/0/0	0/0/0/0
4	NAG	B	1384	1	-	0/6/23/26	0/1/1/1
5	SO4	B	1385	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1386	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1387	-	-	0/0/0/0	0/0/0/0
4	NAG	C	1384	1	-	0/6/23/26	0/1/1/1
5	SO4	C	1385	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1386	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	C	1387	-	-	0/0/0/0	0/0/0/0
4	NAG	D	1384	1	-	0/6/23/26	0/1/1/1
5	SO4	D	1385	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1386	-	-	0/0/0/0	0/0/0/0
5	SO4	D	1387	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1384	NAG	C1-C2	2.32	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1384	NAG	C2-N2-C7	-2.95	119.25	123.04
4	B	1384	NAG	C2-N2-C7	-2.33	120.05	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1384	NAG	1	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	362/362 (100%)	-0.38	5 (1%) 78 73	28, 49, 75, 102	0
1	B	362/362 (100%)	-0.38	6 (1%) 73 68	32, 48, 73, 92	0
1	C	362/362 (100%)	-0.02	14 (3%) 43 36	33, 71, 106, 117	0
1	D	362/362 (100%)	-0.15	13 (3%) 46 40	31, 61, 91, 108	0
All	All	1448/1448 (100%)	-0.23	38 (2%) 59 53	28, 55, 95, 117	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	ARG	5.2
1	B	363	PHE	4.6
1	D	366	GLN	4.5
1	C	363	PHE	4.2
1	D	212	TRP	4.0
1	C	145	ARG	3.9
1	D	363	PHE	3.8
1	D	96	VAL	3.4
1	D	365	GLY	3.0
1	D	65	HIS	3.0
1	B	211	ALA	2.9
1	B	145	ARG	2.9
1	C	95	SER	2.9
1	A	95	SER	2.8
1	D	22	TYR	2.7
1	C	144	ARG	2.7
1	C	366	GLN	2.6
1	C	63	ASN	2.6
1	D	137	LEU	2.5
1	C	136	ASP	2.4
1	B	95	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	138	ALA	2.3
1	D	95	SER	2.3
1	C	212	TRP	2.3
1	A	167	PRO	2.3
1	A	145	ARG	2.2
1	C	176	ALA	2.2
1	D	144	ARG	2.2
1	D	82	THR	2.2
1	B	362	SER	2.2
1	C	365	GLY	2.1
1	B	135	LEU	2.1
1	C	137	LEU	2.1
1	C	86	ARG	2.1
1	C	289	LYS	2.1
1	D	136	ASP	2.1
1	A	136	ASP	2.0
1	A	26	CYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	C	2	15/15	0.89	0.33	6.46	98,100,101,101	0
3	NAG	D	2	15/15	0.91	0.25	4.10	69,74,78,80	0
3	NAG	A	2	15/15	0.95	0.20	3.36	63,66,69,69	0
3	NAG	B	2	15/15	0.95	0.19	2.36	64,66,68,69	0
3	NAG	B	1	14/15	0.95	0.16	0.73	65,68,70,72	0
3	NAG	B	-2	14/15	0.94	0.17	0.72	55,65,68,69	0
3	NAG	C	-2	14/15	0.86	0.18	0.10	93,100,102,103	0
3	NAG	A	1	14/15	0.95	0.14	0.08	66,68,70,71	0
3	NAG	A	-1	14/15	0.94	0.16	0.03	57,62,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	1	14/15	0.91	0.16	-0.25	69,71,75,77	0
3	NAG	A	-2	14/15	0.92	0.14	-0.26	60,65,66,68	0
3	NAG	D	-2	14/15	0.93	0.15	-0.27	58,66,67,68	0
3	NAG	D	-1	14/15	0.94	0.15	-0.70	61,67,68,69	0
3	NAG	C	-1	14/15	0.92	0.16	-0.71	98,99,100,100	0
3	NAG	C	1	14/15	0.89	0.13	-0.89	94,99,99,99	0
3	NAG	B	-1	14/15	0.94	0.12	-1.15	64,67,68,68	0
2	NAG	B	-5	15/15	0.88	0.23	-	89,92,93,93	0
2	NAG	A	-6	14/15	0.90	0.14	-	97,101,103,106	0
2	NAG	B	-6	14/15	0.90	0.20	-	90,94,95,98	0
2	NAG	A	-7	14/15	0.88	0.31	-	109,111,111,112	0
2	NAG	C	-7	14/15	0.88	0.39	-	129,130,133,133	0
2	NAG	D	-6	14/15	0.91	0.23	-	93,95,96,97	0
2	NAG	D	-5	15/15	0.86	0.27	-	93,95,96,99	0
2	NAG	A	-5	15/15	0.92	0.18	-	93,98,100,100	0
2	NAG	B	-7	14/15	0.84	0.25	-	98,100,102,104	0
2	NAG	C	-6	14/15	0.85	0.25	-	118,122,123,127	0
2	NAG	C	-5	15/15	0.86	0.33	-	115,117,119,120	0
2	NAG	D	-7	14/15	0.89	0.33	-	98,99,101,101	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	1385	5/5	0.87	0.28	3.54	138,138,138,138	0
4	NAG	B	1384	14/15	0.92	0.22	1.35	64,66,69,71	0
5	SO4	A	1387	5/5	0.93	0.20	1.28	101,101,102,102	0
4	NAG	A	1384	14/15	0.91	0.20	0.73	62,64,67,67	0
5	SO4	A	1385	5/5	0.93	0.16	0.63	102,102,103,103	0
5	SO4	C	1385	5/5	0.89	0.18	0.36	137,137,138,138	0
4	NAG	D	1384	14/15	0.94	0.19	-0.16	86,87,88,89	0
5	SO4	C	1386	5/5	0.89	0.17	-0.23	142,142,142,142	0
5	SO4	D	1386	5/5	0.94	0.18	-0.26	117,118,119,119	0
4	NAG	C	1384	14/15	0.88	0.20	-0.50	102,104,105,107	0
5	SO4	B	1387	5/5	0.96	0.12	-0.50	87,87,88,88	0
5	SO4	D	1385	5/5	0.97	0.13	-0.67	86,87,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	1386	5/5	0.89	0.24	-	115,115,116,116	0
5	SO4	C	1387	5/5	0.84	0.24	-	139,140,140,140	0
5	SO4	A	1386	5/5	0.87	0.18	-	103,104,105,105	0
5	SO4	D	1387	5/5	0.93	0.20	-	102,102,103,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.