



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:41 AM GMT

PDB ID : 2XWB  
Title : Crystal Structure of Complement C3b in complex with Factors B and D  
Authors : Forneris, F.; Ricklin, D.; Wu, J.; Tzekou, A.; Wallace, R.S.; Lambris, J.D.; Gros, P.  
Deposited on : 2010-11-01  
Resolution : 3.49 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

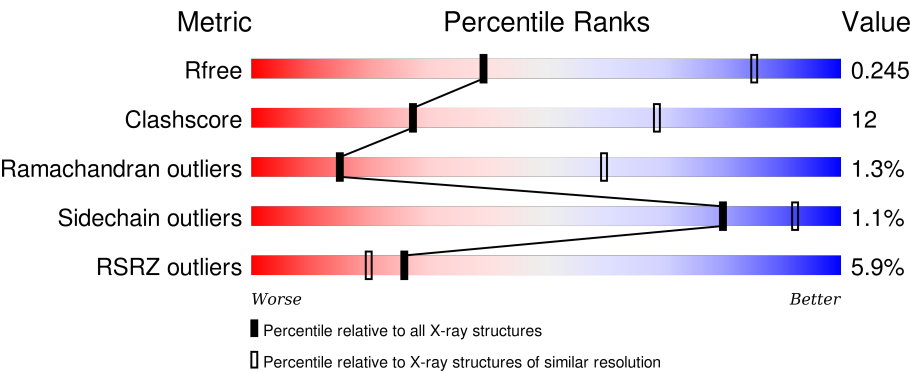
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	642	
1	C	642	
2	B	912	
2	D	912	
3	F	732	

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Mol	Chain	Length	Quality of chain
3	H	732	
4	I	228	
4	J	228	

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
5	NAG	C	2063	-	-	X	-
6	MG	H	1742	-	-	-	X
7	NAG	F	1747	X	-	-	-
9	GOL	I	1229	-	-	-	X
9	GOL	J	1229	-	-	X	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 39285 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 COMPLEMENT C3B BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	C	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	D	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	SEE REMARK 999	UNP P01024
D	991	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	714	Total	C	N	O	S	0	0	0
			5627	3536	979	1079	33			
3	H	711	Total	C	N	O	S	0	0	0
			5608	3523	976	1076	33			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	254	GLY	ASP	ENGINEERED MUTATION	UNP P00751
F	260	ASP	ASN	ENGINEERED MUTATION	UNP P00751

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Chain	Residue	Modelled	Actual	Comment	Reference
F	740	ALA	-	EXPRESSION TAG	UNP P00751
F	741	ALA	-	EXPRESSION TAG	UNP P00751
H	254	GLY	ASP	ENGINEERED MUTATION	UNP P00751
H	260	ASP	ASN	ENGINEERED MUTATION	UNP P00751
H	740	ALA	-	EXPRESSION TAG	UNP P00751
H	741	ALA	-	EXPRESSION TAG	UNP P00751

- Molecule 4 is a protein called COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	228	Total	C	N	O	S	0	0	0
			1710	1058	325	317	10			
4	J	228	Total	C	N	O	S	0	0	0
			1710	1058	325	317	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	183	ALA	SER	ENGINEERED MUTATION	UNP P00746
J	183	ALA	SER	ENGINEERED MUTATION	UNP P00746

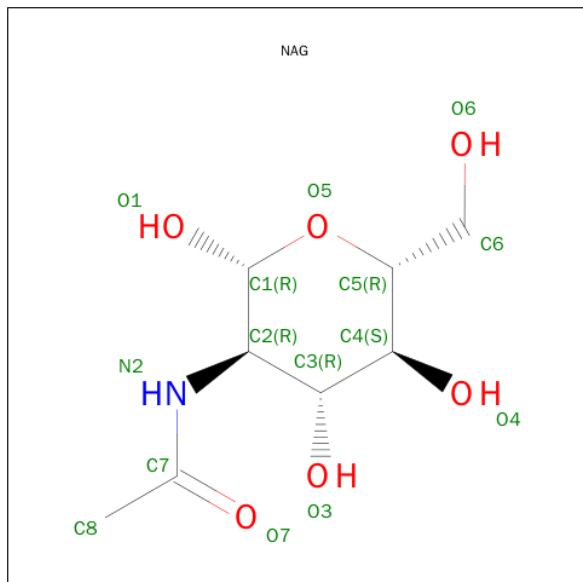
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	3	Total	C	N	O	0	0
			39	22	2	15		
8	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			6	3	3		
9	J	1	Total	C	O	0	0
			6	3	3		

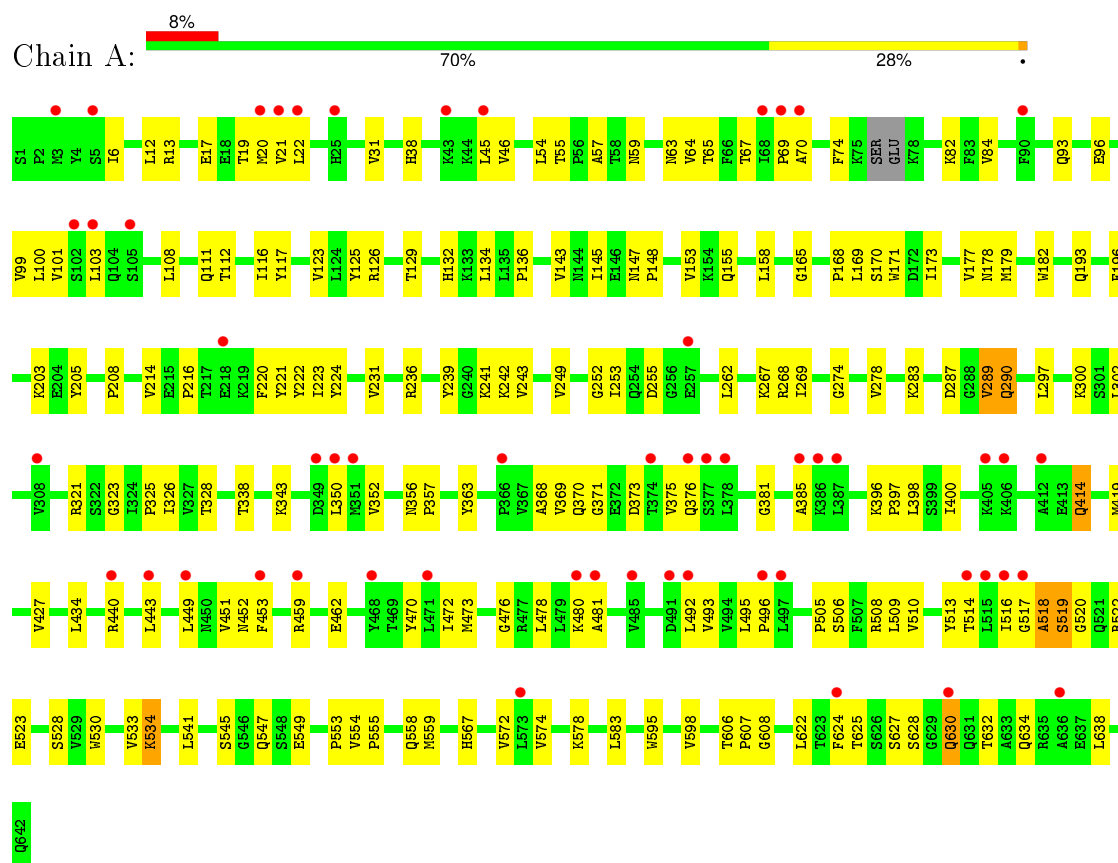
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	2	Total	O	0	0
			2	2		
10	H	2	Total	O	0	0
			2	2		

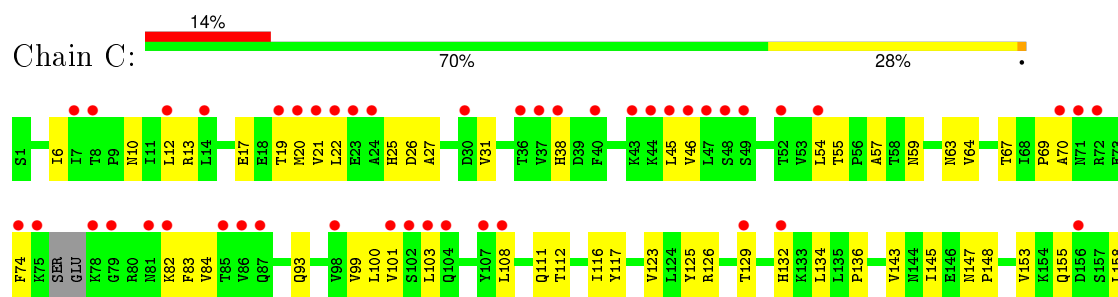
### 3 Residue-property plots

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.

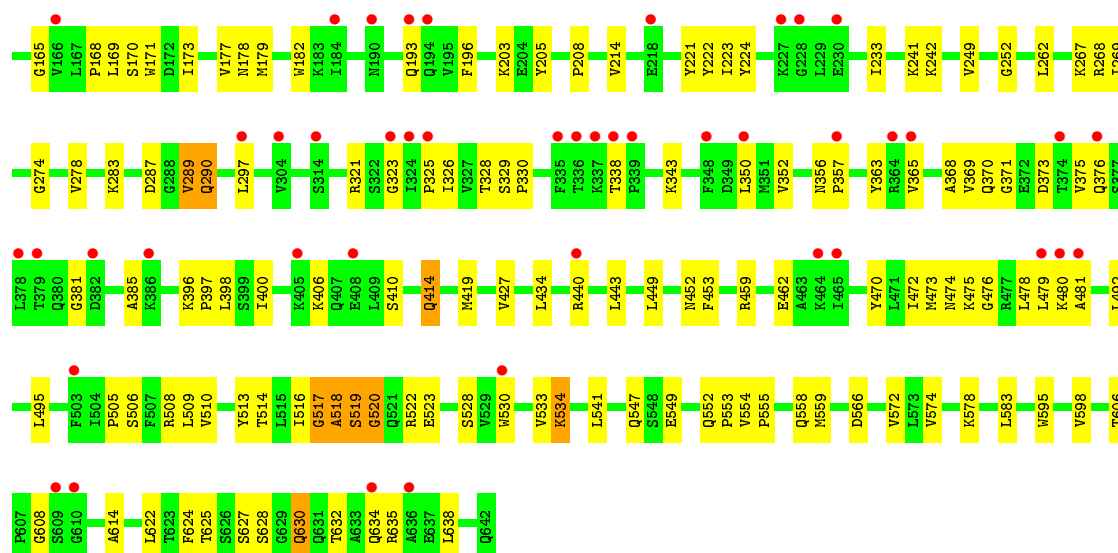
#### • Molecule 1: COMPLEMENT C3B BETA CHAIN



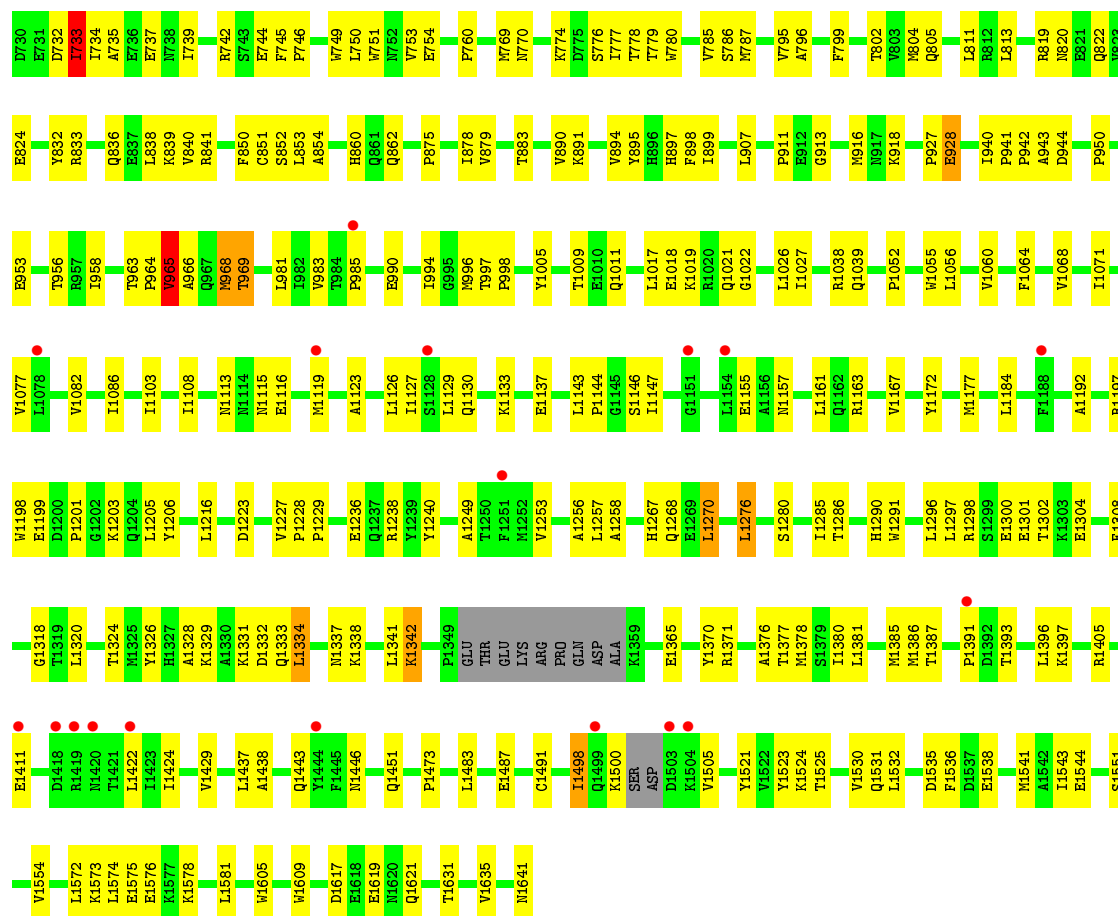
#### • Molecule 1: COMPLEMENT C3B BETA CHAIN





