



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:39 PM GMT

PDB ID : 3RKI  
Title : Structural basis for immunization with post-fusion RSV F to elicit high neutralizing antibody titers  
Authors : Swanson, K.A.; Settembre, E.C.; Shaw, C.A.; Dey, A.K.; Rappuoli, R.; Mandl, C.W.; Dormitzer, P.D.; Carfi, A.  
Deposited on : 2011-04-18  
Resolution : 3.20 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

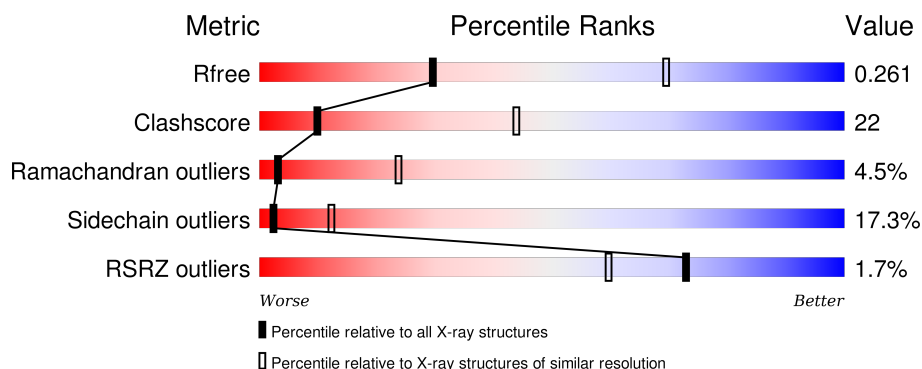
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	528	<div> <div>2%</div> <div>43% 30% 9% • 16%</div> </div>
1	B	528	<div> <div>43% 30% 8% • 17%</div> </div>
1	C	528	<div> <div>2%</div> <div>47% 27% 8% • 17%</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
2	NAG	A	1535	X	-	-	-
2	NAG	B	1535	X	-	-	-
2	NAG	C	1535	X	-	-	-
3	NAG	A	1525	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10438 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3424	2155	569	679	21			
1	B	439	Total	C	N	O	S	0	0	0
			3413	2149	567	676	21			
1	C	439	Total	C	N	O	S	0	0	0
			3419	2152	568	678	21			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ALA	PRO	VARIANT	UNP P03420
A	?	-	PHE	DELETION	UNP P03420
A	?	-	LEU	DELETION	UNP P03420
A	?	-	GLY	DELETION	UNP P03420
A	?	-	PHE	DELETION	UNP P03420
A	?	-	LEU	DELETION	UNP P03420
A	?	-	LEU	DELETION	UNP P03420
A	?	-	GLY	DELETION	UNP P03420
A	?	-	VAL	DELETION	UNP P03420
A	?	-	GLY	DELETION	UNP P03420
A	379	VAL	ILE	VARIANT	UNP P03420
A	447	VAL	MET	VARIANT	UNP P03420
A	525	GLY	-	EXPRESSION TAG	UNP P03420
A	526	GLY	-	EXPRESSION TAG	UNP P03420
A	527	SER	-	EXPRESSION TAG	UNP P03420
A	528	ALA	-	EXPRESSION TAG	UNP P03420
A	529	GLY	-	EXPRESSION TAG	UNP P03420
A	530	SER	-	EXPRESSION TAG	UNP P03420
A	531	GLY	-	EXPRESSION TAG	UNP P03420
A	532	HIS	-	EXPRESSION TAG	UNP P03420
A	533	HIS	-	EXPRESSION TAG	UNP P03420
A	534	HIS	-	EXPRESSION TAG	UNP P03420
A	535	HIS	-	EXPRESSION TAG	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	536	HIS	-	EXPRESSION TAG	UNP P03420
A	537	HIS	-	EXPRESSION TAG	UNP P03420
B	111	ALA	PRO	VARIANT	UNP P03420
B	?	-	PHE	DELETION	UNP P03420
B	?	-	LEU	DELETION	UNP P03420
B	?	-	GLY	DELETION	UNP P03420
B	?	-	PHE	DELETION	UNP P03420
B	?	-	LEU	DELETION	UNP P03420
B	?	-	LEU	DELETION	UNP P03420
B	?	-	GLY	DELETION	UNP P03420
B	?	-	VAL	DELETION	UNP P03420
B	?	-	GLY	DELETION	UNP P03420
B	379	VAL	ILE	VARIANT	UNP P03420
B	447	VAL	MET	VARIANT	UNP P03420
B	525	GLY	-	EXPRESSION TAG	UNP P03420
B	526	GLY	-	EXPRESSION TAG	UNP P03420
B	527	SER	-	EXPRESSION TAG	UNP P03420
B	528	ALA	-	EXPRESSION TAG	UNP P03420
B	529	GLY	-	EXPRESSION TAG	UNP P03420
B	530	SER	-	EXPRESSION TAG	UNP P03420
B	531	GLY	-	EXPRESSION TAG	UNP P03420
B	532	HIS	-	EXPRESSION TAG	UNP P03420
B	533	HIS	-	EXPRESSION TAG	UNP P03420
B	534	HIS	-	EXPRESSION TAG	UNP P03420
B	535	HIS	-	EXPRESSION TAG	UNP P03420
B	536	HIS	-	EXPRESSION TAG	UNP P03420
B	537	HIS	-	EXPRESSION TAG	UNP P03420
C	111	ALA	PRO	VARIANT	UNP P03420
C	?	-	PHE	DELETION	UNP P03420
C	?	-	LEU	DELETION	UNP P03420
C	?	-	GLY	DELETION	UNP P03420
C	?	-	PHE	DELETION	UNP P03420
C	?	-	LEU	DELETION	UNP P03420
C	?	-	LEU	DELETION	UNP P03420
C	?	-	GLY	DELETION	UNP P03420
C	?	-	VAL	DELETION	UNP P03420
C	?	-	GLY	DELETION	UNP P03420
C	379	VAL	ILE	VARIANT	UNP P03420
C	447	VAL	MET	VARIANT	UNP P03420
C	525	GLY	-	EXPRESSION TAG	UNP P03420
C	526	GLY	-	EXPRESSION TAG	UNP P03420
C	527	SER	-	EXPRESSION TAG	UNP P03420

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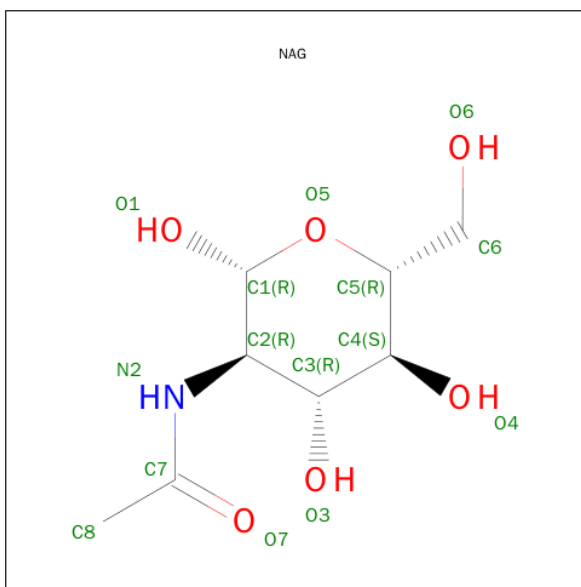
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Chain	Residue	Modelled	Actual	Comment	Reference
C	528	ALA	-	EXPRESSION TAG	UNP P03420
C	529	GLY	-	EXPRESSION TAG	UNP P03420
C	530	SER	-	EXPRESSION TAG	UNP P03420
C	531	GLY	-	EXPRESSION TAG	UNP P03420
C	532	HIS	-	EXPRESSION TAG	UNP P03420
C	533	HIS	-	EXPRESSION TAG	UNP P03420
C	534	HIS	-	EXPRESSION TAG	UNP P03420
C	535	HIS	-	EXPRESSION TAG	UNP P03420
C	536	HIS	-	EXPRESSION TAG	UNP P03420
C	537	HIS	-	EXPRESSION TAG	UNP P03420

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

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

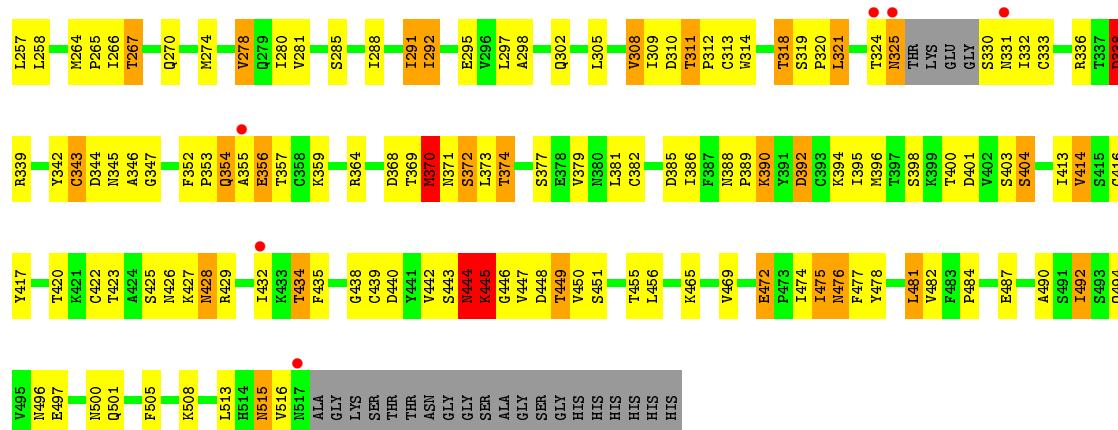
- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



