



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2016 – 02:26 PM EDT

PDB ID : 5FOB  
Title : Crystal Structure of Human Complement C3b in complex with Smallpox Inhibitor of Complement (SPICE)  
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.  
Deposited on : 2015-11-18  
Resolution : 2.60 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
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) : rb-20027674

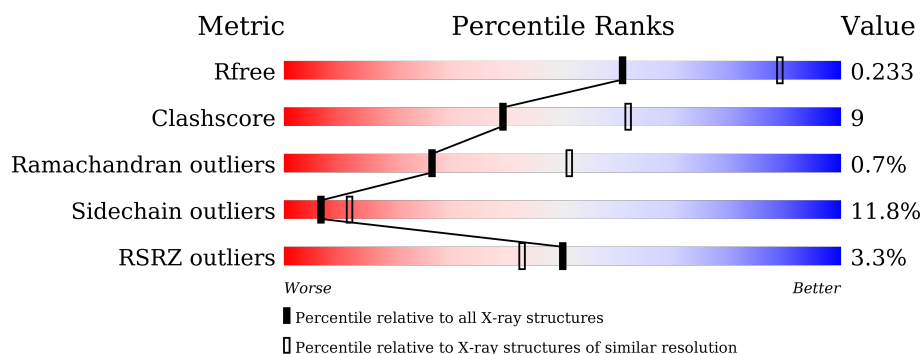
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	645	<div> <div>0%</div> <div>70%</div> <div>25%</div> <div>.</div> </div>
2	B	915	<div> <div>2%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
3	C	245	<div> <div>14%</div> <div>64%</div> <div>27%</div> <div>7%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	A	1062	-	-	-	X
4	NAG	A	1063	X	-	-	-
5	CL	B	2682	-	-	-	X
6	GOL	A	1668	-	-	-	X
6	GOL	A	1671	-	-	-	X
6	GOL	A	1672	-	-	-	X
6	GOL	A	1673	-	-	-	X
6	GOL	A	1674	-	-	-	X
6	GOL	A	1675	-	-	-	X
6	GOL	B	2672	-	-	-	X
6	GOL	C	1260	-	-	-	X
7	NA	B	2677	-	-	-	X
8	IOD	B	2678	-	-	X	-
8	IOD	B	2679	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14474 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 C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	3	0
			5011	3193	846	956	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	902	Total	C	N	O	S	0	0	0
			7199	4563	1210	1388	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called SMALLPOX INHIBITOR OF COMPLEMENT SPICE, D15L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	2	0
			1822	1138	309	356	19			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	C	2	Total	Cl	0	0
			2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	4	Total I 4 4	0	0
8	A	3	Total I 3 3	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

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

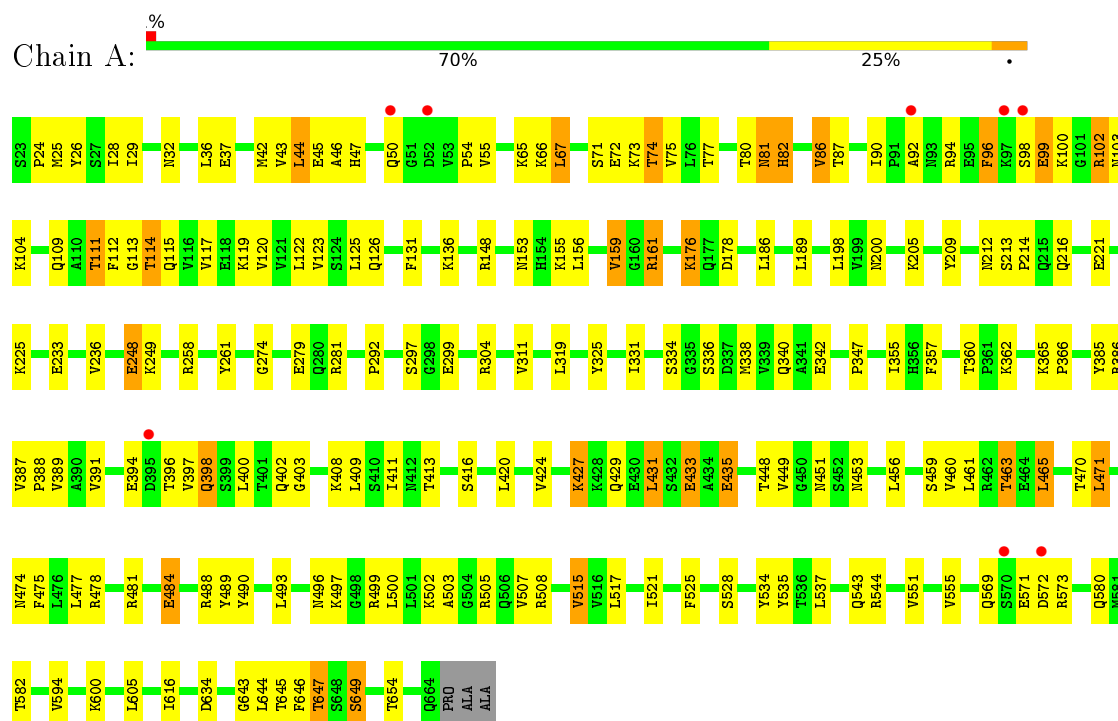
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	98	Total O 98 98	0	0
10	B	92	Total O 92 92	0	0
10	C	17	Total O 17 17	0	0