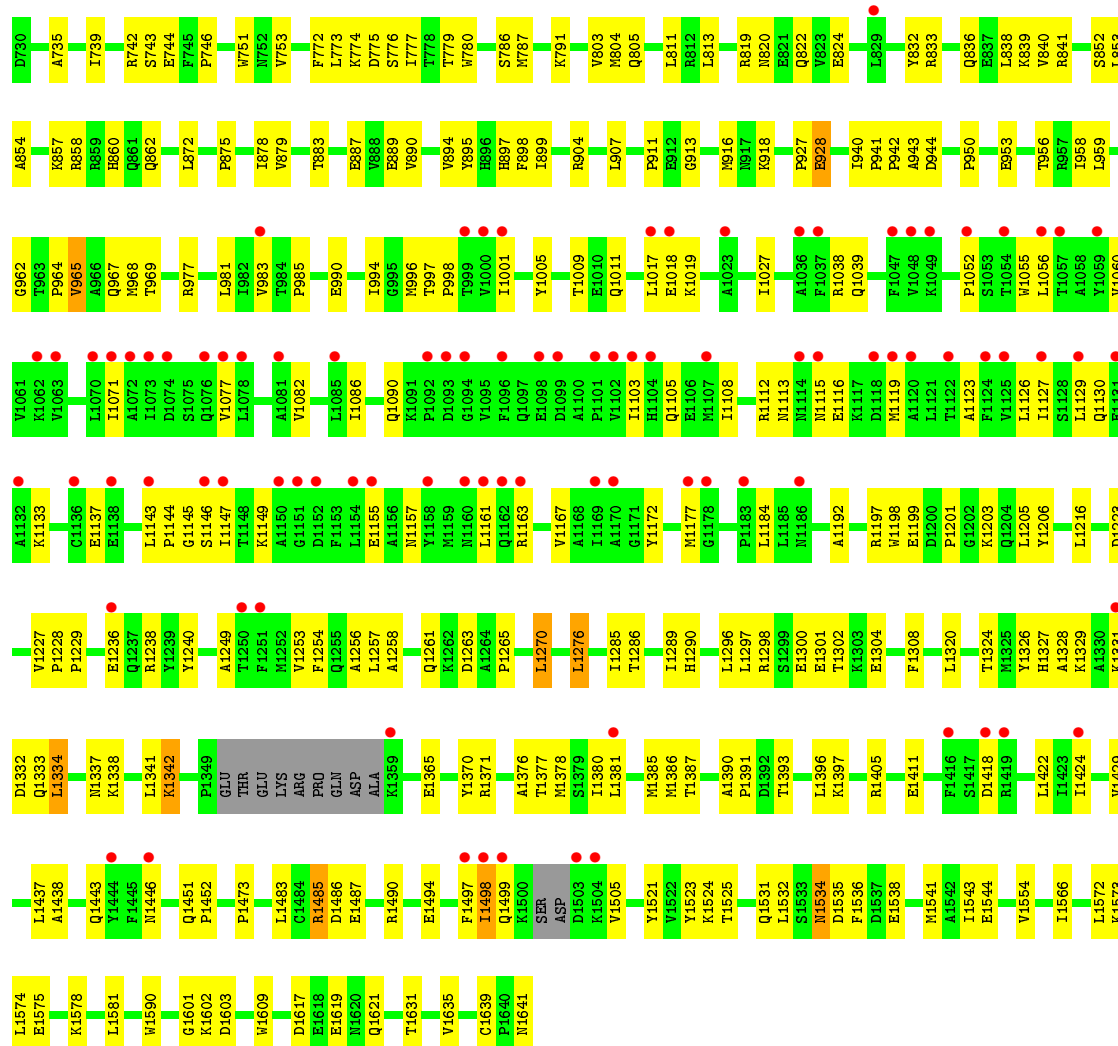


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



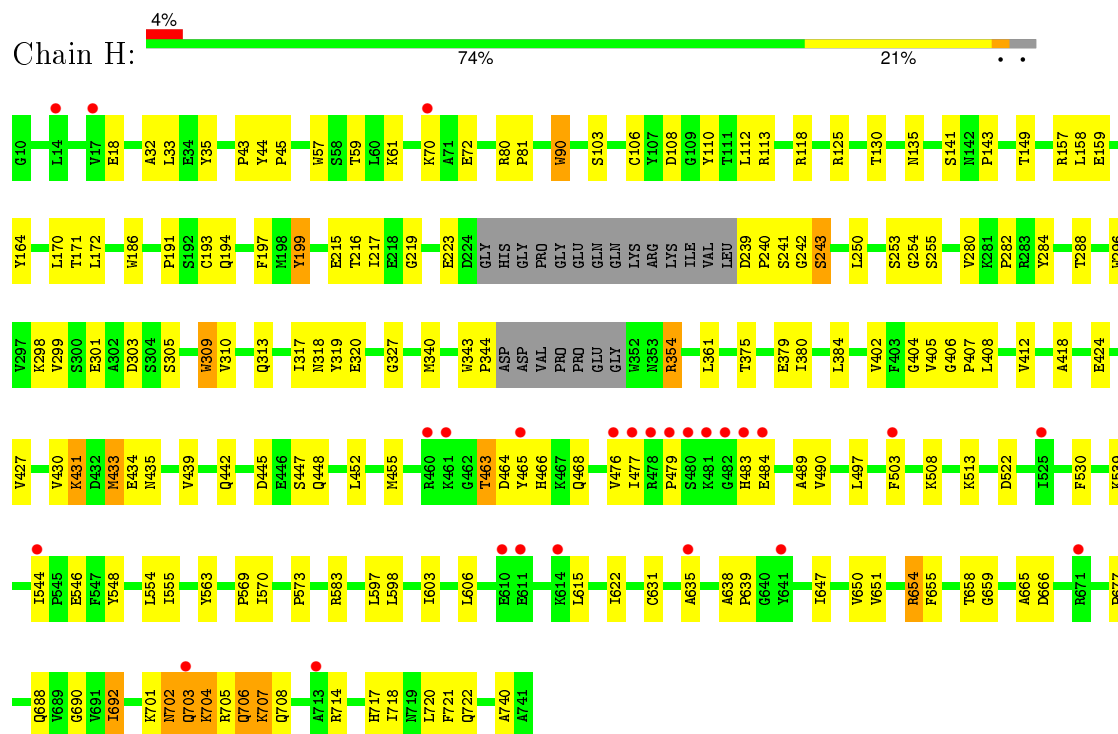


### • Molecule 3: COMPLEMENT FACTOR B

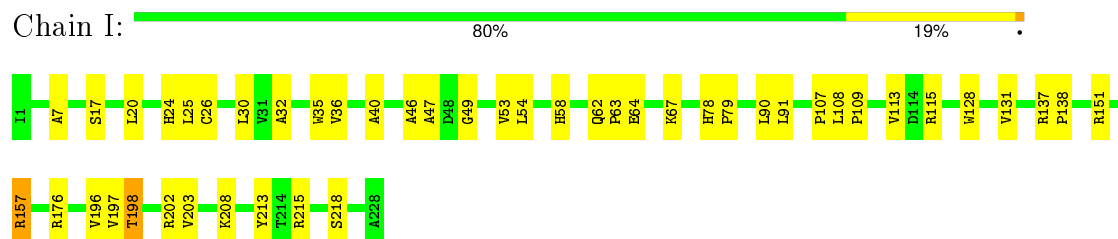


N702  
Q703  
K704  
R705  
Q706  
K707  
Q708  
V709  
P710  
R714  
H717  
I718  
N719  
L720  
F721  
Q722  
A740  
A741

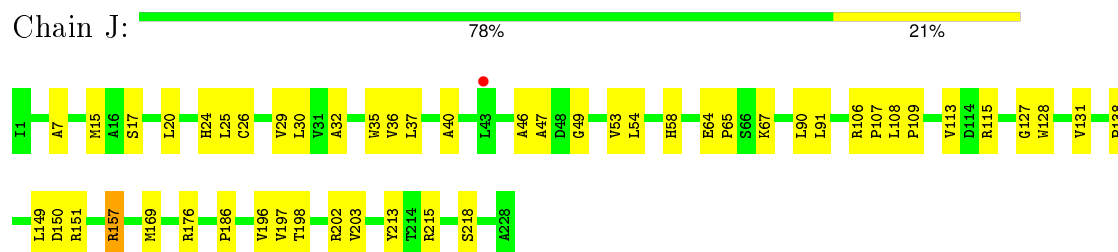
• Molecule 3: COMPLEMENT FACTOR B



• Molecule 4: COMPLEMENT FACTOR D



• Molecule 4: COMPLEMENT FACTOR D



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.28Å 135.78Å 149.97Å 95.47° 110.69° 113.39°	Depositor
Resolution (Å)	65.95 – 3.49 67.46 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.95-3.49) 83.2 (67.46-3.49)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, $R_{free}$	0.189 , 0.244 0.197 , 0.245	Depositor DCC
$R_{free}$ test set	4098 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 89.5	EDS
Estimated twinning fraction	0.045 for h,-h-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 81364 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	39285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

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	0.20	0/5092	0.37	0/6917
1	C	0.21	0/5092	0.39	0/6917
2	B	0.20	0/7340	0.36	0/9936
2	D	0.20	0/7340	0.36	0/9936
3	F	0.21	0/5754	0.37	0/7786
3	H	0.22	0/5733	0.37	0/7758
4	I	0.19	0/1745	0.36	0/2376
4	J	0.18	0/1745	0.36	0/2376
All	All	0.21	0/39841	0.37	0/54002

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
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	964	PRO	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	4992	0	5055	137	0
1	C	4992	0	5056	144	0
2	B	7197	0	7124	199	0
2	D	7197	0	7124	189	0
3	F	5627	0	5476	124	0
3	H	5608	0	5456	119	0
4	I	1710	0	1698	30	0
4	J	1710	0	1698	32	0
5	A	28	0	25	2	0
5	B	28	0	25	1	0
5	C	28	0	25	10	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	D	14	0	13	0	0
7	F	28	0	26	1	0
7	H	28	0	26	0	0
8	F	39	0	34	1	0
8	H	39	0	34	0	0
9	I	6	0	8	3	0
9	J	6	0	8	4	0
10	F	2	0	0	0	0
10	H	2	0	0	1	0
All	All	39285	0	38911	932	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 12.