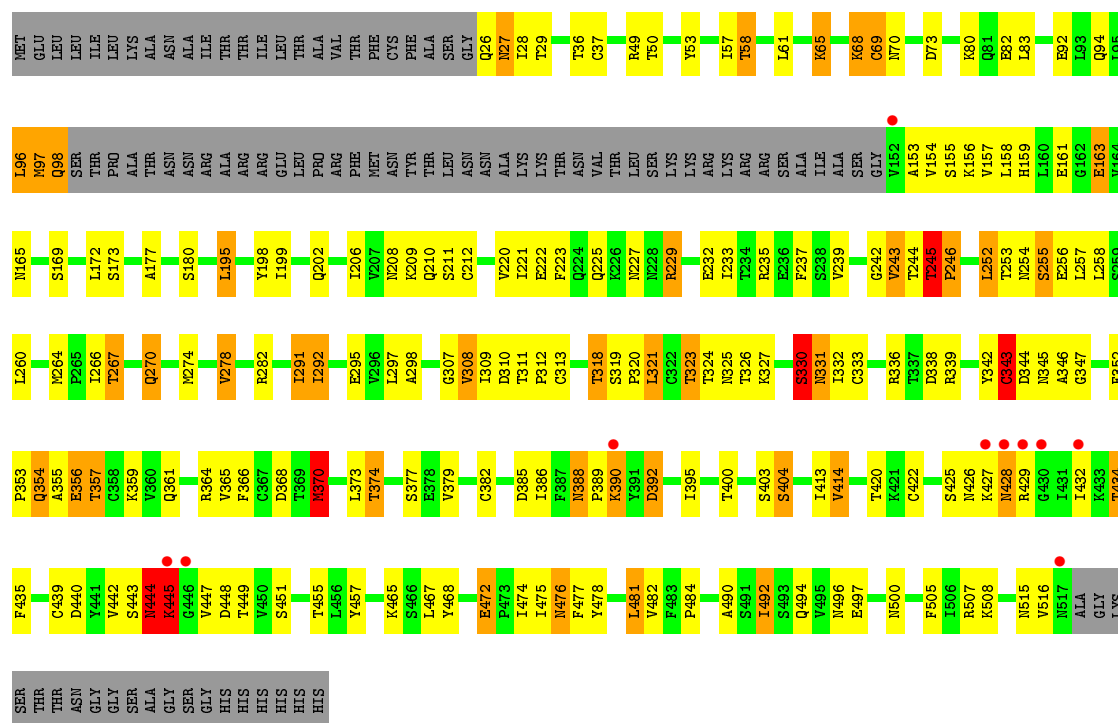
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		







● Molecule 1: Fusion glycoprotein F0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.93Å 113.16Å 311.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	77.0 (30.00-3.20) 77.1 (29.52-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.228 , 0.264 0.225 , 0.261	Depositor DCC
$R_{free}$ test set	2065 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 40186 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: 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	1.05	9/3471 (0.3%)	0.95	6/4703 (0.1%)
1	B	0.84	2/3460 (0.1%)	0.86	3/4688 (0.1%)
1	C	0.93	3/3467 (0.1%)	0.92	5/4698 (0.1%)
All	All	0.94	14/10398 (0.1%)	0.91	14/14089 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	5
2	A	1	0
2	B	1	0
2	C	1	0
All	All	3	16

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	CYS	CB-SG	-11.88	1.62	1.82
1	A	313	CYS	CB-SG	-8.06	1.68	1.82
1	C	343	CYS	CB-SG	-7.20	1.70	1.82
1	A	393	CYS	CB-SG	-6.42	1.71	1.82
1	A	322	CYS	CB-SG	-6.38	1.71	1.82
1	B	338	ASP	CB-CG	6.29	1.65	1.51
1	A	416	CYS	CB-SG	-6.11	1.71	1.82
1	A	394	LYS	CD-CE	5.79	1.65	1.51
1	A	472	GLU	CG-CD	5.79	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	472	GLU	CG-CD	5.76	1.60	1.51
1	C	472	GLU	CG-CD	5.49	1.60	1.51
1	A	459	VAL	CB-CG2	-5.17	1.42	1.52
1	A	477	PHE	CE1-CZ	5.05	1.47	1.37
1	C	212	CYS	CB-SG	-5.04	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	THR	C-N-CD	-9.15	100.46	120.60
1	B	245	THR	C-N-CD	-7.10	104.98	120.60
1	A	245	THR	C-N-CD	-7.01	105.19	120.60
1	A	212	CYS	CA-CB-SG	-6.72	101.90	114.00
1	B	212	CYS	CA-CB-SG	-5.90	103.38	114.00
1	A	432	ILE	CB-CA-C	-5.83	99.94	111.60
1	C	96	LEU	CA-CB-CG	-5.78	102.01	115.30
1	A	446	GLY	N-CA-C	-5.58	99.15	113.10
1	C	212	CYS	CA-CB-SG	-5.50	104.09	114.00
1	B	446	GLY	N-CA-C	-5.45	99.48	113.10
1	A	393	CYS	N-CA-CB	-5.35	100.96	110.60
1	C	243	VAL	CB-CA-C	-5.35	101.23	111.40
1	C	69	CYS	CA-CB-SG	-5.30	104.45	114.00
1	A	477	PHE	N-CA-CB	-5.13	101.36	110.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1535	NAG	C1
2	B	1535	NAG	C1
2	C	1535	NAG	C1

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	VAL	Peptide
1	A	245	THR	Peptide
1	A	392	ASP	Peptide
1	A	444	ASN	Peptide
1	A	445	LYS	Peptide
1	A	476	ASN	Peptide
1	B	245	THR	Peptide
1	B	392	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	434	THR	Peptide
1	B	444	ASN	Peptide
1	B	476	ASN	Peptide
1	C	245	THR	Peptide
1	C	392	ASP	Peptide
1	C	434	THR	Peptide
1	C	444	ASN	Peptide
1	C	476	ASN	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	3424	0	3456	193	1
1	B	3413	0	3447	178	0
1	C	3419	0	3453	173	0
2	A	56	0	50	0	0
2	B	56	0	50	2	0
2	C	56	0	50	1	0
3	A	14	0	13	0	0
All	All	10438	0	10519	462	1

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 22.