All (932) 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:C:63:ASN:HD21	5:C:2063:NAG:C1	1.35	1.30
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.36	1.06
1:C:69:PRO:HA	1:C:70:ALA:HB3	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:ILE:HD11	2:B:841:ARG:HH21	1.32	0.94
1:A:628:SER:HB2	1:A:630:GLN:HE22	1.32	0.93
3:F:222:ALA:N	3:F:223:GLU:HA	1.82	0.93
1:C:628:SER:HB2	1:C:630:GLN:HE22	1.32	0.92
1:A:268:ARG:HH11	2:B:1378:MET:HE3	1.36	0.89
3:H:706:GLN:O	3:H:708:GLN:N	2.08	0.87
3:F:705:ARG:HH11	3:F:705:ARG:HG2	1.37	0.87
2:B:1331:LYS:HA	2:B:1332:ASP:HB2	1.56	0.87
2:B:733:ILE:HG22	2:B:895:TYR:HA	1.55	0.87
2:D:1331:LYS:HA	2:D:1332:ASP:HB2	1.58	0.86
1:C:268:ARG:HH11	2:D:1378:MET:HE3	1.40	0.86
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.41	0.84
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.42	0.84
2:D:840:VAL:HG22	2:D:894:VAL:HG12	1.58	0.83
1:C:517:GLY:O	1:C:518:ALA:O	1.97	0.83
1:C:158:LEU:HD21	1:C:169:LEU:HD21	1.60	0.81
3:H:706:GLN:HG3	3:H:706:GLN:O	1.81	0.80
1:A:158:LEU:HD21	1:A:169:LEU:HD21	1.63	0.79
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.63	0.79
3:H:489:ALA:HB2	3:H:677:PRO:HG3	1.64	0.78
2:D:1205:LEU:HD12	2:D:1249:ALA:HB2	1.65	0.78
3:F:489:ALA:HB2	3:F:677:PRO:HG3	1.65	0.78
2:B:1205:LEU:HD12	2:B:1249:ALA:HB2	1.65	0.78
2:B:840:VAL:HG22	2:B:894:VAL:HG12	1.65	0.77
3:H:539:LYS:HB3	3:H:544:ILE:HB	1.68	0.76
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.21	0.75
3:F:361:LEU:HD21	3:F:402:VAL:HG22	1.69	0.75
3:F:539:LYS:HB3	3:F:544:ILE:HB	1.67	0.75
1:C:223:ILE:H	1:C:223:ILE:HD12	1.52	0.75
3:H:361:LEU:HD21	3:H:402:VAL:HG22	1.69	0.75
1:C:168:PRO:HB3	3:H:108:ASP:HB3	1.69	0.74
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.70	0.74
3:H:705:ARG:O	3:H:707:LYS:N	2.21	0.74
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.70	0.74
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.70	0.74
4:J:150:ASP:HA	9:J:1229:GOL:H2	1.69	0.73
1:C:443:LEU:HD21	1:C:449:LEU:HD13	1.70	0.73
2:B:850:PHE:HZ	2:B:907:LEU:HD21	1.53	0.73
2:B:964:PRO:HA	2:B:965:VAL:HG12	1.71	0.73
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.70	0.72
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:H	1:A:223:ILE:HD12	1.52	0.72
1:C:505:PRO:HG3	1:C:595:TRP:CE3	2.25	0.72
1:C:100:LEU:HD21	1:C:638:LEU:HD23	1.72	0.71
3:F:143:PRO:HG3	3:F:186:TRP:CE2	2.25	0.71
2:B:1333:GLN:HA	2:B:1334:LEU:CB	2.21	0.70
3:H:508:LYS:HA	3:H:508:LYS:HE2	1.73	0.70
4:J:151:ARG:H	9:J:1229:GOL:H11	1.56	0.70
1:C:414:GLN:HE21	1:C:414:GLN:HA	1.57	0.70
1:A:414:GLN:HA	1:A:414:GLN:HE21	1.56	0.70
3:H:430:VAL:HG11	3:H:433:MET:HE1	1.72	0.70
1:A:547:GLN:HE22	1:A:559:MET:HA	1.56	0.70
1:C:480:LYS:HA	5:C:2063:NAG:H81	1.73	0.70
2:D:1333:GLN:HA	2:D:1334:LEU:CB	2.20	0.70
2:B:1103:ILE:HD12	2:B:1103:ILE:H	1.56	0.70
1:C:547:GLN:HE22	1:C:559:MET:HA	1.56	0.69
1:C:63:ASN:HD21	5:C:2063:NAG:C2	2.03	0.69
1:A:443:LEU:HD21	1:A:449:LEU:HD13	1.73	0.69
3:H:143:PRO:HG3	3:H:186:TRP:CE2	2.28	0.69
2:D:858:ARG:HH22	2:D:1494:GLU:HA	1.56	0.69
3:F:705:ARG:NH1	3:F:705:ARG:HG2	2.03	0.68
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.73	0.68
3:F:508:LYS:HE2	3:F:508:LYS:HA	1.76	0.68
1:C:63:ASN:CG	5:C:2063:NAG:C1	2.61	0.67
3:F:706:GLN:O	3:F:708:GLN:N	2.27	0.67
2:B:785:VAL:HG22	2:B:795:VAL:HG12	1.74	0.67
1:C:55:THR:HG22	1:C:57:ALA:H	1.59	0.67
1:C:443:LEU:HD11	1:C:449:LEU:HD22	1.76	0.67
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.76	0.67
2:D:1333:GLN:HA	2:D:1334:LEU:HB3	1.77	0.66
1:C:518:ALA:O	1:C:520:GLY:N	2.28	0.66
2:D:804:MET:HG2	2:D:805:GLN:H	1.60	0.66
3:F:464:ASP:O	3:F:465:TYR:HB2	1.95	0.66
2:B:1333:GLN:HA	2:B:1334:LEU:HB3	1.78	0.66
3:F:430:VAL:HG11	3:F:433:MET:HE1	1.78	0.66
2:D:967:GLN:HG2	2:D:968:MET:H	1.61	0.65
2:B:819:ARG:HH12	2:B:1487:GLU:HG2	1.60	0.65
2:B:819:ARG:NH1	2:B:1487:GLU:HG2	2.12	0.65
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.77	0.65
4:J:32:ALA:HB3	4:J:35:TRP:HB2	1.78	0.65
2:D:857:LYS:HD2	2:D:1602:LYS:HE2	1.79	0.65
4:J:64:GLU:HB2	4:J:67:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:64:GLU:HB2	4:I:67:LYS:HG3	1.78	0.64
1:A:55:THR:HG22	1:A:57:ALA:H	1.61	0.64
2:D:927:PRO:O	2:D:928:GLU:HB2	1.98	0.64
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.32	0.64
2:B:1280:SER:HA	3:F:390:ARG:HD3	1.80	0.64
2:B:927:PRO:O	2:B:928:GLU:HB2	1.98	0.63
1:C:208:PRO:HD3	1:C:583:LEU:HD11	1.80	0.63
3:H:318:ASN:HD21	3:H:320:GLU:HG2	1.64	0.63
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.80	0.63
1:C:506:SER:HB2	1:C:530:TRP:HE1	1.63	0.63
1:C:606:THR:HG22	1:C:608:GLY:H	1.63	0.63
4:I:32:ALA:HB3	4:I:35:TRP:HB2	1.79	0.63
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.81	0.63
2:D:1490:ARG:HD2	2:D:1590:TRP:CZ3	2.33	0.63
2:B:819:ARG:HE	2:B:883:THR:HG23	1.63	0.63
1:A:606:THR:HG22	1:A:608:GLY:H	1.63	0.63
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.81	0.63
1:A:69:PRO:HA	1:A:70:ALA:CB	2.17	0.62
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.11	0.62
1:C:19:THR:HB	1:C:478:LEU:HB2	1.80	0.62
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.82	0.62
1:C:69:PRO:HA	1:C:70:ALA:CB	2.18	0.62
1:A:19:THR:HB	1:A:478:LEU:HB2	1.81	0.62
3:H:598:LEU:HA	3:H:603:ILE:HD13	1.81	0.62
1:C:368:ALA:HB2	1:C:376:GLN:HG2	1.82	0.62
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.65	0.62
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.64	0.62
1:A:452:ASN:HB3	1:A:492:LEU:HD11	1.82	0.62
2:B:943:ALA:HB2	2:B:1324:THR:HG21	1.82	0.61
1:C:45:LEU:H	1:C:45:LEU:HD23	1.65	0.61
2:D:1531:GLN:HB2	2:D:1538:GLU:HB2	1.82	0.61
2:D:819:ARG:HE	2:D:883:THR:HG23	1.64	0.61
1:A:208:PRO:HD3	1:A:583:LEU:HD11	1.83	0.61
3:F:705:ARG:O	3:F:707:LYS:N	2.34	0.61
2:D:958:ILE:HG21	2:D:1276:LEU:HD13	1.83	0.61
1:C:452:ASN:HB3	1:C:492:LEU:HD11	1.83	0.61
3:F:299:VAL:H	3:F:340:MET:HE3	1.65	0.60
4:I:108:LEU:HD12	4:I:109:PRO:HD2	1.83	0.60
3:H:113:ARG:HH22	3:H:141:SER:HB2	1.65	0.60
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.66	0.60
1:A:45:LEU:HD23	1:A:45:LEU:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:958:ILE:HG21	2:B:1276:LEU:HD13	1.84	0.60
3:F:598:LEU:HA	3:F:603:ILE:HD13	1.83	0.60
4:J:108:LEU:HD12	4:J:109:PRO:HD2	1.82	0.60
3:H:239:ASP:CB	3:H:240:PRO:HD2	2.32	0.60
2:B:853:LEU:HB2	2:B:860:HIS:CD2	2.37	0.59
2:D:943:ALA:HB2	2:D:1324:THR:HG21	1.84	0.59
1:A:368:ALA:HB2	1:A:376:GLN:HG2	1.83	0.59
2:D:1113:ASN:HB3	2:D:1163:ARG:HH12	1.67	0.59
1:C:479:LEU:O	5:C:2063:NAG:H83	2.03	0.59
2:D:853:LEU:HB2	2:D:860:HIS:CD2	2.37	0.59
1:A:396:LYS:HD2	1:A:397:PRO:HD2	1.83	0.59
3:H:442:GLN:HE22	4:J:176:ARG:HH22	1.50	0.59
1:C:126:ARG:HG3	2:D:751:TRP:CZ2	2.38	0.58
3:H:318:ASN:ND2	3:H:320:GLU:HG2	2.18	0.58
2:D:1534:ASN:O	2:D:1566:ILE:HG13	2.04	0.58
3:F:631:CYS:SG	3:F:714:ARG:HD2	2.43	0.58
2:D:1276:LEU:HG	2:D:1285:ILE:HB	1.86	0.58
2:D:811:LEU:HD22	2:D:890:VAL:HG22	1.85	0.58
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.14	0.58
1:C:6:ILE:HD11	1:C:20:MET:HG2	1.86	0.58
3:F:690:GLY:HA2	3:F:718:ILE:O	2.04	0.58
2:B:813:LEU:HD23	2:B:907:LEU:HB3	1.86	0.57
1:C:396:LYS:HD2	1:C:397:PRO:HD2	1.85	0.57
1:A:352:VAL:HB	1:A:385:ALA:HB3	1.86	0.57
2:D:1126:LEU:HD21	2:D:1177:MET:HE3	1.87	0.57
1:A:221:TYR:HD2	1:A:326:ILE:HG23	1.70	0.57
2:B:1113:ASN:HB3	2:B:1163:ARG:HH12	1.69	0.57
1:A:239:TYR:HB2	2:B:804:MET:HE2	1.86	0.57
3:H:563:TYR:CZ	3:H:569:PRO:HG3	2.40	0.57
4:J:131:VAL:HG13	4:J:138:PRO:HG3	1.86	0.57
1:C:514:THR:OG1	1:C:522:ARG:HD2	2.04	0.57
1:A:168:PRO:HB3	3:F:108:ASP:HB3	1.87	0.57
2:D:997:THR:N	2:D:998:PRO:HD2	2.20	0.57
1:C:289:VAL:HG21	1:C:297:LEU:HD21	1.86	0.57
2:B:811:LEU:HD22	2:B:890:VAL:HG22	1.86	0.57
2:D:1027:ILE:HG22	2:D:1071:ILE:HD13	1.86	0.57
2:B:883:THR:HG21	2:B:911:PRO:HG3	1.85	0.56
1:A:514:THR:OG1	1:A:522:ARG:HD2	2.05	0.56
3:H:622:ILE:HA	3:H:658:THR:HG22	1.87	0.56
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	1.87	0.56
4:I:131:VAL:HG13	4:I:138:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASN:ND2	5:C:2063:NAG:O5	2.34	0.56
2:D:804:MET:HG2	2:D:805:GLN:N	2.19	0.56
2:D:1525:THR:HG22	2:D:1543:ILE:HA	1.86	0.56
4:J:20:LEU:HD11	4:J:49:GLY:HA3	1.87	0.56
1:A:289:VAL:HG21	1:A:297:LEU:HD21	1.87	0.56
3:H:299:VAL:H	3:H:340:MET:HE3	1.69	0.56
4:I:20:LEU:HD11	4:I:49:GLY:HA3	1.87	0.56
1:A:6:ILE:HD11	1:A:20:MET:HG2	1.87	0.56
1:C:480:LYS:HA	5:C:2063:NAG:C8	2.36	0.56
3:H:690:GLY:HA2	3:H:718:ILE:O	2.06	0.56
5:A:1643:NAG:C1	5:A:1643:NAG:O4	2.52	0.56
2:B:1302:THR:HG22	2:B:1304:GLU:H	1.71	0.56
1:A:289:VAL:O	1:A:290:GLN:HG2	2.06	0.56
1:C:134:LEU:HD11	1:C:598:VAL:HG21	1.87	0.56
2:B:1376:ALA:HB3	2:B:1429:VAL:HG23	1.88	0.56
2:B:997:THR:N	2:B:998:PRO:HD2	2.20	0.56
2:D:1238:ARG:HG2	2:D:1240:TYR:OH	2.06	0.56
3:H:172:LEU:HD11	3:H:191:PRO:HB3	1.88	0.55
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.88	0.55
3:F:622:ILE:HA	3:F:658:THR:HG22	1.88	0.55
1:C:289:VAL:O	1:C:290:GLN:HG2	2.06	0.55
2:D:1302:THR:HG22	2:D:1304:GLU:H	1.70	0.55
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.22	0.55
2:B:1331:LYS:CA	2:B:1332:ASP:HB2	2.32	0.55
3:H:597:LEU:HD12	3:H:721:PHE:HZ	1.72	0.55
1:C:221:TYR:HD2	1:C:326:ILE:HG23	1.70	0.55
1:A:363:TYR:HD1	1:A:381:GLY:HA2	1.72	0.55
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.87	0.55
2:D:889:GLU:HB2	2:D:904:ARG:HG3	1.89	0.55
2:B:1126:LEU:HD21	2:B:1177:MET:HE3	1.89	0.55
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.89	0.55
2:D:742:ARG:HH12	2:D:777:ILE:HG13	1.72	0.55
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.89	0.55
1:C:241:LYS:HG3	2:D:832:TYR:CE1	2.42	0.55
2:D:911:PRO:HD2	2:D:1327:HIS:HE1	1.72	0.55
1:C:363:TYR:HD1	1:C:381:GLY:HA2	1.72	0.55
3:F:113:ARG:HH22	3:F:141:SER:HB2	1.71	0.54
1:C:352:VAL:HB	1:C:385:ALA:HB3	1.88	0.54
1:A:517:GLY:O	1:A:518:ALA:O	2.25	0.54
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.88	0.54
3:F:563:TYR:CZ	3:F:569:PRO:HG3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:VAL:HG23	2:B:897:HIS:HB2	1.90	0.54
3:H:659:GLY:HA2	3:H:666:ASP:HB2	1.90	0.54
2:B:1238:ARG:HG2	2:B:1240:TYR:OH	2.07	0.54
2:B:964:PRO:HA	2:B:965:VAL:CG1	2.36	0.54
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.88	0.54
3:F:172:LEU:HD11	3:F:191:PRO:HB3	1.90	0.54
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.23	0.54
2:D:956:THR:HG23	2:D:1324:THR:HG22	1.90	0.54
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.72	0.54
3:H:631:CYS:SG	3:H:714:ARG:HD2	2.48	0.54
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.43	0.54
3:F:216:THR:HG22	3:F:216:THR:O	2.08	0.54
2:D:1376:ALA:HB3	2:D:1429:VAL:HG23	1.90	0.54
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.90	0.54
2:D:1370:TYR:CD1	2:D:1376:ALA:HB2	2.43	0.54
3:F:573:PRO:HB3	3:F:721:PHE:CZ	2.43	0.54
3:F:18:GLU:HG2	3:F:70:LYS:NZ	2.23	0.54
2:B:956:THR:HG23	2:B:1324:THR:HG22	1.90	0.53
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.43	0.53
3:H:284:TYR:HB2	3:H:310:VAL:HG21	1.90	0.53
3:F:468:GLN:HG2	3:F:608:VAL:HG21	1.88	0.53
2:B:1276:LEU:HG	2:B:1285:ILE:HB	1.89	0.53
1:C:578:LYS:HG3	2:D:779:THR:O	2.09	0.53
3:F:284:TYR:HB2	3:F:310:VAL:HG21	1.88	0.53
1:C:193:GLN:CD	1:C:193:GLN:H	2.11	0.53
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.74	0.53
1:A:193:GLN:CD	1:A:193:GLN:H	2.11	0.53
3:F:149:THR:HG22	3:F:193:CYS:SG	2.48	0.53
2:B:1005:TYR:HD1	2:B:1258:ALA:HB2	1.73	0.53
2:D:894:VAL:HG23	2:D:897:HIS:HB2	1.91	0.53
3:F:433:MET:C	3:F:435:ASN:H	2.13	0.53
3:H:573:PRO:HB3	3:H:721:PHE:CZ	2.43	0.53
2:D:1203:LYS:HG3	2:D:1206:TYR:CE2	2.44	0.53
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.89	0.53
4:J:197:VAL:HG22	4:J:213:TYR:HE2	1.73	0.53
5:C:2063:NAG:O6	5:C:2064:NAG:N2	2.36	0.53
2:B:776:SER:HB2	2:B:780:TRP:HZ2	1.72	0.53
3:F:503:PHE:CZ	3:F:555:ILE:HD11	2.43	0.53
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.91	0.53
3:F:659:GLY:HA2	3:F:666:ASP:HB2	1.91	0.53
1:A:134:LEU:HD11	1:A:598:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:959:LEU:HD11	2:D:1297:LEU:HD22	1.91	0.53
3:H:219:GLY:HA2	3:H:455:MET:CE	2.39	0.53
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.91	0.52
3:F:348:PRO:N	3:F:349:PRO:HD3	2.24	0.52
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	1.89	0.52
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.44	0.52
3:F:442:GLN:HE22	4:I:176:ARG:HH22	1.58	0.52
1:C:126:ARG:HG3	2:D:751:TRP:HZ2	1.74	0.52
2:B:742:ARG:NH1	2:B:777:ILE:HG13	2.24	0.52
2:D:894:VAL:CG2	2:D:899:ILE:HB	2.40	0.52
3:H:239:ASP:HB3	3:H:240:PRO:HD2	1.92	0.52
2:B:965:VAL:HG21	2:B:1268:GLN:HE21	1.75	0.52
2:B:742:ARG:HH12	2:B:777:ILE:HG13	1.74	0.52
2:B:1572:LEU:HB3	2:B:1574:LEU:HG	1.91	0.52
2:D:950:PRO:HD3	2:D:1329:LYS:HE2	1.92	0.52
3:H:18:GLU:HG2	3:H:70:LYS:NZ	2.25	0.52
2:D:1525:THR:HB	2:D:1541:MET:HB3	1.92	0.52
3:F:407:PRO:HB2	3:F:408:LEU:HD22	1.91	0.52
2:B:1203:LYS:HG3	2:B:1206:TYR:CE2	2.44	0.52
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.44	0.52
3:H:219:GLY:HA2	3:H:455:MET:HE1	1.92	0.52
4:I:196:VAL:O	4:I:198:THR:HG22	2.09	0.52
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.10	0.52
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.10	0.52
2:D:744:GLU:C	2:D:746:PRO:HD3	2.31	0.52
3:H:503:PHE:CZ	3:H:555:ILE:HD11	2.44	0.52
4:I:24:HIS:CE1	4:I:128:TRP:HB2	2.45	0.52
2:D:1331:LYS:CA	2:D:1332:ASP:HB2	2.34	0.52
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.92	0.52
3:H:216:THR:HG22	3:H:216:THR:O	2.09	0.52
3:H:430:VAL:HG21	3:H:433:MET:CE	2.40	0.51
2:D:1133:LYS:O	2:D:1137:GLU:HB2	2.10	0.51
2:D:967:GLN:HG2	2:D:968:MET:N	2.25	0.51
2:B:819:ARG:HH12	2:B:1487:GLU:CG	2.23	0.51
4:J:24:HIS:CE1	4:J:128:TRP:HB2	2.45	0.51
1:C:223:ILE:HD13	1:C:328:THR:HG22	1.92	0.51
1:C:84:VAL:HG13	1:C:101:VAL:HG21	1.92	0.51
4:J:149:LEU:O	9:J:1229:GOL:H31	2.10	0.51
2:D:1498:ILE:HA	2:D:1602:LYS:O	2.11	0.51
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.76	0.51
4:J:113:VAL:HG12	4:J:115:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:773:LEU:HD13	2:D:803:VAL:HG21	1.91	0.51
1:A:13:ARG:NH1	1:A:132:HIS:HB3	2.25	0.51
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	1.92	0.51
4:I:197:VAL:HG22	4:I:213:TYR:HE2	1.75	0.51
2:B:1575:GLU:HB2	2:B:1578:LYS:HD2	1.93	0.51
2:B:894:VAL:CG2	2:B:899:ILE:HB	2.41	0.51
1:C:136:PRO:HG3	2:D:787:MET:SD	2.50	0.51
3:F:463:THR:O	3:F:466:HIS:HB2	2.11	0.51
2:D:1103:ILE:H	2:D:1103:ILE:HD12	1.74	0.51
1:A:223:ILE:HD13	1:A:328:THR:HG22	1.91	0.51
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.93	0.51
1:C:147:ASN:HA	1:C:182:TRP:CE3	2.46	0.51
3:H:242:GLY:O	3:H:243:SER:HB2	2.11	0.51
3:H:253:SER:HB3	10:H:2001:HOH:O	2.11	0.51
3:H:407:PRO:HB2	3:H:408:LEU:HD22	1.93	0.51
3:H:250:LEU:HB3	3:H:288:THR:HG22	1.92	0.51
2:B:1530:VAL:HG23	2:B:1576:GLU:HG2	1.92	0.51
1:C:13:ARG:NH1	1:C:132:HIS:HB3	2.26	0.51
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.29	0.51
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.46	0.51
3:H:298:LYS:HZ2	3:H:340:MET:HA	1.77	0.51
2:D:1572:LEU:HB3	2:D:1574:LEU:HG	1.92	0.51
2:B:950:PRO:HD3	2:B:1329:LYS:HE2	1.93	0.51
2:D:1498:ILE:HG12	2:D:1603:ASP:HA	1.93	0.50
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.93	0.50
4:I:113:VAL:HG12	4:I:115:ARG:HG3	1.92	0.50
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.47	0.50
2:D:1532:LEU:O	2:D:1532:LEU:HD12	2.11	0.50
1:C:241:LYS:HE2	2:D:804:MET:HE1	1.93	0.50
2:D:1113:ASN:HB3	2:D:1163:ARG:NH1	2.26	0.50
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.30	0.50
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.47	0.50
2:B:1133:LYS:O	2:B:1137:GLU:HB2	2.12	0.50
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.12	0.50
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.46	0.50
1:A:470:TYR:HB2	1:A:509:LEU:HD21	1.94	0.50
2:D:1286:THR:HG22	3:H:665:ALA:HB3	1.93	0.50
2:D:1017:LEU:C	2:D:1019:LYS:H	2.15	0.50
4:J:196:VAL:O	4:J:198:THR:HG22	2.12	0.50
3:H:424:GLU:OE2	3:H:583:ARG:HD3	2.11	0.50
3:H:303:ASP:HB3	3:H:309:TRP:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.47	0.50
1:A:96:GLU:OE2	2:B:1021:GLN:HG2	2.12	0.50
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.93	0.49
3:H:433:MET:C	3:H:435:ASN:H	2.15	0.49
2:D:743:SER:HB3	2:D:904:ARG:NH1	2.27	0.49
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.27	0.49
3:H:298:LYS:HB3	3:H:301:GLU:HG3	1.94	0.49
2:B:833:ARG:HD3	2:B:836:GLN:HE21	1.76	0.49
3:F:303:ASP:HB3	3:F:309:TRP:CD1	2.47	0.49
1:C:126:ARG:CZ	1:C:572:VAL:HB	2.43	0.49
3:F:298:LYS:HB3	3:F:301:GLU:HG3	1.94	0.49
2:D:1535:ASP:O	2:D:1536:PHE:HB2	2.12	0.49
1:A:147:ASN:HA	1:A:182:TRP:CE3	2.47	0.49
2:B:746:PRO:HG2	2:B:774:LYS:HE3	1.94	0.49
1:C:153:VAL:HG12	2:D:1297:LEU:HD12	1.94	0.49
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.93	0.49
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.43	0.49
3:H:570:ILE:HD13	3:H:688:GLN:HB2	1.94	0.49
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	1.94	0.49
4:I:157:ARG:HD3	4:I:157:ARG:C	2.32	0.49
1:C:6:ILE:HD11	1:C:20:MET:CG	2.42	0.49
4:I:40:ALA:HA	4:I:91:LEU:HB2	1.95	0.49
2:B:735:ALA:HB1	2:B:737:GLU:OE1	2.12	0.49
3:F:296:TRP:CE2	3:F:317:ILE:HG22	2.47	0.49
2:B:751:TRP:HB3	3:F:107:TYR:CD1	2.48	0.49
3:H:149:THR:HG22	3:H:193:CYS:SG	2.53	0.49
4:J:29:VAL:HB	4:J:186:PRO:HG3	1.95	0.49
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.94	0.49
2:D:1381:LEU:HB2	2:D:1424:ILE:O	2.13	0.49
4:I:25:LEU:HG	4:I:26:CYS:SG	2.52	0.49
3:F:424:GLU:OE2	3:F:583:ARG:HD3	2.12	0.49
3:F:597:LEU:HD12	3:F:721:PHE:HZ	1.76	0.49
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.94	0.49
2:B:1381:LEU:HB2	2:B:1424:ILE:O	2.13	0.49
4:J:40:ALA:HA	4:J:91:LEU:HB2	1.94	0.49
1:A:136:PRO:HG3	2:B:787:MET:SD	2.53	0.48
2:B:850:PHE:CZ	2:B:907:LEU:HD21	2.42	0.48
3:H:430:VAL:HG21	3:H:433:MET:HE2	1.95	0.48
2:D:1285:ILE:HG21	2:D:1300:GLU:HG3	1.95	0.48
3:H:118:ARG:NH1	3:H:130:THR:HA	2.29	0.48
3:F:570:ILE:HD13	3:F:688:GLN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1119:MET:HG3	2:D:1161:LEU:HD21	1.95	0.48
3:H:476:VAL:HB	3:H:484:GLU:HB3	1.95	0.48
1:A:478:LEU:HD21	1:A:622:LEU:HD21	1.94	0.48
2:B:1113:ASN:HB3	2:B:1163:ARG:NH1	2.27	0.48
3:H:158:LEU:O	3:H:159:GLU:HB2	2.13	0.48
1:A:624:PHE:H	1:A:632:THR:CG2	2.27	0.48
4:I:36:VAL:HG21	4:I:53:VAL:HG11	1.95	0.48
2:B:940:ILE:HD12	2:B:1308:PHE:CE2	2.49	0.48
3:F:241:SER:CB	3:F:242:GLY:HA3	2.43	0.48
2:B:1331:LYS:HA	2:B:1332:ASP:CB	2.26	0.48
2:B:744:GLU:C	2:B:746:PRO:HD3	2.34	0.48
1:A:624:PHE:H	1:A:632:THR:HG21	1.78	0.48
3:F:250:LEU:HB3	3:F:288:THR:HG22	1.95	0.48
1:A:242:LYS:HB3	1:A:274:GLY:HA3	1.96	0.48
1:A:369:VAL:HG12	1:A:371:GLY:H	1.79	0.48
8:F:1117:NAG:H61	8:F:1118:NAG:HN2	1.79	0.48
2:B:927:PRO:O	2:B:928:GLU:CB	2.62	0.48
1:A:323:GLY:O	1:A:325:PRO:HD3	2.13	0.48
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.14	0.48
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.94	0.48
2:B:1103:ILE:HD12	2:B:1103:ILE:N	2.27	0.48
1:C:6:ILE:HG22	1:C:625:THR:O	2.13	0.48
2:D:1197:ARG:HE	2:D:1199:GLU:CD	2.17	0.48
2:B:1017:LEU:C	2:B:1019:LYS:H	2.17	0.48
2:D:985:PRO:HG3	2:D:996:MET:HA	1.96	0.48
2:D:990:GLU:O	2:D:994:ILE:HG13	2.14	0.48
2:D:907:LEU:H	2:D:907:LEU:HD23	1.78	0.48
2:B:1301:GLU:HG2	3:F:157:ARG:NH1	2.29	0.48
3:H:706:GLN:O	3:H:706:GLN:CG	2.55	0.47
1:C:470:TYR:HB2	1:C:509:LEU:HD21	1.96	0.47
2:D:883:THR:HG21	2:D:911:PRO:HG3	1.96	0.47
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.49	0.47
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.96	0.47
3:F:433:MET:HG3	3:F:434:GLU:N	2.29	0.47
1:C:148:PRO:HD3	1:C:182:TRP:CE2	2.49	0.47
2:B:968:MET:O	2:B:969:THR:HB	2.14	0.47
2:D:916:MET:HG3	2:D:1328:ALA:CB	2.44	0.47
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.49	0.47
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.94	0.47
1:C:177:VAL:HG22	1:C:178:ASN:N	2.29	0.47
2:D:1005:TYR:HD1	2:D:1258:ALA:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LYS:HB3	1:C:274:GLY:HA3	1.96	0.47
1:C:45:LEU:HB2	1:C:46:VAL:HB	1.97	0.47
2:D:1543:ILE:HD12	2:D:1554:VAL:HG21	1.95	0.47
2:B:732:ASP:O	2:B:733:ILE:HG12	2.15	0.47
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.15	0.47
3:H:296:TRP:CE2	3:H:317:ILE:HG22	2.50	0.47
1:A:177:VAL:HG22	1:A:178:ASN:N	2.29	0.47
2:B:1483:LEU:HD11	2:B:1536:PHE:HB3	1.95	0.47
1:C:624:PHE:H	1:C:632:THR:HG21	1.79	0.47
1:A:179:MET:HG3	1:A:203:LYS:HA	1.96	0.47
4:J:36:VAL:HG21	4:J:53:VAL:HG11	1.96	0.47
1:C:630:GLN:H	1:C:630:GLN:NE2	2.13	0.47
2:D:927:PRO:O	2:D:928:GLU:CB	2.62	0.47
2:D:918:LYS:NZ	2:D:944:ASP:HB3	2.29	0.47
2:B:1581:LEU:HB2	2:B:1609:TRP:HE3	1.79	0.47
3:F:404:GLY:O	3:F:430:VAL:HG22	2.14	0.47
1:A:6:ILE:HD11	1:A:20:MET:CG	2.43	0.47
2:B:940:ILE:HD11	2:B:1320:LEU:HD21	1.97	0.47
1:C:624:PHE:H	1:C:632:THR:CG2	2.28	0.47
1:A:578:LYS:HG3	2:B:779:THR:O	2.15	0.47
3:H:703:GLN:O	3:H:704:LYS:HB2	2.14	0.47
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.96	0.47
4:J:157:ARG:C	4:J:157:ARG:HD3	2.34	0.47
2:D:1263:ASP:O	2:D:1265:PRO:HD3	2.14	0.47
1:A:268:ARG:NH1	2:B:1378:MET:HE3	2.18	0.47
2:B:965:VAL:O	2:B:965:VAL:HG13	2.13	0.47
4:J:197:VAL:HG22	4:J:213:TYR:CE2	2.50	0.47
1:A:177:VAL:HG22	1:A:178:ASN:H	1.80	0.47
3:F:701:LYS:O	3:F:702:ASN:C	2.53	0.47
2:B:739:ILE:HB	2:B:891:LYS:HD3	1.95	0.47
1:C:323:GLY:O	1:C:325:PRO:HD3	2.13	0.47
3:F:118:ARG:NH1	3:F:130:THR:HA	2.30	0.47
2:D:1443:GLN:HE21	2:D:1446:ASN:HA	1.79	0.47
3:H:435:ASN:O	3:H:439:VAL:HG23	2.14	0.47
3:F:344:PRO:O	3:F:345:ASP:HB2	2.15	0.47
2:B:966:ALA:HA	2:B:1267:HIS:HA	1.97	0.47
4:J:215:ARG:NH1	4:J:218:SER:HB2	2.30	0.47
2:B:1119:MET:HG3	2:B:1161:LEU:HD21	1.96	0.47
1:C:179:MET:HG3	1:C:203:LYS:HA	1.97	0.47
3:H:254:GLY:HA2	3:H:319:TYR:OH	2.14	0.47
2:D:1575:GLU:HB2	2:D:1578:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:654:ARG:HG3	3:F:722:GLN:HB3	1.97	0.47
2:B:1531:GLN:HB2	2:B:1538:GLU:HB2	1.95	0.47
1:C:369:VAL:HG12	1:C:371:GLY:H	1.80	0.47
2:D:822:GLN:HA	2:D:879:VAL:HG22	1.97	0.47
2:D:894:VAL:HG22	2:D:899:ILE:HB	1.97	0.47
3:H:433:MET:O	3:H:434:GLU:HB2	2.15	0.47
2:B:804:MET:HG2	2:B:805:GLN:N	2.30	0.47
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.97	0.47
2:D:1581:LEU:HB2	2:D:1609:TRP:HE3	1.80	0.47
3:H:59:THR:HG23	3:H:61:LYS:HG2	1.96	0.47
2:B:1285:ILE:HG21	2:B:1300:GLU:HG3	1.98	0.46
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.96	0.46
2:D:872:LEU:HD13	2:D:1418:ASP:HB3	1.96	0.46
3:F:158:LEU:O	3:F:159:GLU:HB2	2.14	0.46
3:H:433:MET:HG3	3:H:434:GLU:N	2.30	0.46
3:F:503:PHE:HB2	3:F:530:PHE:HZ	1.80	0.46
4:I:151:ARG:H	9:I:1229:GOL:H11	1.80	0.46
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.14	0.46
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.15	0.46
3:H:44:TYR:HB3	3:H:72:GLU:O	2.15	0.46
4:J:169:MET:HB2	9:J:1229:GOL:O3	2.15	0.46
1:A:45:LEU:HB2	1:A:46:VAL:HB	1.97	0.46
1:A:6:ILE:HG22	1:A:625:THR:O	2.15	0.46
2:B:822:GLN:HA	2:B:879:VAL:HG22	1.97	0.46
2:B:985:PRO:HG3	2:B:996:MET:HA	1.97	0.46
3:F:215:GLU:C	3:F:217:ILE:H	2.19	0.46
1:A:453:PHE:HE1	1:A:495:LEU:HB2	1.80	0.46
2:D:916:MET:HG3	2:D:1328:ALA:HB3	1.98	0.46
2:B:1119:MET:SD	2:B:1157:ASN:HB2	2.55	0.46
3:H:375:THR:O	3:H:379:GLU:HG3	2.15	0.46
2:D:1341:LEU:C	2:D:1342:LYS:HD3	2.36	0.46
1:A:630:GLN:H	1:A:630:GLN:NE2	2.13	0.46
3:F:435:ASN:O	3:F:439:VAL:HG23	2.16	0.46
1:A:583:LEU:N	1:A:583:LEU:HD12	2.31	0.46
1:A:6:ILE:HD12	1:A:21:VAL:O	2.15	0.46
2:D:1119:MET:SD	2:D:1157:ASN:HB2	2.55	0.46
1:C:112:THR:HG22	1:C:125:TYR:HB3	1.98	0.46
3:F:59:THR:HG23	3:F:61:LYS:HG2	1.96	0.46
2:D:965:VAL:HG22	2:D:965:VAL:O	2.15	0.46
3:H:215:GLU:C	3:H:217:ILE:H	2.19	0.46
4:I:197:VAL:HG22	4:I:213:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:309:TRP:HZ3	3:F:313:GLN:CD	2.18	0.46
3:H:688:GLN:HG2	3:H:720:LEU:HD11	1.98	0.46
2:D:833:ARG:HD3	2:D:836:GLN:HE21	1.80	0.46
1:A:12:LEU:HG	1:A:99:VAL:HG11	1.97	0.46
3:H:464:ASP:C	3:H:466:HIS:H	2.19	0.46
2:B:1197:ARG:HE	2:B:1199:GLU:CD	2.19	0.46
4:J:25:LEU:HG	4:J:26:CYS:SG	2.55	0.46
1:C:31:VAL:HG13	1:C:54:LEU:HB2	1.97	0.46
2:D:940:ILE:HD11	2:D:1320:LEU:HD21	1.98	0.46
1:C:558:GLN:HG2	2:D:772:PHE:CE2	2.51	0.46
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.98	0.46
2:D:940:ILE:HD12	2:D:1308:PHE:CE2	2.50	0.46
2:D:1639:CYS:O	3:H:327:GLY:HA2	2.16	0.46
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.81	0.46
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.56	0.46
2:D:1385:MET:HA	2:D:1385:MET:HE2	1.98	0.46
2:B:894:VAL:HG22	2:B:899:ILE:HB	1.98	0.46
2:B:913:GLY:O	2:B:1331:LYS:HE3	2.16	0.46
1:C:223:ILE:N	1:C:223:ILE:HD12	2.25	0.46
3:H:404:GLY:O	3:H:430:VAL:HG22	2.15	0.46
3:H:503:PHE:HB2	3:H:530:PHE:HZ	1.81	0.46
1:C:74:PHE:C	1:C:82:LYS:HZ3	2.20	0.46
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.97	0.46
3:F:164:TYR:CD1	3:F:191:PRO:HG2	2.52	0.45
2:B:1525:THR:HB	2:B:1541:MET:HB3	1.97	0.45
3:F:95:TYR:HE2	7:F:1743:NAG:HN2	1.65	0.45
3:H:171:THR:HG23	3:H:412:VAL:HG22	1.99	0.45
1:A:628:SER:HB2	1:A:630:GLN:NE2	2.16	0.45
1:A:268:ARG:HD3	2:B:1378:MET:CE	2.47	0.45
1:A:223:ILE:N	1:A:223:ILE:HD12	2.26	0.45
2:B:1443:GLN:HE21	2:B:1446:ASN:HA	1.80	0.45
2:B:918:LYS:NZ	2:B:944:ASP:HB3	2.31	0.45
1:A:45:LEU:HA	1:A:46:VAL:HA	1.72	0.45
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.51	0.45
1:C:614:ALA:HB1	1:C:632:THR:HA	1.99	0.45
4:I:215:ARG:NH1	4:I:218:SER:HB2	2.31	0.45
1:A:356:ASN:HB3	1:A:357:PRO:HD2	1.97	0.45
3:H:654:ARG:HG3	3:H:722:GLN:HB3	1.98	0.45
1:A:112:THR:HG22	1:A:125:TYR:HB3	1.98	0.45
3:H:606:LEU:HD12	3:H:606:LEU:C	2.37	0.45
3:F:430:VAL:HG21	3:F:433:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:742:ARG:NH1	2:D:777:ILE:HG13	2.32	0.45
1:C:398:LEU:HD22	1:C:400:ILE:HD11	1.98	0.45
1:C:177:VAL:HG22	1:C:178:ASN:H	1.80	0.45
3:H:464:ASP:HB2	3:H:615:LEU:HD12	1.98	0.45
1:C:541:LEU:HD22	2:D:786:SER:CB	2.46	0.45
1:C:222:TYR:HE2	1:C:224:TYR:HB2	1.82	0.45
3:F:703:GLN:O	3:F:704:LYS:HB2	2.15	0.45
2:D:1009:THR:HB	2:D:1011:GLN:HE21	1.82	0.45
1:C:453:PHE:HE1	1:C:495:LEU:HB2	1.82	0.45
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.15	0.45
3:F:655:PHE:HA	3:F:717:HIS:O	2.16	0.45
2:B:1286:THR:HG22	3:F:665:ALA:HB3	1.99	0.45
2:D:1163:ARG:O	2:D:1167:VAL:HG23	2.17	0.45
1:A:222:TYR:HE2	1:A:224:TYR:HB2	1.81	0.45
2:B:1017:LEU:O	2:B:1018:GLU:HB3	2.16	0.45
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.97	0.45
2:B:733:ILE:HD11	2:B:841:ARG:NH2	2.15	0.45
3:H:544:ILE:HD13	3:H:650:VAL:HG12	1.98	0.45
2:B:1333:GLN:HB3	2:B:1334:LEU:C	2.37	0.45
2:B:819:ARG:HE	2:B:883:THR:CG2	2.27	0.45
2:B:990:GLU:O	2:B:994:ILE:HG13	2.17	0.45
2:D:852:SER:HB3	2:D:878:ILE:HG22	1.98	0.45
3:H:477:ILE:HG13	3:H:483:HIS:CE1	2.51	0.45
5:C:2063:NAG:O6	5:C:2064:NAG:C1	2.64	0.45
1:C:223:ILE:H	1:C:223:ILE:CD1	2.26	0.45
2:B:1236:GLU:HA	2:B:1238:ARG:NH2	2.31	0.45
3:H:452:LEU:HD12	3:H:455:MET:HG3	1.99	0.45
3:H:170:LEU:HD23	3:H:193:CYS:HB3	1.98	0.45
2:B:1581:LEU:HB2	2:B:1609:TRP:CE3	2.52	0.45
2:D:1105:GLN:O	2:D:1112:ARG:HD2	2.16	0.45
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.17	0.45
3:F:318:ASN:ND2	3:F:320:GLU:HG2	2.31	0.45
2:B:907:LEU:HD23	2:B:907:LEU:H	1.82	0.45
3:F:345:ASP:O	3:F:348:PRO:HD2	2.16	0.45
3:F:688:GLN:HG2	3:F:720:LEU:HD11	1.99	0.45
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.17	0.45
2:D:1497:PHE:HA	2:D:1601:GLY:O	2.15	0.45
2:D:1631:THR:O	2:D:1635:VAL:HG23	2.17	0.45
2:B:840:VAL:HG12	2:B:841:ARG:N	2.33	0.44
2:D:819:ARG:HE	2:D:883:THR:CG2	2.28	0.44
2:B:854:ALA:HB2	2:B:860:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HD12	1:C:21:VAL:O	2.17	0.44
3:H:309:TRP:HZ3	3:H:313:GLN:CD	2.21	0.44
2:D:918:LYS:HZ3	2:D:944:ASP:HB3	1.82	0.44
2:B:1641:ASN:OXT	3:F:255:SER:HB3	2.17	0.44
2:D:1301:GLU:HG2	3:H:157:ARG:NH1	2.32	0.44
3:F:125:ARG:HH21	3:F:194:GLN:HE22	1.65	0.44
2:B:1341:LEU:C	2:B:1342:LYS:HD3	2.37	0.44
3:F:606:LEU:C	3:F:606:LEU:HD12	2.38	0.44
1:C:63:ASN:HD22	5:C:2063:NAG:C1	2.06	0.44
4:I:17:SER:HB3	4:I:54:LEU:HB3	1.98	0.44
2:D:1483:LEU:HB3	2:D:1490:ARG:HG2	2.00	0.44
2:D:1581:LEU:HB2	2:D:1609:TRP:CE3	2.53	0.44
1:C:554:VAL:HG13	1:C:555:PRO:HD2	1.99	0.44
3:F:375:THR:O	3:F:379:GLU:HG3	2.17	0.44
3:H:199:TYR:CE1	3:H:431:LYS:HD3	2.51	0.44
3:H:655:PHE:HA	3:H:717:HIS:O	2.16	0.44
3:H:32:ALA:HA	3:H:57:TRP:HZ3	1.83	0.44
1:A:74:PHE:C	1:A:82:LYS:HZ3	2.20	0.44
1:C:518:ALA:O	1:C:519:SER:C	2.54	0.44
3:F:544:ILE:HD13	3:F:650:VAL:HG12	1.98	0.44
2:D:1333:GLN:HB3	2:D:1334:LEU:C	2.37	0.44
2:B:833:ARG:HD2	2:B:838:LEU:HD21	1.99	0.44
3:F:546:GLU:HB3	3:F:548:TYR:CE1	2.52	0.44
2:B:1551:SER:HB3	3:F:371:GLY:HA3	1.99	0.44
2:B:916:MET:HG3	2:B:1328:ALA:CB	2.47	0.44
3:F:110:TYR:CE1	3:F:135:ASN:HB3	2.52	0.44
3:F:433:MET:O	3:F:434:GLU:HB2	2.17	0.44
2:D:1103:ILE:N	2:D:1103:ILE:HD12	2.31	0.44
1:A:93:GLN:HE21	1:A:627:SER:HB2	1.82	0.44
2:D:1365:GLU:HA	2:D:1438:ALA:HB2	1.99	0.44
1:C:583:LEU:HD12	1:C:583:LEU:N	2.33	0.44
1:A:541:LEU:HG	2:B:796:ALA:HB2	1.99	0.44
3:F:513:LYS:HB3	3:F:522:ASP:HB3	1.99	0.44
2:D:941:PRO:HA	2:D:942:PRO:HD3	1.90	0.44
2:B:1385:MET:HA	2:B:1385:MET:HE2	1.98	0.44
2:B:964:PRO:HA	2:B:965:VAL:CB	2.47	0.44
2:B:1276:LEU:HD23	2:B:1276:LEU:H	1.83	0.44
2:D:1017:LEU:O	2:D:1018:GLU:HB3	2.17	0.44
1:C:338:THR:HG21	1:C:419:MET:HE1	2.00	0.44
2:B:733:ILE:HG13	2:B:734:ILE:N	2.31	0.44