All (462) 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:A:154:VAL:CG1	1:A:155:SER:H	1.46	1.26
1:A:154:VAL:HG13	1:A:155:SER:H	1.07	1.09
1:A:65:LYS:HZ2	1:B:475:ILE:HA	0.97	1.08
1:A:475:ILE:O	1:A:477:PHE:HD2	1.35	1.07
1:B:475:ILE:O	1:B:477:PHE:HD2	1.37	1.07
1:A:154:VAL:CG1	1:A:155:SER:N	2.21	1.02
1:C:475:ILE:O	1:C:477:PHE:HD2	1.41	1.01
1:A:65:LYS:HZ2	1:B:475:ILE:CA	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASN:HD22	1:B:481:LEU:H	1.00	0.98
1:A:481:LEU:H	1:C:208:ASN:HD22	1.03	0.98
1:A:152:VAL:HG13	1:A:154:VAL:HB	1.44	0.97
1:C:389:PRO:O	1:C:390:LYS:HB2	1.63	0.97
1:B:389:PRO:O	1:B:390:LYS:HB2	1.66	0.96
1:A:65:LYS:NZ	1:B:475:ILE:HA	1.80	0.96
1:B:208:ASN:HD22	1:C:481:LEU:H	1.13	0.93
1:B:149:ALA:H	1:C:158:LEU:CD1	1.83	0.91
1:C:497:GLU:OE1	1:C:497:GLU:HA	1.69	0.90
1:B:97:MET:CE	1:B:97:MET:HA	2.02	0.90
1:A:245:THR:HG22	1:A:246:PRO:CD	2.03	0.89
1:B:267:THR:HG23	1:B:270:GLN:NE2	1.86	0.89
1:B:149:ALA:HB2	1:C:155:SER:HB2	1.54	0.88
1:C:245:THR:HG22	1:C:246:PRO:CD	2.03	0.88
1:A:292:ILE:HD13	1:A:292:ILE:N	1.89	0.88
1:C:159:HIS:CE1	1:C:163:GLU:OE1	2.26	0.87
1:A:497:GLU:OE1	1:A:497:GLU:HA	1.72	0.87
1:B:65:LYS:HZ1	1:C:475:ILE:HA	1.39	0.87
1:A:475:ILE:HA	1:C:65:LYS:HZ2	1.40	0.87
1:C:292:ILE:HD13	1:C:292:ILE:N	1.90	0.87
1:A:208:ASN:HD22	1:B:481:LEU:N	1.72	0.87
1:A:385:ASP:O	1:A:386:ILE:HB	1.73	0.86
1:C:311:THR:HG21	1:C:344:ASP:O	1.76	0.86
1:A:389:PRO:O	1:A:390:LYS:HB2	1.75	0.86
1:B:497:GLU:HA	1:B:497:GLU:OE1	1.73	0.85
1:A:481:LEU:N	1:C:208:ASN:HD22	1.74	0.85
1:B:82:GLU:HG2	1:C:225:GLN:NE2	1.94	0.83
1:A:154:VAL:HG13	1:A:155:SER:N	1.88	0.83
1:B:292:ILE:HG23	1:B:297:LEU:HD13	1.61	0.82
1:B:245:THR:HG22	1:B:246:PRO:CD	2.08	0.82
1:C:97:MET:HA	1:C:97:MET:CE	2.10	0.82
1:A:475:ILE:O	1:A:477:PHE:CD2	2.27	0.81
1:B:292:ILE:HD13	1:B:292:ILE:N	1.95	0.81
1:A:154:VAL:HG12	1:A:155:SER:H	1.41	0.81
1:B:475:ILE:O	1:B:477:PHE:CD2	2.29	0.81
1:A:225:GLN:NE2	1:C:82:GLU:HG2	1.96	0.81
1:A:92:GLU:OE2	1:B:253:THR:HG23	1.80	0.80
1:A:253:THR:HG23	1:C:92:GLU:OE2	1.81	0.80
1:B:386:ILE:HG23	1:B:395:ILE:HD11	1.63	0.80
1:A:208:ASN:ND2	1:B:481:LEU:H	1.79	0.80
1:C:475:ILE:O	1:C:477:PHE:CD2	2.32	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:THR:HG21	1:B:344:ASP:O	1.83	0.79
1:A:267:THR:HG23	1:A:270:GLN:NE2	1.97	0.78
1:B:208:ASN:HD22	1:C:481:LEU:N	1.80	0.78
1:A:475:ILE:HG22	1:C:65:LYS:HZ1	1.47	0.77
1:B:65:LYS:NZ	1:C:475:ILE:HA	2.00	0.77
1:C:267:THR:HG23	1:C:270:GLN:NE2	1.99	0.77
1:C:266:ILE:HD12	1:C:270:GLN:HB3	1.67	0.77
1:A:82:GLU:HG2	1:B:225:GLN:NE2	2.00	0.77
1:B:160:LEU:HD21	1:C:161:GLU:HA	1.67	0.76
1:C:385:ASP:O	1:C:386:ILE:HB	1.84	0.76
1:A:428:ASN:O	1:A:429:ARG:HB2	1.85	0.75
1:B:427:LYS:HA	1:B:448:ASP:OD2	1.86	0.75
1:A:154:VAL:HG12	1:A:155:SER:N	1.98	0.75
1:A:481:LEU:H	1:C:208:ASN:ND2	1.82	0.75
1:B:385:ASP:O	1:B:386:ILE:HB	1.86	0.75
1:A:292:ILE:HG23	1:A:297:LEU:HD13	1.70	0.73
1:A:324:THR:O	1:A:325:ASN:ND2	2.21	0.73
1:C:342:TYR:O	1:C:343:CYS:HB2	1.88	0.73
1:B:69:CYS:SG	1:B:70:ASN:N	2.61	0.73
1:B:97:MET:HA	1:B:97:MET:HE3	1.71	0.73
1:B:65:LYS:HZ1	1:C:475:ILE:CA	2.01	0.73
1:A:267:THR:HG23	1:A:270:GLN:HE21	1.54	0.72
1:A:152:VAL:HG12	1:A:153:ALA:H	1.55	0.72
1:A:152:VAL:CG1	1:A:154:VAL:HB	2.17	0.72
1:B:37:CYS:HB2	1:B:321:LEU:HG	1.70	0.72
1:C:292:ILE:HG23	1:C:297:LEU:HD13	1.72	0.72
1:C:370:MET:CE	1:C:370:MET:HA	2.20	0.71
1:B:208:ASN:ND2	1:C:481:LEU:H	1.89	0.71
1:A:151:GLY:O	1:A:154:VAL:HG23	1.91	0.71
1:B:370:MET:CE	1:B:370:MET:HA	2.21	0.71
1:C:69:CYS:SG	1:C:70:ASN:N	2.63	0.71
1:B:370:MET:HE3	1:B:370:MET:HA	1.72	0.70
1:A:97:MET:HA	1:A:97:MET:CE	2.21	0.70
1:C:156:LYS:HG3	1:C:157:VAL:N	2.06	0.69
1:B:319:SER:OG	1:B:320:PRO:HD2	1.91	0.69
1:A:311:THR:HG22	1:A:312:PRO:HD2	1.74	0.69
1:C:37:CYS:HB2	1:C:321:LEU:HG	1.74	0.68
1:B:267:THR:HG23	1:B:270:GLN:HE21	1.56	0.68
1:B:311:THR:HG22	1:B:344:ASP:HB2	1.75	0.68
1:B:97:MET:HA	1:B:97:MET:HE2	1.75	0.68
1:C:245:THR:HG22	1:C:246:PRO:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:THR:HG21	1:C:336:ARG:O	1.94	0.68
1:A:58:THR:HG23	1:A:298:ALA:HB2	1.74	0.67
1:C:442:VAL:HB	1:C:447:VAL:HG21	1.74	0.67
1:C:386:ILE:HG23	1:C:395:ILE:HD11	1.76	0.67
1:A:311:THR:HG21	1:A:344:ASP:O	1.95	0.67
1:B:149:ALA:H	1:C:158:LEU:HD12	1.59	0.67
1:A:245:THR:HG22	1:A:246:PRO:HD3	1.76	0.67
1:A:342:TYR:O	1:A:343:CYS:HB2	1.94	0.66
1:B:318:THR:HG21	1:B:336:ARG:O	1.95	0.66
1:A:475:ILE:HG22	1:C:65:LYS:NZ	2.10	0.66
1:B:444:ASN:OD1	1:B:444:ASN:N	2.25	0.66
1:C:97:MET:HE2	1:C:97:MET:HA	1.79	0.65
1:C:26:GLN:O	1:C:27:ASN:HB2	1.96	0.65
1:A:475:ILE:HA	1:C:65:LYS:NZ	2.10	0.65
1:B:338:ASP:HB3	1:B:394:LYS:NZ	2.12	0.64
1:B:374:THR:HG21	1:C:404:SER:HB3	1.78	0.64
1:A:370:MET:CE	1:A:370:MET:HA	2.27	0.64
1:C:311:THR:HG22	1:C:344:ASP:HB2	1.78	0.64
1:A:475:ILE:CA	1:C:65:LYS:HZ2	2.10	0.64
1:B:229:ARG:O	1:B:233:ILE:HG13	1.98	0.63
1:C:370:MET:HE3	1:C:370:MET:HA	1.81	0.63
1:C:156:LYS:HG3	1:C:157:VAL:H	1.62	0.63
1:B:354:GLN:OE1	1:B:356:GLU:HB2	1.98	0.63
1:B:308:VAL:HG13	1:C:455:THR:HA	1.81	0.63
1:B:148:ILE:N	1:C:158:LEU:HD13	2.14	0.63
1:A:150:SER:O	1:A:151:GLY:C	2.35	0.62
1:C:427:LYS:HA	1:C:448:ASP:OD2	1.99	0.62
1:B:92:GLU:OE2	1:C:253:THR:HG23	1.99	0.62
1:A:253:THR:HG22	1:A:254:ASN:N	2.13	0.62
1:A:26:GLN:N	1:A:26:GLN:OE1	2.33	0.62
1:A:148:ILE:O	1:A:149:ALA:O	2.18	0.62
1:C:97:MET:HE3	1:C:97:MET:HA	1.80	0.62
1:C:267:THR:HG23	1:C:270:GLN:HE21	1.63	0.62
1:B:58:THR:HG23	1:B:298:ALA:HB2	1.81	0.62
1:A:494:GLN:O	1:A:497:GLU:HB2	2.00	0.61
1:A:442:VAL:HB	1:A:447:VAL:HG21	1.82	0.61
1:A:69:CYS:SG	1:A:70:ASN:N	2.73	0.61
1:C:58:THR:HG23	1:C:298:ALA:HB2	1.82	0.61
1:A:158:LEU:HA	1:A:161:GLU:HB3	1.83	0.61
1:A:444:ASN:OD1	1:A:444:ASN:N	2.32	0.61
1:B:235:ARG:O	1:B:239:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:PRO:O	1:C:390:LYS:CB	2.41	0.60
1:B:386:ILE:CG2	1:B:395:ILE:HD11	2.31	0.60
1:A:422:CYS:HB2	1:A:435:PHE:HB2	1.83	0.60
1:B:422:CYS:HB2	1:B:435:PHE:HB2	1.84	0.60
1:C:318:THR:HB	1:C:339:ARG:HG2	1.84	0.60
1:C:444:ASN:N	1:C:444:ASN:OD1	2.36	0.59
1:C:494:GLN:O	1:C:497:GLU:HB2	2.01	0.59
2:C:1535:NAG:H3	2:C:1535:NAG:O7	2.01	0.59
1:B:324:THR:HG22	1:B:325:ASN:HD22	1.68	0.59
1:A:311:THR:HG22	1:A:344:ASP:HB2	1.83	0.59
1:B:311:THR:HG22	1:B:312:PRO:HD2	1.83	0.59
1:B:149:ALA:O	1:B:150:SER:HB3	2.03	0.59
1:A:309:ILE:HG22	1:A:310:ASP:CG	2.23	0.59
1:B:82:GLU:HG2	1:C:225:GLN:HE21	1.65	0.59
1:A:37:CYS:HB2	1:A:321:LEU:HG	1.84	0.59
1:B:266:ILE:HD12	1:B:270:GLN:HB3	1.85	0.58
1:B:222:GLU:HB3	1:C:474:ILE:HD11	1.85	0.58
1:B:426:ASN:C	1:B:426:ASN:OD1	2.40	0.58
1:C:385:ASP:HB3	1:C:388:ASN:HD22	1.68	0.58
1:A:150:SER:O	1:A:152:VAL:N	2.37	0.58
1:B:264:MET:HE1	1:B:274:MET:SD	2.43	0.58
1:A:338:ASP:HB3	1:A:394:LYS:NZ	2.19	0.58