2:D:840:VAL:HG12	2:D:841:ARG:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:298:LYS:HZ2	3:F:340:MET:HA	1.83	0.44
1:A:398:LEU:HD22	1:A:400:ILE:HD11	1.99	0.44
1:C:356:ASN:HB3	1:C:357:PRO:HD2	1.99	0.44
1:A:116:ILE:HG12	1:A:205:TYR:CE2	2.52	0.44
2:B:1333:GLN:CD	2:B:1333:GLN:H	2.21	0.44
1:C:506:SER:HB2	1:C:530:TRP:NE1	2.32	0.44
2:D:1236:GLU:HA	2:D:1238:ARG:NH2	2.33	0.44
1:C:13:ARG:NH2	1:C:476:GLY:HA3	2.33	0.44
1:C:400:ILE:HD12	1:C:400:ILE:N	2.33	0.44
1:A:338:THR:HG21	1:A:419:MET:HE1	1.99	0.44
1:C:329:SER:HA	1:C:330:PRO:HD3	1.84	0.44
2:B:1365:GLU:HA	2:B:1438:ALA:HB2	2.00	0.44
2:D:1380:ILE:N	2:D:1380:ILE:HD12	2.32	0.44
2:B:851:CYS:HB2	2:B:1491:CYS:HB2	1.88	0.44
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.99	0.44
2:D:1333:GLN:CD	2:D:1333:GLN:H	2.21	0.44
2:B:804:MET:HG2	2:B:805:GLN:H	1.83	0.44
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.52	0.44
2:B:918:LYS:HE3	2:B:1326:TYR:OH	2.18	0.44
3:F:222:ALA:N	3:F:223:GLU:CA	2.66	0.43
2:D:1331:LYS:HA	2:D:1332:ASP:CB	2.28	0.43
2:D:819:ARG:NH1	2:D:1487:GLU:HG2	2.33	0.43
1:C:111:GLN:O	1:C:125:TYR:HA	2.17	0.43
3:H:463:THR:OG1	3:H:464:ASP:N	2.51	0.43
1:C:129:THR:OG1	1:C:165:GLY:HA2	2.18	0.43
3:F:479:PRO:C	3:F:481:LYS:H	2.21	0.43
3:H:635:ALA:HB3	3:H:647:ILE:HD11	2.00	0.43
2:B:1296:LEU:O	2:B:1298:ARG:HG3	2.18	0.43
2:B:1535:ASP:OD1	2:B:1535:ASP:N	2.50	0.43
3:H:106:CYS:SG	3:H:112:LEU:HB2	2.58	0.43
2:B:1338:LYS:N	2:B:1338:LYS:HD2	2.33	0.43
2:D:918:LYS:HE3	2:D:1326:TYR:OH	2.19	0.43
2:D:1386:MET:SD	2:D:1473:PRO:HD3	2.57	0.43
3:H:513:LYS:HB3	3:H:522:ASP:HB3	1.99	0.43
3:H:701:LYS:O	3:H:702:ASN:C	2.55	0.43
3:F:106:CYS:SG	3:F:112:LEU:HB2	2.58	0.43
1:C:533:VAL:HG12	1:C:534:LYS:N	2.33	0.43
1:A:17:GLU:HG2	1:A:67:THR:OG1	2.18	0.43
3:H:380:ILE:O	3:H:384:LEU:HG	2.18	0.43
1:C:343:LYS:HD2	1:C:343:LYS:N	2.33	0.43
2:D:854:ALA:HB2	2:D:860:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1337:ASN:HB3	2:B:1338:LYS:H	1.63	0.43
3:H:463:THR:O	3:H:466:HIS:HB2	2.17	0.43
1:C:116:ILE:HG12	1:C:205:TYR:CE2	2.53	0.43
1:A:373:ASP:C	1:A:375:VAL:H	2.21	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.32	0.43
2:D:913:GLY:O	2:D:1331:LYS:HE3	2.18	0.43
3:H:240:PRO:HA	3:H:241:SER:HA	1.52	0.43
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.17	0.43
1:A:255:ASP:HB2	1:A:300:LYS:HG2	2.00	0.43
1:C:283:LYS:O	1:C:287:ASP:HB2	2.18	0.43
1:A:553:PRO:HD2	2:B:802:THR:O	2.19	0.43
1:C:12:LEU:HG	1:C:99:VAL:HG11	2.00	0.43
3:H:433:MET:CG	3:H:434:GLU:H	2.31	0.43
3:H:433:MET:CG	3:H:434:GLU:N	2.82	0.43
2:D:833:ARG:HD2	2:D:838:LEU:HD21	2.00	0.43
2:B:1039:GLN:OE1	2:B:1052:PRO:HG3	2.19	0.43
2:D:1001:ILE:HG13	2:D:1254:PHE:HB2	1.99	0.43
4:J:202:ARG:HB3	4:J:203:VAL:H	1.62	0.43
2:D:1039:GLN:OE1	2:D:1052:PRO:HG3	2.19	0.43
1:A:283:LYS:O	1:A:287:ASP:HB2	2.18	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.53	0.43
3:F:433:MET:CG	3:F:434:GLU:H	2.31	0.43
3:F:433:MET:CG	3:F:434:GLU:N	2.82	0.43
2:D:1498:ILE:HG22	2:D:1499:GLN:HG2	2.00	0.43
1:A:145:ILE:O	1:A:153:VAL:HG22	2.18	0.43
3:F:35:TYR:HB2	3:F:43:PRO:HB3	1.99	0.43
1:A:171:TRP:CZ3	1:A:173:ILE:HG12	2.53	0.43
3:F:380:ILE:O	3:F:384:LEU:HG	2.18	0.43
4:I:7:ALA:O	4:I:58:HIS:HE1	2.02	0.43
4:I:30:LEU:O	4:I:107:PRO:HA	2.19	0.43
2:D:1536:PHE:H	2:D:1566:ILE:HG12	1.83	0.43
4:J:40:ALA:HB2	4:J:90:LEU:O	2.18	0.43
3:H:110:TYR:CE1	3:H:135:ASN:HB3	2.54	0.43
2:D:1390:ALA:HA	2:D:1391:PRO:HD3	1.90	0.43
1:A:269:ILE:HD13	1:A:278:VAL:HB	2.01	0.43
2:D:1145:GLY:O	2:D:1149:LYS:HG2	2.19	0.43
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.18	0.43
3:F:450:LEU:HA	3:F:450:LEU:HD12	1.93	0.43
2:B:785:VAL:HG13	2:B:795:VAL:HG12	1.99	0.43
2:B:819:ARG:O	2:B:820:ASN:HB2	2.19	0.43
1:A:63:ASN:HB3	5:A:1643:NAG:O5	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:19:ILE:HG13	3:F:71:ALA:C	2.39	0.43
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.54	0.43
2:B:1631:THR:O	2:B:1635:VAL:HG23	2.19	0.43
1:A:158:LEU:HD22	1:A:169:LEU:HD11	2.01	0.43
3:H:650:VAL:HG23	3:H:651:VAL:HG23	2.01	0.43
3:F:143:PRO:HG3	3:F:186:TRP:NE1	2.34	0.43
1:C:123:VAL:O	1:C:170:SER:HA	2.19	0.43
1:C:373:ASP:C	1:C:375:VAL:H	2.22	0.43
3:H:447:SER:O	4:I:208:LYS:HE2	2.18	0.43
1:C:566:ASP:OD2	2:D:791:LYS:HG3	2.19	0.43
3:H:35:TYR:HB2	3:H:43:PRO:HB3	2.00	0.43
1:C:269:ILE:HD13	1:C:278:VAL:HB	2.00	0.43
1:A:103:LEU:HD22	1:A:103:LEU:N	2.34	0.43
1:C:552:GLN:HA	1:C:553:PRO:HD3	1.92	0.43
1:A:19:THR:HA	1:A:65:THR:HG22	2.01	0.43
2:B:964:PRO:HB3	2:B:1291:TRP:CZ3	2.54	0.43
3:F:299:VAL:H	3:F:340:MET:CE	2.29	0.43
3:F:490:VAL:O	3:F:569:PRO:HA	2.19	0.43
2:B:1543:ILE:HD12	2:B:1554:VAL:HG21	2.01	0.43
1:A:495:LEU:HA	1:A:496:PRO:HD3	1.89	0.43
1:A:400:ILE:HD12	1:A:400:ILE:N	2.33	0.43
3:H:692:ILE:HA	3:H:717:HIS:ND1	2.34	0.43
2:D:1115:ASN:O	2:D:1116:GLU:HB2	2.19	0.43
3:F:219:GLY:HA2	3:F:455:MET:CE	2.49	0.43
2:B:1380:ILE:N	2:B:1380:ILE:HD12	2.34	0.43
2:B:839:LYS:O	2:B:895:TYR:HD1	2.02	0.42
2:D:1490:ARG:HD2	2:D:1590:TRP:CE3	2.54	0.42
2:D:1338:LYS:N	2:D:1338:LYS:HD2	2.34	0.42
2:B:1531:GLN:C	2:B:1532:LEU:HD12	2.39	0.42
3:F:80:ARG:HA	3:F:81:PRO:HD3	1.94	0.42
2:D:1155:GLU:HG3	2:D:1184:LEU:HD21	2.00	0.42
2:D:811:LEU:HG	2:D:813:LEU:HD13	2.01	0.42
2:B:1064:PHE:O	2:B:1068:VAL:HG13	2.19	0.42
3:F:341:MET:SD	3:F:380:ILE:HG23	2.59	0.42
3:H:80:ARG:HA	3:H:81:PRO:HD3	1.94	0.42
2:D:839:LYS:O	2:D:895:TYR:HD1	2.01	0.42
2:B:963:THR:HG22	2:B:1318:GLY:HA2	2.01	0.42
2:B:1155:GLU:HG3	2:B:1184:LEU:HD21	2.01	0.42
1:A:249:VAL:HG13	1:A:267:LYS:HB2	2.01	0.42
1:A:123:VAL:O	1:A:170:SER:HA	2.19	0.42
3:H:280:VAL:O	3:H:282:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:TRP:CZ3	1:C:173:ILE:HG12	2.54	0.42
1:C:10:ASN:CB	1:C:635:ARG:HH11	2.33	0.42
1:A:440:ARG:HD2	1:A:440:ARG:HA	1.92	0.42
2:B:1115:ASN:O	2:B:1116:GLU:HB2	2.19	0.42
2:B:1498:ILE:HD12	2:B:1605:TRP:HB2	2.00	0.42
3:H:113:ARG:NH2	3:H:141:SER:HB2	2.30	0.42
2:B:1276:LEU:N	2:B:1276:LEU:HD23	2.34	0.42
2:D:959:LEU:HD21	2:D:1297:LEU:CD2	2.49	0.42
2:D:1337:ASN:HB3	2:D:1338:LYS:H	1.63	0.42
1:A:241:LYS:HG3	2:B:832:TYR:CE1	2.54	0.42
1:A:533:VAL:HG12	1:A:534:LYS:N	2.34	0.42
3:F:44:TYR:HB3	3:F:72:GLU:O	2.19	0.42
3:F:90:TRP:CD1	3:F:90:TRP:N	2.85	0.42
1:C:38:HIS:HD2	1:C:45:LEU:HB3	1.85	0.42
1:C:578:LYS:HD3	2:D:779:THR:HB	2.01	0.42
3:F:44:TYR:CD1	3:F:45:PRO:HA	2.55	0.42
2:D:1411:GLU:HG2	2:D:1422:LEU:HD12	2.00	0.42
2:B:749:TRP:CE3	2:B:750:LEU:HB2	2.55	0.42
2:D:1387:THR:HG23	2:D:1387:THR:O	2.19	0.42
3:F:113:ARG:NH2	3:F:141:SER:HB2	2.33	0.42
1:C:145:ILE:O	1:C:153:VAL:HG22	2.19	0.42
2:D:1485:ARG:O	2:D:1486:ASP:HB2	2.20	0.42
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	2.01	0.42
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.42
1:A:414:GLN:HA	1:A:414:GLN:NE2	2.29	0.42
2:D:977:ARG:HD2	2:D:1240:TYR:CE2	2.55	0.42
3:F:701:LYS:O	3:F:703:GLN:N	2.52	0.42
2:B:916:MET:HG3	2:B:1328:ALA:HB3	2.01	0.42
2:D:1296:LEU:O	2:D:1298:ARG:HG3	2.18	0.42
2:B:754:GLU:HG3	2:B:769:MET:SD	2.59	0.42
2:B:1405:ARG:HE	2:B:1437:LEU:HD22	1.84	0.42
2:B:1253:VAL:O	2:B:1257:LEU:HG	2.20	0.42
1:A:129:THR:OG1	1:A:165:GLY:HA2	2.20	0.42
1:C:25:HIS:HA	1:C:26:ASP:HA	1.51	0.42
1:C:547:GLN:NE2	1:C:559:MET:HA	2.29	0.42
4:J:54:LEU:HD21	4:J:67:LYS:HE3	2.01	0.42
1:C:459:ARG:HA	1:C:462:GLU:HG2	2.02	0.42
3:F:497:LEU:HA	3:F:554:LEU:HD23	2.02	0.42
2:B:1524:LYS:O	2:B:1544:GLU:HB2	2.19	0.42
3:H:490:VAL:O	3:H:569:PRO:HA	2.20	0.42
3:H:250:LEU:O	3:H:288:THR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1009:THR:HG22	2:D:1261:GLN:HG3	2.01	0.42
2:D:1391:PRO:HB2	2:D:1396:LEU:HD11	2.02	0.42
3:F:280:VAL:O	3:F:282:PRO:HD3	2.20	0.42
1:C:440:ARG:HA	1:C:440:ARG:HD2	1.92	0.42
3:F:650:VAL:HG23	3:F:651:VAL:HG23	2.02	0.42
1:C:414:GLN:NE2	1:C:414:GLN:HA	2.30	0.42
4:J:64:GLU:HA	4:J:65:PRO:HD3	1.89	0.42
1:A:606:THR:HA	1:A:607:PRO:HD3	1.94	0.42
1:A:541:LEU:HD22	2:B:786:SER:CB	2.49	0.42
1:A:545:SER:HB2	2:B:799:PHE:HZ	1.84	0.42
3:F:32:ALA:HA	3:F:57:TRP:HZ3	1.84	0.42
2:D:1086:ILE:HG23	2:D:1146:SER:HB2	2.00	0.42
2:D:1270:LEU:O	2:D:1290:HIS:HA	2.20	0.42
2:B:1500:LYS:HB2	2:B:1500:LYS:HE3	1.93	0.42
2:B:1297:LEU:HA	2:B:1297:LEU:HD12	1.68	0.42
2:D:1451:GLN:HA	2:D:1452:PRO:HD3	1.95	0.42
1:A:470:TYR:HA	1:A:510:VAL:O	2.20	0.42
1:A:510:VAL:HG21	1:A:622:LEU:HD12	2.01	0.42
2:D:968:MET:O	2:D:969:THR:HB	2.20	0.42
2:D:811:LEU:HG	2:D:813:LEU:CD1	2.50	0.42
2:D:981:LEU:HB3	2:D:998:PRO:O	2.20	0.42
3:F:445:ASP:O	3:F:448:GLN:HG2	2.20	0.42
2:B:1086:ILE:HG23	2:B:1146:SER:HB2	2.02	0.42
3:H:546:GLU:HB3	3:H:548:TYR:CE1	2.55	0.42
2:D:1521:TYR:HB2	2:D:1523:TYR:CZ	2.55	0.42
2:B:941:PRO:HA	2:B:942:PRO:HD3	1.90	0.42
3:H:164:TYR:CD1	3:H:191:PRO:HG2	2.55	0.41
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.50	0.41
4:J:7:ALA:O	4:J:58:HIS:HE1	2.03	0.41
4:I:78:HIS:HA	4:I:79:PRO:HD3	1.89	0.41
2:D:1405:ARG:HE	2:D:1437:LEU:HD22	1.85	0.41
1:C:103:LEU:N	1:C:103:LEU:HD22	2.34	0.41
3:H:706:GLN:C	3:H:708:GLN:H	2.10	0.41
1:C:510:VAL:HG21	1:C:622:LEU:HD12	2.02	0.41
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.34	0.41
2:B:1342:LYS:N	2:B:1342:LYS:HD3	2.35	0.41
3:F:37:CYS:HA	3:F:38:PRO:HD3	1.93	0.41
1:C:93:GLN:HE21	1:C:627:SER:HB2	1.84	0.41
2:D:1276:LEU:N	2:D:1276:LEU:HD23	2.36	0.41
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.56	0.41
3:F:158:LEU:HG	3:F:159:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CD1	1:A:357:PRO:HG2	2.55	0.41
1:A:112:THR:HB	1:A:117:TYR:OH	2.20	0.41
1:C:459:ARG:HA	1:C:462:GLU:CG	2.50	0.41
1:C:365:VAL:HA	1:C:406:LYS:HE2	2.02	0.41
4:J:30:LEU:O	4:J:107:PRO:HA	2.20	0.41
3:H:90:TRP:CD1	3:H:90:TRP:N	2.87	0.41
2:D:819:ARG:O	2:D:820:ASN:HB2	2.21	0.41
2:B:981:LEU:HB3	2:B:998:PRO:O	2.20	0.41
2:B:735:ALA:C	2:B:737:GLU:H	2.23	0.41
1:A:31:VAL:CG1	1:A:54:LEU:HB2	2.50	0.41
3:H:44:TYR:CD1	3:H:45:PRO:HA	2.56	0.41
2:B:916:MET:HA	2:B:916:MET:HE2	2.02	0.41
1:A:236:ARG:HA	1:A:243:VAL:HG23	2.02	0.41
4:I:202:ARG:HB3	4:I:203:VAL:H	1.62	0.41
1:C:143:VAL:O	1:C:155:GLN:HA	2.20	0.41
3:F:499:ALA:HB2	3:F:675:GLY:HA2	2.02	0.41
2:D:1524:LYS:O	2:D:1544:GLU:HB2	2.20	0.41
1:C:480:LYS:HG2	1:C:481:ALA:N	2.35	0.41
4:J:17:SER:HB3	4:J:54:LEU:HB3	2.02	0.41
2:D:1143:LEU:O	2:D:1147:ILE:HG13	2.20	0.41
2:B:1391:PRO:HB2	2:B:1396:LEU:HD11	2.03	0.41
3:H:497:LEU:HA	3:H:554:LEU:HD23	2.02	0.41
1:A:100:LEU:HD12	1:A:101:VAL:H	1.84	0.41
1:C:470:TYR:HA	1:C:510:VAL:O	2.20	0.41
2:B:1376:ALA:HB3	2:B:1429:VAL:CG2	2.50	0.41
2:B:1060:VAL:HG13	2:B:1064:PHE:CE1	2.56	0.41
3:F:219:GLY:HA2	3:F:455:MET:HE1	2.03	0.41
4:J:106:ARG:HA	4:J:107:PRO:HD3	1.91	0.41
3:F:531:HIS:HA	3:F:532:PRO:HD3	1.98	0.41
2:B:1387:THR:O	2:B:1387:THR:HG23	2.21	0.41
2:D:983:VAL:O	2:D:985:PRO:HD3	2.20	0.41
4:I:151:ARG:HB2	9:I:1229:GOL:H12	2.02	0.41
1:C:112:THR:HB	1:C:117:TYR:OH	2.21	0.41
1:C:233:ILE:HG13	1:C:269:ILE:HD11	2.03	0.41
3:H:282:PRO:O	3:H:305:SER:HA	2.21	0.41
3:H:418:ALA:HB3	3:H:427:VAL:HG22	2.02	0.41
3:H:445:ASP:O	3:H:448:GLN:HG2	2.21	0.41
1:C:17:GLU:HG2	1:C:67:THR:OG1	2.21	0.41
2:B:811:LEU:HG	2:B:813:LEU:HD13	2.03	0.41
1:C:83:PHE:CD2	1:C:100:LEU:HA	2.55	0.41
2:B:1617:ASP:C	2:B:1619:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:37:LEU:HD11	4:J:90:LEU:HD22	2.02	0.41
1:A:451:VAL:HB	1:A:495:LEU:HB3	2.03	0.41
1:C:31:VAL:CG1	1:C:54:LEU:HB2	2.51	0.41
4:I:62:GLN:HA	4:I:63:PRO:HD3	1.85	0.41
3:F:393:PRO:O	3:F:394:ARG:HB2	2.21	0.41
2:B:1270:LEU:O	2:B:1290:HIS:HA	2.20	0.41
3:F:706:GLN:C	3:F:708:GLN:H	2.23	0.41
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.20	0.41
3:H:299:VAL:HG22	3:H:340:MET:HE3	2.02	0.41
2:B:1005:TYR:CD1	2:B:1258:ALA:HB2	2.53	0.41
2:B:745:PHE:N	2:B:746:PRO:HD3	2.36	0.41
3:F:94:PRO:HB2	3:F:95:TYR:CD1	2.56	0.41
3:F:452:LEU:HD12	3:F:455:MET:HG3	2.02	0.41
3:H:405:VAL:HG23	3:H:406:GLY:N	2.36	0.41
3:F:620:VAL:HG12	3:F:667:PRO:HD2	2.03	0.41
4:J:15:MET:CE	4:J:127:GLY:HA2	2.51	0.41
3:F:76:ILE:HG23	3:F:197:PHE:CE1	2.55	0.41
3:H:343:TRP:HE3	3:H:344:PRO:HD2	1.86	0.41
3:F:103:SER:HB3	3:F:117:ASN:OD1	2.21	0.41
2:D:1641:ASN:OXT	3:H:255:SER:HB3	2.20	0.41
3:F:196:SER:O	3:F:197:PHE:HB3	2.21	0.41
1:C:158:LEU:HD22	1:C:169:LEU:HD11	2.02	0.41
3:F:539:LYS:HG3	3:F:547:PHE:CD1	2.56	0.41
3:F:299:VAL:HG22	3:F:340:MET:HE3	2.03	0.41
1:A:111:GLN:O	1:A:125:TYR:HA	2.20	0.41
2:B:1378:MET:HE2	2:B:1378:MET:HB3	1.93	0.40
1:A:38:HIS:HD2	1:A:45:LEU:HB3	1.85	0.40
3:F:190:GLU:HA	3:F:191:PRO:HD3	1.81	0.40
2:D:1617:ASP:C	2:D:1619:GLU:H	2.24	0.40
2:B:983:VAL:O	2:B:985:PRO:HD3	2.21	0.40
2:D:1342:LYS:HD3	2:D:1342:LYS:N	2.36	0.40
1:A:216:PRO:HA	1:A:231:VAL:HA	2.02	0.40
3:H:125:ARG:HH21	3:H:194:GLN:HE22	1.69	0.40
2:D:1253:VAL:O	2:D:1257:LEU:HG	2.21	0.40
2:B:1022:GLY:O	2:B:1026:LEU:HG	2.21	0.40
2:D:1276:LEU:H	2:D:1276:LEU:HD23	1.85	0.40
4:I:137:ARG:HA	4:I:138:PRO:HD3	1.90	0.40
3:F:318:ASN:HD21	3:F:320:GLU:HG2	1.86	0.40
1:A:480:LYS:HG2	1:A:481:ALA:N	2.36	0.40
3:H:354:ARG:HD2	3:H:354:ARG:C	2.42	0.40
3:H:33:LEU:HD12	3:H:33:LEU:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:SER:O	1:C:414:GLN:HG2	2.22	0.40
3:H:143:PRO:HB2	3:H:164:TYR:OH	2.20	0.40
3:F:309:TRP:HZ3	3:F:313:GLN:CG	2.35	0.40
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.51	0.40
3:H:464:ASP:O	3:H:465:TYR:HB2	2.21	0.40
2:D:1086:ILE:HA	2:D:1090:GLN:NE2	2.37	0.40
1:A:253:ILE:HG12	1:A:302:LEU:CD2	2.52	0.40
1:A:459:ARG:HA	1:A:462:GLU:HG2	2.03	0.40
5:B:2643:NAG:H5	5:B:2643:NAG:HN2	1.85	0.40
1:C:474:ASN:ND2	1:C:475:LYS:HG3	2.36	0.40
1:C:45:LEU:HA	1:C:46:VAL:HA	1.72	0.40
3:F:119:THR:HB	4:I:115:ARG:NH1	2.36	0.40
1:C:249:VAL:HG13	1:C:267:LYS:HB2	2.03	0.40
3:F:254:GLY:HA2	3:F:319:TYR:OH	2.21	0.40
4:I:54:LEU:HD21	4:I:67:LYS:HE3	2.03	0.40
2:B:1143:LEU:O	2:B:1147:ILE:HG13	2.22	0.40
3:F:408:LEU:HD22	3:F:408:LEU:N	2.37	0.40
3:H:503:PHE:HB2	3:H:530:PHE:CZ	2.56	0.40
3:H:408:LEU:N	3:H:408:LEU:HD22	2.36	0.40
4:I:40:ALA:HB2	4:I:90:LEU:O	2.21	0.40
4:I:151:ARG:N	9:I:1229:GOL:H11	2.37	0.40
4:J:15:MET:HE1	4:J:127:GLY:HA2	2.04	0.40
2:D:962:GLY:HA3	2:D:1289:ILE:HG21	2.03	0.40
3:F:709:VAL:HA	3:F:710:PRO:HD3	1.93	0.40
1:A:143:VAL:O	1:A:155:GLN:HA	2.22	0.40
3:H:638:ALA:HA	3:H:639:PRO:HD3	1.97	0.40
2:D:735:ALA:O	2:D:739:ILE:HG13	2.22	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	636/642 (99%)	569 (90%)	59 (9%)	8 (1%)	15	60
1	C	636/642 (99%)	565 (89%)	61 (10%)	10 (2%)	12	55
2	B	895/912 (98%)	802 (90%)	83 (9%)	10 (1%)	17	63
2	D	895/912 (98%)	795 (89%)	92 (10%)	8 (1%)	21	68
3	F	708/732 (97%)	642 (91%)	55 (8%)	11 (2%)	12	55
3	H	705/732 (96%)	637 (90%)	54 (8%)	14 (2%)	9	51
4	I	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	21	68
4	J	226/228 (99%)	199 (88%)	25 (11%)	2 (1%)	21	68
All	All	4927/5028 (98%)	4410 (90%)	452 (9%)	65 (1%)	15	60