1:B:333:CYS:HB2	1:B:398:SER:HB3	1.84	0.58
1:B:492:ILE:C	1:B:494:GLN:N	2.54	0.58
1:A:36:THR:O	1:A:36:THR:HG22	2.04	0.58
1:A:492:ILE:C	1:A:494:GLN:N	2.56	0.57
1:A:404:SER:HB3	1:C:374:THR:HG21	1.85	0.57
1:A:492:ILE:C	1:A:494:GLN:H	2.08	0.57
1:A:365:VAL:HG12	1:A:366:PHE:N	2.19	0.57
1:A:455:THR:HA	1:C:308:VAL:HG13	1.87	0.57
1:C:311:THR:HG22	1:C:312:PRO:HD2	1.87	0.57
1:A:365:VAL:CG1	1:A:366:PHE:N	2.68	0.57
1:B:389:PRO:O	1:B:390:LYS:CB	2.44	0.56
1:B:245:THR:HG22	1:B:246:PRO:HD3	1.86	0.56
1:C:426:ASN:OD1	1:C:426:ASN:C	2.42	0.56
1:A:223:PHE:O	1:A:227:ASN:HB2	2.05	0.56
1:A:152:VAL:HG12	1:A:153:ALA:N	2.18	0.56
1:A:318:THR:HG22	1:A:339:ARG:CZ	2.35	0.56
1:C:223:PHE:O	1:C:227:ASN:HB2	2.05	0.56
1:B:149:ALA:CB	1:C:155:SER:HB2	2.31	0.56
1:C:492:ILE:C	1:C:494:GLN:N	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:ILE:C	1:B:494:GLN:H	2.07	0.56
1:C:98:GLN:N	1:C:98:GLN:OE1	2.39	0.56
1:B:252:LEU:HD13	1:B:257:LEU:HB2	1.88	0.55
1:A:199:ILE:HD11	1:B:199:ILE:HD11	1.88	0.55
1:A:199:ILE:HD11	1:C:199:ILE:HD11	1.88	0.55
1:A:97:MET:HE2	1:A:97:MET:HA	1.87	0.55
1:B:442:VAL:HB	1:B:447:VAL:HG21	1.87	0.55
1:B:445:LYS:HA	1:B:445:LYS:CE	2.36	0.55
1:C:492:ILE:C	1:C:494:GLN:H	2.09	0.55
1:C:229:ARG:O	1:C:233:ILE:HG13	2.07	0.55
1:C:319:SER:OG	1:C:320:PRO:HD2	2.07	0.55
1:A:208:ASN:ND2	1:B:481:LEU:N	2.48	0.55
1:A:229:ARG:O	1:A:233:ILE:HG13	2.06	0.55
1:A:225:GLN:HE21	1:C:82:GLU:HG2	1.71	0.55
1:B:318:THR:HB	1:B:339:ARG:HG2	1.89	0.54
1:A:82:GLU:HG2	1:B:225:GLN:HE21	1.70	0.54
1:A:428:ASN:O	1:A:429:ARG:CB	2.54	0.54
1:C:253:THR:HG22	1:C:254:ASN:N	2.21	0.54
1:B:169:SER:HA	1:B:172:LEU:HD12	1.90	0.54
1:A:427:LYS:HA	1:A:448:ASP:OD2	2.07	0.54
1:A:266:ILE:HD12	1:A:270:GLN:HB3	1.89	0.54
1:A:386:ILE:HG23	1:A:395:ILE:HD11	1.89	0.54
1:B:505:PHE:HB3	1:C:177:ALA:HB2	1.90	0.54
1:C:309:ILE:HG22	1:C:310:ASP:CG	2.27	0.54
1:A:237:PHE:CD2	1:A:242:GLY:HA2	2.43	0.54
1:C:235:ARG:O	1:C:239:VAL:HG23	2.08	0.54
1:A:318:THR:HG21	1:A:336:ARG:O	2.08	0.54
1:B:221:ILE:O	1:B:225:GLN:HG3	2.08	0.54
1:A:354:GLN:OE1	1:A:356:GLU:HB2	2.08	0.54
1:C:379:VAL:O	1:C:382:CYS:HB2	2.08	0.54
1:B:223:PHE:O	1:B:227:ASN:HB2	2.08	0.53
1:A:318:THR:HG22	1:A:318:THR:O	2.09	0.53
1:B:494:GLN:O	1:B:497:GLU:HB2	2.09	0.53
1:B:309:ILE:HG22	1:B:310:ASP:CG	2.29	0.53
1:B:342:TYR:O	1:B:343:CYS:HB2	2.08	0.53
1:A:292:ILE:CD1	1:A:292:ILE:N	2.62	0.53
1:A:314:TRP:NE1	1:A:342:TYR:HB2	2.24	0.53
1:B:385:ASP:HB3	1:B:388:ASN:HD22	1.73	0.53
1:B:253:THR:HG22	1:B:255:SER:H	1.74	0.52
1:C:308:VAL:O	1:C:309:ILE:HD13	2.08	0.52
1:A:318:THR:HB	1:A:339:ARG:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASN:O	1:A:500:ASN:HB2	2.09	0.52
1:A:97:MET:HA	1:A:97:MET:HE3	1.92	0.52
1:A:198:TYR:O	1:A:202:GLN:HB2	2.09	0.52
1:B:445:LYS:HE3	1:B:445:LYS:HA	1.91	0.52
1:A:152:VAL:HG13	1:A:154:VAL:CB	2.31	0.52
1:C:354:GLN:OE1	1:C:356:GLU:HB2	2.08	0.52
1:C:386:ILE:CG2	1:C:395:ILE:HD11	2.40	0.52
1:A:225:GLN:HE22	1:C:82:GLU:HG2	1.73	0.52
1:B:58:THR:HB	1:C:468:TYR:HD1	1.75	0.52
1:A:291:ILE:C	1:A:292:ILE:HD13	2.30	0.52
1:A:313:CYS:HA	1:A:343:CYS:HA	1.92	0.52
1:C:291:ILE:C	1:C:292:ILE:HD13	2.29	0.51
1:C:253:THR:HG22	1:C:255:SER:H	1.76	0.51
1:C:422:CYS:HB2	1:C:435:PHE:HB2	1.91	0.51
1:A:468:TYR:HD1	1:C:58:THR:HB	1.75	0.51
1:A:232:GLU:OE2	1:C:235:ARG:NH1	2.43	0.51
1:C:321:LEU:O	1:C:333:CYS:HA	2.10	0.51
1:B:148:ILE:O	1:B:149:ALA:HB3	2.10	0.51
1:A:494:GLN:HA	1:A:497:GLU:HG2	1.92	0.51
1:C:428:ASN:O	1:C:429:ARG:HB2	2.10	0.51
1:B:318:THR:HG22	1:B:339:ARG:CZ	2.41	0.51
1:C:264:MET:HE1	1:C:274:MET:SD	2.50	0.51
1:B:379:VAL:O	1:B:382:CYS:HB2	2.11	0.51
1:A:389:PRO:O	1:A:390:LYS:CB	2.50	0.51
1:C:313:CYS:HA	1:C:343:CYS:HA	1.93	0.51
1:A:369:THR:O	1:A:370:MET:C	2.49	0.51
1:A:46:SER:HB2	1:A:48:LEU:HD21	1.92	0.51
1:A:161:GLU:O	1:A:165:ASN:HB2	2.11	0.51
1:B:426:ASN:OD1	1:B:428:ASN:N	2.42	0.51
1:B:314:TRP:NE1	1:B:342:TYR:HB2	2.25	0.51
1:C:426:ASN:OD1	1:C:428:ASN:N	2.40	0.51
1:A:278:VAL:O	1:A:282:ARG:HG3	2.11	0.51
1:C:36:THR:O	1:C:36:THR:HG22	2.11	0.50
1:A:449:THR:HG23	1:A:456:LEU:HD11	1.94	0.50
1:C:321:LEU:HD22	1:C:323:THR:O	2.11	0.50
1:B:291:ILE:C	1:B:292:ILE:HD13	2.30	0.50
1:B:265:PRO:HB2	1:C:429:ARG:HH22	1.76	0.50
1:C:445:LYS:CE	1:C:445:LYS:HA	2.42	0.50
1:C:496:ASN:O	1:C:500:ASN:HB2	2.11	0.50
1:B:159:HIS:NE2	1:B:163:GLU:OE1	2.44	0.50
1:A:338:ASP:HB3	1:A:394:LYS:HZ2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:PHE:CD2	1:C:242:GLY:HA2	2.47	0.49
1:A:474:ILE:HD11	1:C:222:GLU:HB3	1.94	0.49
1:B:50:THR:HB	1:C:457:TYR:HA	1.93	0.49
1:A:169:SER:HA	1:A:172:LEU:HD12	1.94	0.49
1:A:65:LYS:HD2	1:A:65:LYS:H	1.77	0.49
1:B:36:THR:O	1:B:36:THR:HG22	2.11	0.49
1:B:413:ILE:HG22	1:B:414:VAL:N	2.27	0.49
1:A:426:ASN:C	1:A:426:ASN:OD1	2.50	0.49
2:B:1535:NAG:H61	2:B:1536:NAG:H2	1.94	0.49
1:B:82:GLU:HG2	1:C:225:GLN:HE22	1.75	0.49
1:C:254:ASN:ND2	1:C:258:LEU:HD12	2.28	0.49
1:B:496:ASN:O	1:B:500:ASN:HB2	2.12	0.49
1:C:494:GLN:HA	1:C:497:GLU:HG2	1.95	0.49
1:C:36:THR:O	1:C:37:CYS:C	2.51	0.49
1:B:469:VAL:O	1:B:469:VAL:HG12	2.11	0.49
1:A:322:CYS:SG	1:A:417:TYR:CD1	3.06	0.49
1:A:168:LYS:NZ	1:B:516:VAL:O	2.40	0.49
1:B:199:ILE:HD11	1:C:199:ILE:HD11	1.95	0.49
1:B:254:ASN:ND2	1:B:258:LEU:HD12	2.27	0.49
1:B:345:ASN:O	1:B:347:GLY:N	2.47	0.48
1:C:292:ILE:CD1	1:C:292:ILE:N	2.64	0.48
1:C:311:THR:CG2	1:C:344:ASP:HB2	2.43	0.48
1:A:67:ASN:HD22	1:B:476:ASN:HB3	1.79	0.48
1:B:220:VAL:O	1:B:223:PHE:HB3	2.14	0.48
1:B:324:THR:HG22	1:B:325:ASN:ND2	2.29	0.48
1:A:468:TYR:CD1	1:C:58:THR:HB	2.49	0.48
1:A:507:ARG:HB3	1:A:507:ARG:HE	1.36	0.48
1:A:237:PHE:HD2	1:A:242:GLY:HA2	1.77	0.47
1:A:370:MET:HE3	1:A:370:MET:HA	1.96	0.47
1:A:308:VAL:HG13	1:B:455:THR:HA	1.95	0.47
1:A:492:ILE:O	1:A:494:GLN:N	2.47	0.47
1:A:417:TYR:CE2	1:A:438:GLY:HA2	2.50	0.47
1:A:65:LYS:CE	1:B:475:ILE:HA	2.45	0.47
1:C:490:ALA:O	1:C:494:GLN:HB2	2.15	0.47
1:B:57:ILE:HG12	1:C:467:LEU:HB2	1.96	0.47
1:B:208:ASN:HA	1:B:211:SER:HB2	1.95	0.47
1:C:169:SER:HA	1:C:172:LEU:HD12	1.95	0.47
1:C:49:ARG:NH1	1:C:368:ASP:OD1	2.48	0.47
1:C:507:ARG:HE	1:C:507:ARG:HB3	1.48	0.47
1:B:208:ASN:ND2	1:C:481:LEU:N	2.55	0.47
1:A:68:LYS:HB2	1:A:68:LYS:HE2	1.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.54	0.47
1:B:237:PHE:CD2	1:B:242:GLY:HA2	2.49	0.47
1:A:357:THR:HG22	1:A:368:ASP:HB3	1.97	0.47
1:A:28:ILE:H	1:A:28:ILE:HG13	1.49	0.47
1:A:481:LEU:N	1:C:208:ASN:ND2	2.51	0.46
1:B:311:THR:CG2	1:B:344:ASP:HB2	2.44	0.46
1:A:386:ILE:CG2	1:A:395:ILE:HD11	2.44	0.46
1:A:311:THR:CG2	1:A:344:ASP:HB2	2.45	0.46
1:A:378:GLU:OE1	1:A:378:GLU:N	2.48	0.46
1:A:235:ARG:O	1:A:236:GLU:C	2.54	0.46
1:C:97:MET:HB2	1:C:98:GLN:OE1	2.16	0.46
1:B:36:THR:O	1:B:37:CYS:C	2.52	0.46
1:B:444:ASN:C	1:B:445:LYS:O	2.54	0.46
1:B:428:ASN:O	1:B:429:ARG:HB2	2.15	0.46
1:A:404:SER:OG	1:A:405:SER:N	2.47	0.46
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.70	0.46
1:A:324:THR:HG21	1:A:437:ASN:ND2	2.30	0.46
1:A:47:ALA:C	1:A:48:LEU:HD23	2.36	0.46
1:A:477:PHE:CD2	1:A:477:PHE:N	2.82	0.46
1:A:253:THR:CG2	1:A:254:ASN:N	2.78	0.46
1:B:53:TYR:HB2	1:B:305:LEU:HD21	1.98	0.46
1:B:338:ASP:HB3	1:B:394:LYS:HZ1	1.79	0.46
1:A:467:LEU:HB2	1:C:57:ILE:HG12	1.98	0.46
1:A:379:VAL:HG12	1:A:380:ASN:N	2.32	0.45
1:B:195:LEU:HA	1:B:195:LEU:HD23	1.66	0.45
1:B:151:GLY:O	1:B:152:VAL:C	2.54	0.45
1:B:245:THR:HG22	1:B:246:PRO:N	2.32	0.45
1:A:413:ILE:HG22	1:A:414:VAL:N	2.31	0.45
1:C:198:TYR:O	1:C:202:GLN:HB2	2.17	0.45
1:B:494:GLN:HA	1:B:497:GLU:HG2	1.98	0.45
1:C:257:LEU:HD23	1:C:278:VAL:HG12	1.97	0.45
1:A:386:ILE:HA	1:A:393:CYS:SG	2.57	0.45
1:C:445:LYS:HE3	1:C:445:LYS:HA	1.97	0.45
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.66	0.45
1:A:220:VAL:O	1:A:221:ILE:C	2.54	0.45
1:A:36:THR:O	1:A:37:CYS:C	2.54	0.45
1:B:68:LYS:HE2	1:B:68:LYS:HB2	1.76	0.45
1:A:423:THR:O	1:A:450:VAL:HA	2.16	0.45
1:B:65:LYS:O	1:B:65:LYS:HD3	2.16	0.45
1:A:65:LYS:HZ1	1:B:475:ILE:HG22	1.82	0.45
1:B:325:ASN:HD22	1:B:325:ASN:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:HG22	1:C:65:LYS:CE	2.47	0.45
1:C:345:ASN:O	1:C:347:GLY:N	2.50	0.45
1:C:444:ASN:C	1:C:445:LYS:O	2.55	0.44
1:C:326:THR:O	1:C:327:LYS:C	2.55	0.44
1:B:352:PHE:HA	1:B:353:PRO:HD3	1.72	0.44
1:C:53:TYR:HE2	1:C:260:LEU:HD22	1.81	0.44
1:A:484:PRO:O	1:A:485:SER:C	2.56	0.44
1:C:221:ILE:O	1:C:225:GLN:HG3	2.18	0.44
1:A:457:TYR:HA	1:C:50:THR:HB	1.99	0.44
1:A:177:ALA:HB2	1:C:505:PHE:HB3	1.99	0.44
1:A:148:ILE:O	1:A:149:ALA:C	2.56	0.44
1:B:314:TRP:CE2	1:B:342:TYR:HB2	2.52	0.44
1:C:96:LEU:HA	1:C:96:LEU:HD23	1.35	0.44
1:C:413:ILE:HG22	1:C:414:VAL:N	2.32	0.44
1:A:221:ILE:O	1:A:225:GLN:HG3	2.17	0.44
1:A:467:LEU:O	1:C:57:ILE:HA	2.18	0.44
1:A:352:PHE:HA	1:A:353:PRO:HD3	1.73	0.44
1:B:426:ASN:HD21	1:B:428:ASN:ND2	2.15	0.44
1:B:153:ALA:C	1:B:155:SER:N	2.70	0.44
1:A:30:GLU:HA	1:A:40:VAL:O	2.17	0.44
1:C:154:VAL:HG12	1:C:155:SER:O	2.18	0.43
1:B:149:ALA:N	1:C:158:LEU:HD12	2.31	0.43
1:A:148:ILE:O	1:A:148:ILE:HG23	2.18	0.43
1:A:314:TRP:CE2	1:A:342:TYR:HB2	2.53	0.43
1:A:308:VAL:O	1:A:309:ILE:HD13	2.17	0.43
1:A:67:ASN:H	1:B:476:ASN:HD22	1.65	0.43
1:B:423:THR:O	1:B:450:VAL:HA	2.18	0.43
1:C:28:ILE:O	1:C:28:ILE:HD12	2.19	0.43
1:A:313:CYS:HB3	1:A:342:TYR:O	2.18	0.43
1:B:313:CYS:HA	1:B:343:CYS:HA	2.00	0.43
1:C:365:VAL:CG1	1:C:366:PHE:N	2.81	0.43
1:A:245:THR:CG2	1:A:246:PRO:N	2.81	0.43
1:A:245:THR:HG22	1:A:246:PRO:N	2.33	0.43
1:B:492:ILE:O	1:B:494:GLN:N	2.51	0.43
1:B:369:THR:O	1:B:371:ASN:N	2.52	0.43
1:C:26:GLN:O	1:C:27:ASN:CB	2.66	0.43
1:A:513:LEU:C	1:A:515:ASN:H	2.21	0.43
1:A:345:ASN:O	1:A:347:GLY:N	2.52	0.43
1:A:148:ILE:H	1:C:156:LYS:HB3	1.84	0.43
1:B:206:ILE:HA	1:B:209:LYS:HB2	2.01	0.43
1:C:352:PHE:HA	1:C:353:PRO:HD3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:PHE:CD2	1:C:477:PHE:N	2.86	0.43
1:B:245:THR:CG2	1:B:246:PRO:N	2.82	0.43
1:A:53:TYR:OH	1:A:263:ASP:OD2	2.35	0.43
1:B:333:CYS:SG	1:B:401:ASP:HA	2.59	0.43
1:B:240:ASN:HB3	1:B:243:VAL:O	2.19	0.43
1:B:65:LYS:H	1:B:65:LYS:HD2	1.84	0.43
1:A:374:THR:HG21	1:B:404:SER:HB3	2.01	0.43
1:A:211:SER:OG	1:C:210:GLN:NE2	2.49	0.43
1:A:156:LYS:O	1:A:157:VAL:C	2.56	0.43
1:A:151:GLY:C	1:A:152:VAL:CG2	2.87	0.42
1:A:467:LEU:HD23	1:A:467:LEU:HA	1.71	0.42
1:B:285:SER:HB3	1:B:302:GLN:O	2.19	0.42
1:A:154:VAL:O	1:A:155:SER:C	2.58	0.42
1:A:436:SER:O	1:A:437:ASN:C	2.58	0.42
1:B:264:MET:HB2	1:B:264:MET:HE3	1.71	0.42
1:B:369:THR:O	1:B:372:SER:N	2.46	0.42
1:A:455:THR:HA	1:C:307:GLY:O	2.19	0.42
1:A:65:LYS:NZ	1:B:475:ILE:HG22	2.34	0.42
1:B:369:THR:O	1:B:370:MET:C	2.58	0.42
1:B:235:ARG:NH1	1:C:232:GLU:OE2	2.52	0.42
1:B:292:ILE:N	1:B:292:ILE:CD1	2.69	0.42
1:B:67:ASN:HD22	1:C:476:ASN:HB3	1.84	0.42
1:B:513:LEU:C	1:B:515:ASN:H	2.22	0.42
1:B:477:PHE:N	1:B:477:PHE:CD2	2.88	0.42
1:C:388:ASN:HA	1:C:389:PRO:HD2	1.75	0.42
1:A:253:THR:CG2	1:C:92:GLU:OE2	2.61	0.42
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.73	0.42
1:A:240:ASN:HB3	1:A:243:VAL:O	2.20	0.42
1:A:388:ASN:HA	1:A:389:PRO:HD2	1.78	0.42
1:B:352:PHE:CD1	1:B:352:PHE:N	2.87	0.42
1:B:417:TYR:CE2	1:B:438:GLY:HA2	2.55	0.42
1:B:65:LYS:HZ1	1:C:475:ILE:CB	2.33	0.42
1:B:505:PHE:CB	1:C:177:ALA:HB2	2.50	0.42
1:B:28:ILE:O	1:B:28:ILE:HD12	2.20	0.42
1:B:65:LYS:CE	1:C:475:ILE:HA	2.50	0.41
1:C:208:ASN:HA	1:C:211:SER:HB2	2.01	0.41
1:C:467:LEU:HA	1:C:467:LEU:HD23	1.87	0.41
1:A:235:ARG:O	1:A:239:VAL:HG23	2.19	0.41
1:A:206:ILE:HA	1:A:209:LYS:HB2	2.02	0.41
1:C:318:THR:HG22	1:C:339:ARG:CZ	2.50	0.41
1:A:233:ILE:HG23	1:A:251:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:PHE:HD2	1:C:242:GLY:HA2	1.85	0.41
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.74	0.41
1:B:88:ASN:O	1:B:89:ALA:C	2.58	0.41
1:B:264:MET:CE	1:B:274:MET:SD	3.06	0.41
1:B:388:ASN:HA	1:B:389:PRO:HD2	1.79	0.41
1:C:245:THR:CG2	1:C:246:PRO:N	2.83	0.41
1:B:490:ALA:O	1:B:494:GLN:HB2	2.20	0.41
1:C:260:LEU:HA	1:C:260:LEU:HD23	1.75	0.41
1:A:385:ASP:O	1:A:386:ILE:CB	2.52	0.41
1:C:264:MET:HE3	1:C:264:MET:HB2	1.78	0.41
1:C:252:LEU:HD22	1:C:256:GLU:HB2	2.03	0.41
1:A:490:ALA:O	1:A:494:GLN:HB2	2.21	0.41
1:A:369:THR:O	1:A:371:ASN:N	2.53	0.41
1:B:308:VAL:HG22	1:C:455:THR:HG23	2.03	0.41
1:C:220:VAL:O	1:C:223:PHE:HB3	2.21	0.41
1:C:357:THR:HG22	1:C:368:ASP:HB3	2.02	0.41
1:B:395:ILE:CG2	1:B:396:MET:N	2.84	0.41
1:B:280:ILE:O	1:B:281:VAL:C	2.59	0.41
1:A:63:ASN:O	1:B:474:ILE:HG22	2.21	0.41
2:B:1535:NAG:H5	2:B:1535:NAG:N2	2.36	0.41
1:B:449:THR:HG23	1:B:456:LEU:HD11	2.02	0.41
1:A:163:GLU:HG3	1:C:516:VAL:HG13	2.03	0.41
1:A:492:ILE:O	1:A:495:VAL:N	2.54	0.41
1:C:253:THR:CG2	1:C:254:ASN:N	2.84	0.41
1:B:198:TYR:O	1:B:202:GLN:HB2	2.21	0.41
1:B:156:LYS:H	1:B:156:LYS:HG3	1.63	0.41
1:C:365:VAL:HG12	1:C:366:PHE:N	2.36	0.41
1:A:87:LYS:O	1:A:90:VAL:HB	2.21	0.41
1:C:278:VAL:O	1:C:282:ARG:HG3	2.21	0.40
1:C:330:SER:HB3	1:C:331:ASN:H	1.65	0.40
1:A:475:ILE:HA	1:C:65:LYS:CE	2.52	0.40
1:A:388:ASN:C	1:A:389:PRO:O	2.59	0.40
1:B:58:THR:HB	1:C:468:TYR:CD1	2.53	0.40
1:B:47:ALA:C	1:B:48:LEU:HD23	2.41	0.40
1:B:497:GLU:O	1:B:501:GLN:HB2	2.20	0.40
1:B:198:TYR:O	1:B:199:ILE:C	2.59	0.40
1:B:152:VAL:HG13	1:B:155:SER:OG	2.21	0.40
1:A:270:GLN:HB2	1:A:270:GLN:HE21	1.72	0.40
1:A:483:PHE:HA	1:A:484:PRO:HD2	1.87	0.40
1:B:49:ARG:NH1	1:B:368:ASP:OD1	2.54	0.40
1:C:245:THR:HG22	1:C:246:PRO:HD2	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:HD13	1:A:257:LEU:HB2	2.04	0.40
1:A:88:ASN:O	1:A:89:ALA:C	2.59	0.40
1:B:30:GLU:HA	1:B:40:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:SER:CB	1:A:395:ILE:O[2_555]	2.09	0.11