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	VAL
1	A	518	ALA
2	B	733	ILE
2	B	965	VAL
2	B	1498	ILE
1	C	289	VAL
1	C	518	ALA
1	C	519	SER
2	D	1498	ILE
3	F	197	PHE
3	F	702	ASN
3	F	706	GLN
3	F	707	LYS
3	H	197	PHE
3	H	702	ASN
3	H	706	GLN
3	H	707	LYS
1	A	290	GLN
1	A	534	LYS
2	B	968	MET
2	B	1377	THR
2	B	1505	VAL
1	C	290	GLN
1	C	534	LYS
2	D	928	GLU
2	D	965	VAL
2	D	1377	THR

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Mol	Chain	Res	Type
2	D	1505	VAL
3	F	199	TYR
3	F	704	LYS
3	F	740	ALA
3	H	199	TYR
3	H	463	THR
3	H	704	LYS
3	H	740	ALA
1	A	519	SER
1	A	549	GLU
2	B	928	GLU
1	C	517	GLY
1	C	549	GLU
2	D	774	LYS
2	D	1534	ASN
3	F	431	LYS
3	F	703	GLN
3	H	431	LYS
3	H	703	GLN
4	I	46	ALA
4	I	47	ALA
4	J	46	ALA
4	J	47	ALA
1	A	574	VAL
2	B	778	THR
2	B	969	THR
1	C	574	VAL
3	F	479	PRO
3	H	433	MET
1	C	27	ALA
3	H	223	GLU
3	H	479	PRO
2	D	1201	PRO
3	H	692	ILE
2	B	1201	PRO
1	C	520	GLY
1	A	520	GLY
3	F	692	ILE