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	435/528 (82%)	370 (85%)	43 (10%)	22 (5%)	2	20
1	B	433/528 (82%)	366 (84%)	49 (11%)	18 (4%)	3	26
1	C	435/528 (82%)	371 (85%)	45 (10%)	19 (4%)	3	24
All	All	1303/1584 (82%)	1107 (85%)	137 (10%)	59 (4%)	3	24

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	149	ALA
1	A	150	SER
1	A	153	ALA
1	A	246	PRO
1	A	356	GLU
1	A	370	MET
1	A	372	SER
1	A	445	LYS

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Mol	Chain	Res	Type
1	A	465	LYS
1	B	68	LYS
1	B	152	VAL
1	B	246	PRO
1	B	355	ALA
1	B	356	GLU
1	B	370	MET
1	B	445	LYS
1	B	465	LYS
1	C	27	ASN
1	C	68	LYS
1	C	153	ALA
1	C	246	PRO
1	C	330	SER
1	C	331	ASN
1	C	356	GLU
1	C	370	MET
1	C	445	LYS
1	C	465	LYS
1	A	148	ILE
1	A	151	GLY
1	A	154	VAL
1	A	346	ALA
1	A	355	ALA
1	B	278	VAL
1	B	331	ASN
1	B	346	ALA
1	B	372	SER
1	B	390	LYS
1	C	73	ASP
1	C	278	VAL
1	C	332	ILE
1	C	346	ALA
1	C	355	ALA
1	C	390	LYS
1	A	73	ASP
1	A	343	CYS
1	A	390	LYS
1	B	73	ASP
1	B	149	ALA
1	B	343	CYS
1	B	484	PRO

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Mol	Chain	Res	Type
1	C	343	CYS
1	A	484	PRO
1	B	151	GLY
1	C	484	PRO
1	A	155	SER
1	A	386	ILE
1	A	388	ASN
1	C	388	ASN

### 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	406/477 (85%)	339 (84%)	67 (16%)	3	13
1	B	405/477 (85%)	329 (81%)	76 (19%)	2	10
1	C	406/477 (85%)	338 (83%)	68 (17%)	3	13
All	All	1217/1431 (85%)	1006 (83%)	211 (17%)	2	12

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	50	THR
1	A	58	THR
1	A	65	LYS
1	A	68	LYS
1	A	80	LYS
1	A	83	LEU
1	A	94	GLN
1	A	97	MET
1	A	98	GLN
1	A	146	SER
1	A	152	VAL
1	A	154	VAL
1	A	156	LYS

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Mol	Chain	Res	Type
1	A	165	ASN
1	A	173	SER
1	A	180	SER
1	A	195	LEU
1	A	206	ILE
1	A	209	LYS
1	A	243	VAL
1	A	244	THR
1	A	252	LEU
1	A	255	SER
1	A	267	THR
1	A	270	GLN
1	A	278	VAL
1	A	288	ILE
1	A	291	ILE
1	A	292	ILE
1	A	295	GLU
1	A	308	VAL
1	A	318	THR
1	A	321	LEU
1	A	323	THR
1	A	324	THR
1	A	354	GLN
1	A	357	THR
1	A	359	LYS
1	A	361	GLN
1	A	364	ARG
1	A	370	MET
1	A	373	LEU
1	A	374	THR
1	A	377	SER
1	A	392	ASP
1	A	400	THR
1	A	403	SER
1	A	404	SER
1	A	420	THR
1	A	425	SER
1	A	428	ASN
1	A	434	THR
1	A	439	CYS
1	A	440	ASP
1	A	443	SER

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Mol	Chain	Res	Type
1	A	444	ASN
1	A	445	LYS
1	A	449	THR
1	A	451	SER
1	A	472	GLU
1	A	475	ILE
1	A	478	TYR
1	A	482	VAL
1	A	492	ILE
1	A	508	LYS
1	A	515	ASN
1	B	26	GLN
1	B	29	THR
1	B	58	THR
1	B	65	LYS
1	B	68	LYS
1	B	80	LYS
1	B	83	LEU
1	B	94	GLN
1	B	97	MET
1	B	98	GLN
1	B	152	VAL
1	B	154	VAL
1	B	155	SER
1	B	158	LEU
1	B	163	GLU
1	B	165	ASN
1	B	173	SER
1	B	180	SER
1	B	195	LEU
1	B	206	ILE
1	B	209	LYS
1	B	229	ARG
1	B	243	VAL
1	B	244	THR
1	B	252	LEU
1	B	255	SER
1	B	267	THR
1	B	278	VAL
1	B	288	ILE
1	B	291	ILE
1	B	292	ILE

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Mol	Chain	Res	Type
1	B	295	GLU
1	B	308	VAL
1	B	311	THR
1	B	318	THR
1	B	321	LEU
1	B	325	ASN
1	B	330	SER
1	B	332	ILE
1	B	338	ASP
1	B	354	GLN
1	B	357	THR
1	B	359	LYS
1	B	364	ARG
1	B	370	MET
1	B	373	LEU
1	B	374	THR
1	B	377	SER
1	B	381	LEU
1	B	392	ASP
1	B	400	THR
1	B	403	SER
1	B	404	SER
1	B	414	VAL
1	B	416	CYS
1	B	420	THR
1	B	425	SER
1	B	428	ASN
1	B	432	ILE
1	B	434	THR
1	B	439	CYS
1	B	440	ASP
1	B	443	SER
1	B	444	ASN
1	B	445	LYS
1	B	449	THR
1	B	451	SER
1	B	472	GLU
1	B	475	ILE
1	B	478	TYR
1	B	481	LEU
1	B	482	VAL
1	B	487	GLU

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Mol	Chain	Res	Type
1	B	492	ILE
1	B	508	LYS
1	B	515	ASN
1	C	29	THR
1	C	58	THR
1	C	61	LEU
1	C	65	LYS
1	C	68	LYS
1	C	80	LYS
1	C	83	LEU
1	C	94	GLN
1	C	97	MET
1	C	98	GLN
1	C	163	GLU
1	C	165	ASN
1	C	173	SER
1	C	180	SER
1	C	195	LEU
1	C	206	ILE
1	C	209	LYS
1	C	229	ARG
1	C	243	VAL
1	C	244	THR
1	C	252	LEU
1	C	255	SER
1	C	267	THR
1	C	270	GLN
1	C	291	ILE
1	C	292	ILE
1	C	295	GLU
1	C	308	VAL
1	C	318	THR
1	C	321	LEU
1	C	323	THR
1	C	324	THR
1	C	325	ASN
1	C	330	SER
1	C	338	ASP
1	C	354	GLN
1	C	357	THR
1	C	359	LYS
1	C	361	GLN

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Mol	Chain	Res	Type
1	C	364	ARG
1	C	370	MET
1	C	373	LEU
1	C	374	THR
1	C	377	SER
1	C	392	ASP
1	C	400	THR
1	C	403	SER
1	C	404	SER
1	C	414	VAL
1	C	420	THR
1	C	425	SER
1	C	428	ASN
1	C	432	ILE
1	C	434	THR
1	C	439	CYS
1	C	440	ASP
1	C	443	SER
1	C	444	ASN
1	C	445	LYS
1	C	449	THR
1	C	451	SER
1	C	472	GLU
1	C	478	TYR
1	C	481	LEU
1	C	482	VAL
1	C	492	ILE
1	C	508	LYS
1	C	515	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	67	ASN
1	A	81	GLN
1	A	159	HIS
1	A	208	ASN
1	A	254	ASN
1	A	270	GLN
1	A	345	ASN
1	A	388	ASN

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Mol	Chain	Res	Type
1	A	437	ASN
1	B	26	GLN
1	B	67	ASN
1	B	81	GLN
1	B	208	ASN
1	B	254	ASN
1	B	270	GLN
1	B	317	HIS
1	B	325	ASN
1	B	388	ASN
1	B	428	ASN
1	C	67	ASN
1	C	81	GLN
1	C	159	HIS
1	C	197	ASN
1	C	208	ASN
1	C	210	GLN
1	C	254	ASN
1	C	270	GLN
1	C	345	ASN
1	C	388	ASN
1	C	428	ASN