### 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	564/566 (100%)	557 (99%)	7 (1%)	78	92
1	C	564/566 (100%)	558 (99%)	6 (1%)	80	92
2	B	797/807 (99%)	788 (99%)	9 (1%)	80	92
2	D	797/807 (99%)	789 (99%)	8 (1%)	82	93
3	F	620/635 (98%)	612 (99%)	8 (1%)	76	91
3	H	618/635 (97%)	611 (99%)	7 (1%)	80	92
4	I	181/181 (100%)	179 (99%)	2 (1%)	80	92
4	J	181/181 (100%)	180 (99%)	1 (1%)	90	97
All	All	4322/4378 (99%)	4274 (99%)	48 (1%)	80	92

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	370	GLN
1	A	414	GLN
1	A	516	ILE
1	A	519	SER
1	A	630	GLN
1	A	634	GLN
2	B	733	ILE
2	B	898	PHE
2	B	953	GLU
2	B	965	VAL
2	B	1270	LEU
2	B	1276	LEU
2	B	1334	LEU
2	B	1342	LYS
2	B	1573	LYS
1	C	59	ASN
1	C	370	GLN
1	C	414	GLN

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Mol	Chain	Res	Type
1	C	516	ILE
1	C	630	GLN
1	C	634	GLN
2	D	898	PHE
2	D	953	GLU
2	D	1270	LEU
2	D	1276	LEU
2	D	1334	LEU
2	D	1342	LYS
2	D	1485	ARG
2	D	1573	LYS
3	F	90	TRP
3	F	103	SER
3	F	241	SER
3	F	309	TRP
3	F	468	GLN
3	F	611	GLU
3	F	654	ARG
3	F	705	ARG
3	H	90	TRP
3	H	103	SER
3	H	243	SER
3	H	309	TRP
3	H	354	ARG
3	H	468	GLN
3	H	654	ARG
4	I	157	ARG
4	I	198	THR
4	J	157	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	59	ASN
1	A	104	GLN
1	A	132	HIS
1	A	311	HIS
1	A	370	GLN
1	A	414	GLN
1	A	558	GLN
1	A	587	ASN

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Mol	Chain	Res	Type
1	A	630	GLN
1	A	634	GLN
2	B	770	ASN
2	B	836	GLN
2	B	860	HIS
2	B	1090	GLN
2	B	1130	GLN
2	B	1176	GLN
2	B	1268	GLN
2	B	1545	GLN
1	C	38	HIS
1	C	59	ASN
1	C	63	ASN
1	C	104	GLN
1	C	132	HIS
1	C	311	HIS
1	C	356	ASN
1	C	370	GLN
1	C	414	GLN
1	C	558	GLN
1	C	587	ASN
1	C	630	GLN
1	C	634	GLN
2	D	770	ASN
2	D	836	GLN
2	D	860	HIS
2	D	1090	GLN
2	D	1130	GLN
2	D	1176	GLN
2	D	1267	HIS
2	D	1545	GLN
3	F	63	GLN
3	F	194	GLN
3	F	357	HIS
3	F	423	ASN
3	F	591	GLN
3	H	63	GLN
3	H	194	GLN
3	H	318	ASN
3	H	357	HIS
3	H	483	HIS
3	H	591	GLN

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Mol	Chain	Res	Type
4	I	10	HIS
4	J	10	HIS

### 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 ⓘ

12 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	$\# Z  > 2$
5	NAG	A	1643	1,5	14,14,15	0.48	0	15,19,21	1.24	1 (6%)
5	NAG	A	1644	5	14,14,15	0.55	0	15,19,21	1.35	2 (13%)
5	NAG	B	2642	2,5	14,14,15	0.52	0	15,19,21	0.56	0
5	NAG	B	2643	5	14,14,15	0.51	0	15,19,21	0.72	0
5	NAG	C	2063	1,5	14,14,15	0.54	0	15,19,21	0.60	0
5	NAG	C	2064	5	14,14,15	0.54	0	15,19,21	0.59	0
8	NAG	F	1117	8,3	14,14,15	0.57	0	15,19,21	1.32	2 (13%)
8	NAG	F	1118	8	14,14,15	0.58	0	15,19,21	1.16	2 (13%)
8	BMA	F	1119	8	11,11,12	0.26	0	14,15,17	0.60	0
8	NAG	H	1117	8,3	14,14,15	0.45	0	15,19,21	1.93	3 (20%)
8	NAG	H	1118	8	14,14,15	0.51	0	15,19,21	1.61	4 (26%)
8	BMA	H	1119	8	11,11,12	1.68	2 (18%)	14,15,17	3.61	10 (71%)

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
5	NAG	A	1643	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1644	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2642	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2643	5	-	0/6/23/26	0/1/1/1
5	NAG	C	2063	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2064	5	-	0/6/23/26	0/1/1/1
8	NAG	F	1117	8,3	-	0/6/23/26	0/1/1/1
8	NAG	F	1118	8	-	0/6/23/26	0/1/1/1
8	BMA	F	1119	8	-	0/2/19/22	0/1/1/1
8	NAG	H	1117	8,3	-	0/6/23/26	0/1/1/1
8	NAG	H	1118	8	-	0/6/23/26	0/1/1/1
8	BMA	H	1119	8	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1119	BMA	C4-C3	2.99	1.60	1.52
8	H	1119	BMA	C2-C3	3.66	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1644	NAG	C1-O5-C5	-3.77	107.47	112.25
8	F	1117	NAG	C2-N2-C7	-2.43	119.91	123.04
8	H	1117	NAG	C6-C5-C4	-2.35	107.22	113.02
8	H	1118	NAG	C4-C3-C2	-2.31	107.64	111.23
8	H	1118	NAG	C6-C5-C4	-2.24	107.49	113.02
8	F	1118	NAG	C1-O5-C5	-2.06	109.64	112.25
5	A	1644	NAG	C2-N2-C7	-2.01	120.46	123.04
8	H	1119	BMA	C1-O5-C5	2.35	115.22	112.25
8	H	1118	NAG	C2-N2-C7	2.43	126.16	123.04
8	F	1118	NAG	C3-C4-C5	2.55	114.64	110.20
8	H	1119	BMA	C3-C4-C5	2.81	115.09	110.20
8	H	1119	BMA	O6-C6-C5	2.95	121.08	111.33
8	H	1118	NAG	O3-C3-C2	3.12	115.28	109.11
5	A	1643	NAG	C1-O5-C5	3.33	116.48	112.25
8	F	1117	NAG	C1-O5-C5	3.52	116.71	112.25
8	H	1119	BMA	O4-C4-C3	3.52	118.26	110.34
8	H	1117	NAG	C1-O5-C5	4.06	117.40	112.25
8	H	1119	BMA	O4-C4-C5	4.47	121.09	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1119	BMA	O2-C2-C3	4.56	119.29	110.12
8	H	1119	BMA	O3-C3-C2	4.76	118.59	110.00
8	H	1117	NAG	C2-N2-C7	4.81	129.22	123.04
8	H	1119	BMA	O3-C3-C4	4.92	121.42	110.34
8	H	1119	BMA	O2-C2-C1	5.12	119.47	109.21
8	H	1119	BMA	O5-C5-C6	5.24	118.69	107.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1643	NAG	2	0
5	B	2643	NAG	1	0
5	C	2063	NAG	10	0
5	C	2064	NAG	2	0
8	F	1117	NAG	1	0
8	F	1118	NAG	1	0