### 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
2	NAG	A	1535	1,2	14,14,15	0.95	0	15,19,21	2.46	6 (40%)
2	NAG	A	1536	2	14,14,15	0.94	1 (7%)	15,19,21	2.02	4 (26%)
2	NAG	A	1545	1,2	14,14,15	1.24	1 (7%)	15,19,21	2.07	5 (33%)
2	NAG	A	1546	2	14,14,15	1.01	1 (7%)	15,19,21	3.20	3 (20%)
2	NAG	B	1535	1,2	14,14,15	1.02	1 (7%)	15,19,21	1.88	3 (20%)
2	NAG	B	1536	2	14,14,15	1.39	1 (7%)	15,19,21	1.55	3 (20%)
2	NAG	B	1545	1,2	14,14,15	0.83	1 (7%)	15,19,21	1.74	5 (33%)
2	NAG	B	1546	2	14,14,15	1.57	3 (21%)	15,19,21	2.99	6 (40%)
2	NAG	C	1535	1,2	14,14,15	1.44	1 (7%)	15,19,21	2.76	4 (26%)
2	NAG	C	1536	2	14,14,15	1.04	1 (7%)	15,19,21	1.78	2 (13%)
2	NAG	C	1545	1,2	14,14,15	1.31	1 (7%)	15,19,21	3.24	7 (46%)
2	NAG	C	1546	2	14,14,15	0.96	1 (7%)	15,19,21	2.07	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1535	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1536	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1545	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1546	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1535	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1536	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1545	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1546	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1535	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	1536	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1545	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1546	2	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1536	NAG	C1-C2	2.10	1.55	1.52
2	B	1546	NAG	C3-C2	2.22	1.57	1.52
2	B	1545	NAG	C1-C2	2.37	1.55	1.52
2	A	1545	NAG	C4-C5	2.57	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1535	NAG	C1-C2	2.59	1.56	1.52
2	A	1546	NAG	C1-C2	2.59	1.56	1.52
2	B	1546	NAG	C2-N2	2.59	1.50	1.46
2	C	1546	NAG	C1-C2	2.65	1.56	1.52
2	C	1536	NAG	C1-C2	2.89	1.56	1.52
2	C	1545	NAG	C1-C2	3.82	1.57	1.52
2	C	1535	NAG	C1-C2	4.11	1.58	1.52
2	B	1546	NAG	C1-C2	4.25	1.58	1.52
2	B	1536	NAG	C1-C2	4.35	1.58	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1545	NAG	C4-C3-C2	-3.89	105.17	111.23
2	A	1535	NAG	O7-C7-C8	-2.93	116.68	122.06
2	B	1546	NAG	O7-C7-C8	-2.89	116.75	122.06
2	C	1545	NAG	C3-C4-C5	-2.85	105.22	110.20
2	C	1535	NAG	O7-C7-C8	-2.17	118.08	122.06
2	B	1545	NAG	C3-C2-N2	-2.09	105.56	110.56
2	B	1536	NAG	O7-C7-C8	-2.06	118.29	122.06
2	C	1545	NAG	O3-C3-C4	2.08	115.01	110.34
2	B	1545	NAG	O4-C4-C3	2.11	115.08	110.34
2	A	1535	NAG	C1-O5-C5	2.15	114.97	112.25
2	A	1535	NAG	O5-C5-C6	2.16	112.02	107.35
2	A	1535	NAG	O7-C7-N2	2.19	126.33	121.86
2	B	1535	NAG	C1-O5-C5	2.19	115.03	112.25
2	C	1545	NAG	O4-C4-C5	2.36	115.50	109.24
2	C	1545	NAG	O3-C3-C2	2.37	113.80	109.11
2	A	1546	NAG	O3-C3-C2	2.41	113.90	109.11
2	B	1546	NAG	O7-C7-N2	2.43	126.82	121.86
2	A	1535	NAG	C3-C2-N2	2.50	116.55	110.56
2	B	1545	NAG	O5-C5-C6	2.50	112.77	107.35
2	B	1536	NAG	C4-C3-C2	2.52	115.14	111.23
2	A	1545	NAG	O6-C6-C5	2.58	119.86	111.33
2	C	1536	NAG	C1-O5-C5	2.71	115.69	112.25
2	A	1536	NAG	O5-C5-C6	2.84	113.50	107.35
2	B	1535	NAG	O4-C4-C3	2.84	116.74	110.34
2	B	1545	NAG	C2-N2-C7	2.85	126.70	123.04
2	B	1546	NAG	C3-C4-C5	2.96	115.36	110.20
2	A	1545	NAG	C6-C5-C4	3.06	120.57	113.02
2	A	1545	NAG	C1-O5-C5	3.37	116.53	112.25
2	A	1536	NAG	C1-O5-C5	3.44	116.62	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1545	NAG	O5-C5-C6	3.63	115.22	107.35
2	B	1545	NAG	C1-O5-C5	3.66	116.89	112.25
2	B	1536	NAG	C2-N2-C7	3.75	127.86	123.04
2	A	1545	NAG	O4-C4-C5	3.76	119.21	109.24
2	C	1546	NAG	C2-N2-C7	3.87	128.01	123.04
2	C	1535	NAG	O4-C4-C5	3.88	119.52	109.24
2	A	1536	NAG	C4-C3-C2	4.14	117.66	111.23
2	A	1536	NAG	C3-C4-C5	4.15	117.43	110.20
2	B	1535	NAG	O5-C5-C6	4.69	117.50	107.35
2	C	1536	NAG	C2-N2-C7	4.91	129.35	123.04
2	B	1546	NAG	C4-C3-C2	5.30	119.46	111.23
2	A	1546	NAG	C2-N2-C7	5.34	129.91	123.04
2	C	1546	NAG	C1-O5-C5	5.47	119.19	112.25
2	B	1546	NAG	C2-N2-C7	5.69	130.35	123.04
2	C	1545	NAG	C2-N2-C7	5.78	130.46	123.04
2	C	1535	NAG	C6-C5-C4	5.87	127.49	113.02
2	B	1546	NAG	C1-O5-C5	6.87	120.97	112.25
2	C	1535	NAG	C2-N2-C7	6.97	132.00	123.04
2	A	1535	NAG	C2-N2-C7	7.27	132.38	123.04
2	C	1545	NAG	C1-O5-C5	8.47	123.00	112.25
2	A	1546	NAG	C1-O5-C5	10.42	125.48	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1535	NAG	C1
2	C	1535	NAG	C1
2	B	1535	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1535	NAG	2	0
2	B	1536	NAG	1	0
2	C	1535	NAG	1	0

## 5.6 Ligand geometry

1 ligand is 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	1525	1	14,14,15	2.30	3 (21%)	15,19,21	3.58	7 (46%)

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	1525	1	1/1/5/7	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1525	NAG	C3-C2	3.10	1.59	1.52
3	A	1525	NAG	C2-N2	3.72	1.52	1.46
3	A	1525	NAG	C1-C2	6.27	1.61	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1525	NAG	O7-C7-C8	-2.90	116.74	122.06
3	A	1525	NAG	O7-C7-N2	2.27	126.48	121.86
3	A	1525	NAG	O5-C5-C6	2.72	113.24	107.35
3	A	1525	NAG	O3-C3-C2	2.91	114.87	109.11
3	A	1525	NAG	C6-C5-C4	3.40	121.40	113.02
3	A	1525	NAG	C4-C3-C2	4.07	117.56	111.23
3	A	1525	NAG	C2-N2-C7	11.28	137.53	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1525	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	441/528 (83%)	-0.47	5 (1%)	82 72	22, 47, 89, 116	5 (1%)
1	B	439/528 (83%)	-0.33	7 (1%)	74 62	28, 62, 91, 108	5 (1%)
1	C	439/528 (83%)	-0.27	10 (2%)	64 49	18, 57, 114, 137	5 (1%)
All	All	1319/1584 (83%)	-0.36	22 (1%)	73 60	18, 55, 101, 137	15 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	ASN	4.8
1	B	324	THR	4.5
1	B	325	ASN	4.4
1	B	432	ILE	3.7
1	C	432	ILE	3.5
1	C	446	GLY	3.4
1	C	152	VAL	3.3
1	C	430	GLY	3.3
1	C	429	ARG	3.1
1	A	325	ASN	3.0
1	C	427	LYS	2.8
1	C	445	LYS	2.8
1	C	428	ASN	2.7
1	B	331	ASN	2.7
1	B	26	GLN	2.7
1	C	517	ASN	2.6
1	A	330	SER	2.5
1	C	390	LYS	2.3
1	A	355	ALA	2.3
1	B	355	ALA	2.3
1	B	517	ASN	2.2
1	A	507	ARG	2.1

## 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
2	NAG	C	1536	14/15	0.70	0.62	-	101,103,104,104	0
2	NAG	A	1536	14/15	0.77	0.56	-	106,109,110,110	0
2	NAG	A	1535	14/15	0.89	0.50	-	80,91,95,101	0
2	NAG	C	1546	14/15	0.78	0.45	-	88,93,96,97	0
2	NAG	A	1545	14/15	0.77	0.39	-	63,75,79,85	0
2	NAG	C	1535	14/15	0.83	0.45	-	76,87,91,96	0
2	NAG	B	1546	14/15	0.58	0.49	-	93,95,98,99	0
2	NAG	C	1545	14/15	0.83	0.32	-	67,80,84,87	0
2	NAG	B	1536	14/15	0.72	0.54	-	104,106,109,110	0
2	NAG	B	1545	14/15	0.87	0.28	-	66,78,83,86	0
2	NAG	A	1546	14/15	0.83	0.51	-	90,93,95,96	0
2	NAG	B	1535	14/15	0.77	0.46	-	78,87,92,99	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
3	NAG	A	1525	14/15	0.74	0.43	-	51,61,64,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.