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z  > 2$
7	NAG	D	2642	2	14,14,15	0.54	0	15,19,21	0.60	0
7	NAG	F	1743	3	14,14,15	0.52	0	15,19,21	0.55	0
7	NAG	F	1747	3	14,14,15	0.56	0	15,19,21	0.68	0
7	NAG	H	1743	3	14,14,15	0.50	0	15,19,21	0.62	0
7	NAG	H	1747	3	14,14,15	0.47	0	15,19,21	0.73	0
9	GOL	I	1229	-	5,5,5	0.35	0	5,5,5	0.13	0
9	GOL	J	1229	-	5,5,5	0.35	0	5,5,5	0.26	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
7	NAG	D	2642	2	-	0/6/23/26	0/1/1/1
7	NAG	F	1743	3	-	0/6/23/26	0/1/1/1
7	NAG	F	1747	3	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	H	1743	3	-	0/6/23/26	0/1/1/1
7	NAG	H	1747	3	-	0/6/23/26	0/1/1/1
9	GOL	I	1229	-	-	0/4/4/4	0/0/0/0
9	GOL	J	1229	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	F	1747	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1743	NAG	1	0
9	I	1229	GOL	3	0
9	J	1229	GOL	4	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	640/642 (99%)	0.43	54 (8%) 14 12	58, 134, 189, 278	0
1	C	640/642 (99%)	0.75	91 (14%) 4 4	67, 134, 189, 281	0
2	B	901/912 (98%)	0.18	18 (1%) 68 59	60, 122, 203, 330	0
2	D	901/912 (98%)	0.36	91 (10%) 9 9	60, 125, 205, 328	0
3	F	714/732 (97%)	0.04	10 (1%) 78 68	37, 82, 154, 272	0
3	H	711/732 (97%)	0.17	26 (3%) 45 36	37, 84, 153, 222	0
4	I	228/228 (100%)	-0.19	0 100 100	46, 79, 125, 218	0
4	J	228/228 (100%)	-0.15	1 (0%) 93 90	42, 79, 125, 220	0
All	All	4963/5028 (98%)	0.27	291 (5%) 26 20	37, 109, 189, 330	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1073	ILE	8.5
2	D	1151	GLY	8.4
3	F	482	GLY	8.1
2	D	1154	LEU	7.5
1	C	636	ALA	7.2
2	D	1136	CYS	6.4
2	D	1503	ASP	6.3
1	C	337	LYS	6.2
1	C	78	LYS	6.1
1	C	74	PHE	6.1
1	C	47	LEU	6.1
1	C	46	VAL	6.0
1	A	378	LEU	6.0
1	C	102	SER	5.8
1	C	45	LEU	5.7
2	D	1118	ASP	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	69	PRO	5.7
2	D	1092	PRO	5.4
2	B	1499	GLN	5.4
2	D	1093	ASP	5.2
2	D	1115	ASN	5.1
3	F	480	SER	5.1
2	D	1057	THR	5.1
1	C	103	LEU	5.1
1	C	48	SER	5.0
2	D	1169	ILE	5.0
1	A	70	ALA	4.9
2	D	1074	ASP	4.9
3	H	480	SER	4.9
1	C	20	MET	4.8
2	D	1072	ALA	4.7
1	C	408	GLU	4.7
2	D	1077	VAL	4.6
2	D	1499	GLN	4.5
3	H	460	ARG	4.4
2	D	1078	LEU	4.4
2	D	1504	LYS	4.3
1	C	44	LYS	4.3
2	D	1122	THR	4.3
3	F	483	HIS	4.3
2	D	1107	MET	4.2
1	A	374	THR	4.2
2	D	1131	GLU	4.2
1	C	40	PHE	4.2
2	D	1096	PHE	4.1
1	C	22	LEU	4.1
2	D	1081	ALA	4.1
2	D	1049	LYS	4.1
3	H	479	PRO	4.0
1	C	314	SER	4.0
2	D	1071	ILE	4.0
2	B	1419	ARG	3.9
2	D	1150	ALA	3.9
2	D	1103	ILE	3.9
1	C	323	GLY	3.9
2	D	1158	TYR	3.8
1	C	107	TYR	3.8
2	D	1099	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	194	GLN	3.7
1	A	497	LEU	3.7
2	D	1162	GLN	3.7
3	H	483	HIS	3.7
2	D	1098	GLU	3.7
3	H	484	GLU	3.7
2	D	1177	MET	3.7
1	C	37	VAL	3.7
1	C	75	LYS	3.7
2	D	1059	TYR	3.7
1	C	374	THR	3.7
2	D	1120	ALA	3.6
2	D	1070	LEU	3.6
1	C	19	THR	3.6
2	D	1161	LEU	3.6
1	C	36	THR	3.6
2	D	1424	ILE	3.5
2	D	1155	GLU	3.5
1	C	21	VAL	3.5
2	D	1119	MET	3.5
1	C	70	ALA	3.5
1	C	350	LEU	3.5
2	D	1056	LEU	3.5
1	A	102	SER	3.4
2	D	1444	TYR	3.4
2	D	1018	GLU	3.4
1	C	24	ALA	3.3
1	C	378	LEU	3.3
1	C	81	ASN	3.3
1	C	166	VAL	3.3
1	C	610	GLY	3.3
1	C	382	ASP	3.3
1	C	634	GLN	3.3
3	H	703	GLN	3.3
1	A	468	TYR	3.3
3	F	343	TRP	3.3
1	C	52	THR	3.3
1	A	405	LYS	3.2
1	A	376	GLN	3.2
1	A	20	MET	3.2
2	B	1119	MET	3.2
2	D	1036	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	90	PHE	3.2
1	C	230	GLU	3.2
1	C	440	ARG	3.2
2	D	1076	GLN	3.2
2	D	1419	ARG	3.2
1	A	514	THR	3.1
1	C	104	GLN	3.1
1	C	72	ARG	3.1
1	C	190	ASN	3.1
3	H	477	ILE	3.1
1	A	21	VAL	3.1
2	D	1023	ALA	3.1
1	C	336	THR	3.0
2	B	985	PRO	3.0
1	A	481	ALA	3.0
1	C	365	VAL	3.0
3	H	70	LYS	3.0
2	D	1085	LEU	3.0
2	B	1444	TYR	3.0
1	C	228	GLY	3.0
2	D	1418	ASP	3.0
2	D	1102	VAL	3.0
1	A	105	SER	3.0
1	C	609	SER	3.0
2	B	1078	LEU	2.9
3	H	461	LYS	2.9
1	C	465	ILE	2.9
1	C	87	GLN	2.9
1	C	101	VAL	2.9
2	D	1152	ASP	2.9
1	C	530	TRP	2.9
2	B	1411	GLU	2.9
2	B	1418	ASP	2.9
1	A	515	LEU	2.9
2	D	1048	VAL	2.9
2	D	1147	ILE	2.9
3	F	481	LYS	2.8
1	A	449	LEU	2.8
2	D	1143	LEU	2.8
1	A	349	ASP	2.8
1	A	68	ILE	2.8
2	D	1331	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	1186	ASN	2.8
1	C	38	HIS	2.7
1	C	405	LYS	2.7
1	C	156	ASP	2.7
1	A	636	ALA	2.7
3	H	476	VAL	2.7
1	A	480	LYS	2.7
1	C	30	ASP	2.7
1	C	379	THR	2.7
2	D	1178	GLY	2.7
1	C	82	LYS	2.7
1	A	440	ARG	2.7
1	C	386	LYS	2.7
3	H	482	GLY	2.7
2	D	1359	LYS	2.6
3	H	611	GLU	2.6
1	A	22	LEU	2.6
1	A	3	MET	2.6
1	A	351	MET	2.6
1	C	98	VAL	2.6
1	A	386	LYS	2.6
2	D	1114	ASN	2.6
2	D	1251	PHE	2.6
3	H	641	TYR	2.6
2	B	1188	PHE	2.6
2	D	1062	LYS	2.6
2	D	1132	ALA	2.5
1	C	54	LEU	2.5
2	D	1017	LEU	2.5
2	D	1236	GLU	2.5
1	C	348	PHE	2.5
2	D	1160	ASN	2.5
2	D	1498	ILE	2.5
2	D	1054	THR	2.5
1	A	25	HIS	2.5
2	D	1125	VAL	2.5
3	H	17	VAL	2.5
1	C	481	ALA	2.5
4	J	43	LEU	2.5
1	C	12	LEU	2.5
2	D	1250	THR	2.4
1	C	480	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	71	ASN	2.4
1	C	7	ILE	2.4
1	C	324	ILE	2.4
2	B	1154	LEU	2.4
1	A	43	LYS	2.4
1	A	387	LEU	2.4
1	C	304	VAL	2.4
1	A	350	LEU	2.4
2	D	1124	PHE	2.4
2	D	1170	ALA	2.4
1	A	630	GLN	2.4
2	D	1104	HIS	2.4
2	D	999	THR	2.4
2	B	1151	GLY	2.4
1	C	8	THR	2.4
1	C	49	SER	2.4
1	C	129	THR	2.4
3	H	610	GLU	2.4
2	D	1037	PHE	2.4
1	C	339	PRO	2.4
2	D	1127	ILE	2.4
2	D	1063	VAL	2.4
3	H	465	TYR	2.4
2	D	1446	ASN	2.3
1	A	496	PRO	2.3
3	H	525	ILE	2.3
3	H	478	ARG	2.3
3	H	713	ALA	2.3
1	C	184	ILE	2.3
3	H	544	ILE	2.3
2	D	1163	ARG	2.3
1	A	385	ALA	2.3
1	A	516	ILE	2.3
2	D	1183	PRO	2.3
3	H	481	LYS	2.3
3	H	635	ALA	2.3
1	A	517	GLY	2.3
1	C	297	LEU	2.3
2	D	1146	SER	2.3
3	H	503	PHE	2.3
2	B	1420	ASN	2.3
3	H	614	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	1129	LEU	2.2
1	A	624	PHE	2.2
2	B	1391	PRO	2.2
1	C	86	VAL	2.2
1	C	23	GLU	2.2
1	C	464	LYS	2.2
1	A	45	LEU	2.2
2	D	1416	PHE	2.2
1	A	257	GLU	2.2
2	D	1052	PRO	2.2
2	B	1422	LEU	2.2
1	A	377	SER	2.2
1	A	443	LEU	2.2
1	C	335	PHE	2.2
2	B	1504	LYS	2.2
2	D	1381	LEU	2.2
1	A	218	GLU	2.2
3	F	641	TYR	2.2
1	C	193	GLN	2.2
2	B	1503	ASP	2.2
1	C	108	LEU	2.2
2	D	1094	GLY	2.2
1	A	5	SER	2.2
2	D	1047	PHE	2.2
1	C	479	LEU	2.1
3	F	460	ARG	2.1
1	A	491	ASP	2.1
3	H	14	LEU	2.1
2	B	1128	SER	2.1
2	D	983	VAL	2.1
1	C	85	THR	2.1
2	D	1138	GLU	2.1
1	C	14	LEU	2.1
1	C	325	PRO	2.1
1	A	453	PHE	2.1
1	C	338	THR	2.1
1	C	218	GLU	2.1
1	A	412	ALA	2.1
1	A	366	PRO	2.1
1	C	227	LYS	2.1
2	D	1497	PHE	2.1
1	A	485	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	406	LYS	2.1
1	C	79	GLY	2.1
3	F	459	HIS	2.1
1	C	376	GLN	2.1
1	A	573	LEU	2.1
2	D	1001	ILE	2.0
1	A	103	LEU	2.0
2	B	1251	PHE	2.0
3	H	671	ARG	2.0
1	C	357	PRO	2.0
1	A	459	ARG	2.0
1	A	471	LEU	2.0
1	C	364	ARG	2.0
1	C	503	PHE	2.0
2	D	1101	PRO	2.0
3	F	348	PRO	2.0
1	A	492	LEU	2.0
2	D	829	LEU	2.0
1	A	308	VAL	2.0
2	D	1000	VAL	2.0
3	F	478	ARG	2.0
1	C	43	LYS	2.0
1	C	132	HIS	2.0

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

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

## 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<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	NAG	A	1643	14/15	0.88	0.26	-1.25	129,188,212,214	0
5	NAG	C	2063	14/15	0.74	0.24	-1.47	123,187,212,212	0
8	NAG	F	1118	14/15	0.84	0.21	-	118,138,166,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	H	1118	14/15	0.64	0.31	-	160,172,206,213	0
5	NAG	A	1644	14/15	0.78	0.17	-	160,201,217,223	0
8	NAG	H	1117	14/15	0.89	0.23	-	96,122,150,154	0
8	NAG	F	1117	14/15	0.85	0.22	-	91,116,131,137	0
8	BMA	H	1119	11/12	0.56	0.29	-	132,155,186,196	0
5	NAG	B	2642	14/15	0.88	0.20	-	102,141,165,192	0
5	NAG	C	2064	14/15	0.36	0.35	-	155,202,219,222	0
8	BMA	F	1119	11/12	0.69	0.32	-	128,162,204,271	0
5	NAG	B	2643	14/15	0.84	0.24	-	114,185,200,200	0

## 6.4 Ligands [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<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
9	GOL	I	1229	6/6	0.97	0.38	5.75	73,107,124,127	0
6	MG	H	1742	1/1	0.84	0.30	2.92	140,140,140,140	0
9	GOL	J	1229	6/6	0.95	0.26	2.20	58,74,87,95	0
6	MG	F	1742	1/1	0.99	0.20	1.26	67,67,67,67	0
7	NAG	F	1743	14/15	0.72	0.37	-	97,143,202,215	0
7	NAG	D	2642	14/15	0.81	0.23	-	104,146,166,179	0
7	NAG	F	1747	14/15	0.83	0.27	-	135,154,184,195	0
7	NAG	H	1747	14/15	0.81	0.28	-	118,163,182,198	0
6	MG	C	1645	1/1	0.89	0.03	-	127,127,127,127	0
7	NAG	H	1743	14/15	0.86	0.27	-	117,167,189,193	0
6	MG	A	1645	1/1	0.91	0.12	-	108,108,108,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.