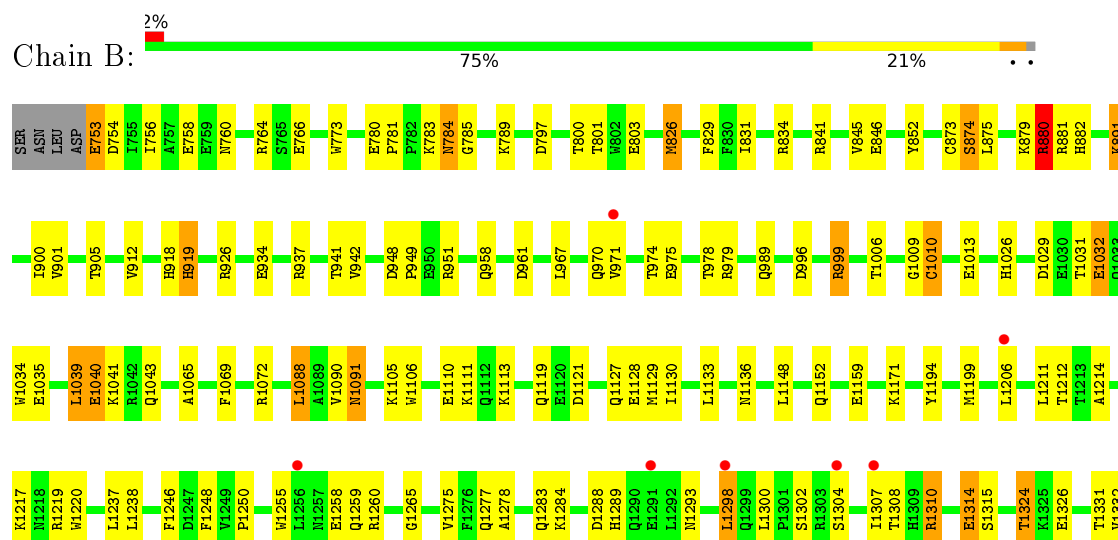
### 3 Residue-property plots

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

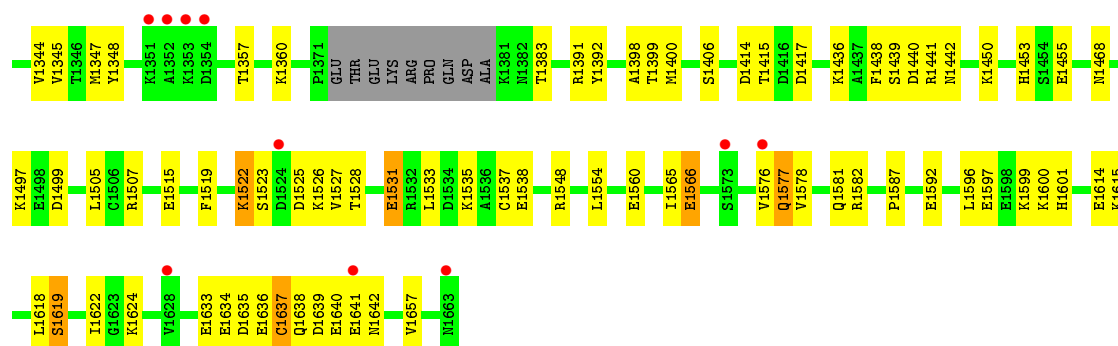
#### • Molecule 1: COMPLEMENT C3 BETA CHAIN



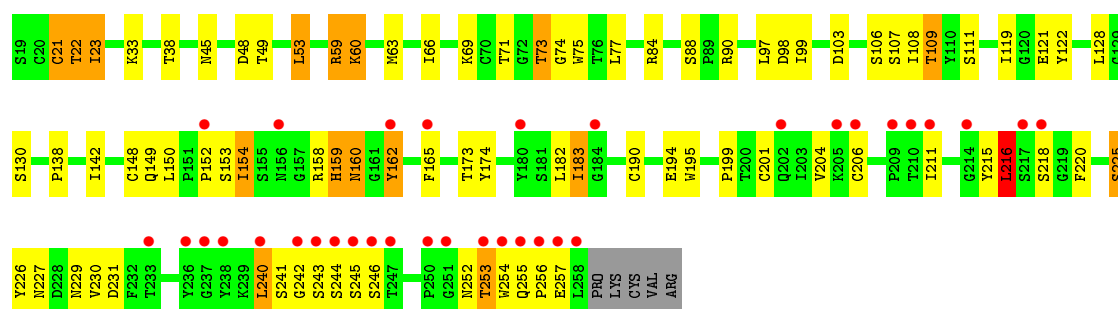
#### • Molecule 2: COMPLEMENT C3B ALPHA' CHAIN







● Molecule 3: SMALLPOX INHIBITOR OF COMPLEMENT SPICE, D15L



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.89Å 83.31Å 127.38Å 75.03° 76.20° 68.50°	Depositor
Resolution (Å)	42.36 – 2.60 42.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.36-2.60) 90.8 (42.36-2.60)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.198 , 0.230 0.200 , 0.233	Depositor DCC
$R_{free}$ test set	2248 reflections (2.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

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

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

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	0.26	0/5121	0.47	0/6958
2	B	0.26	0/7343	0.47	2/9943 (0.0%)
3	C	0.29	0/1877	0.54	0/2550
All	All	0.27	0/14341	0.48	2/19451 (0.0%)

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
4	A	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1009	GLY	C-N-CA	5.79	136.18	121.70
2	B	880	ARG	NE-CZ-NH1	-5.03	117.79	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1063	NAG	C1

There are no planarity outliers.

## 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	5011	0	5068	98	0
2	B	7199	0	7116	116	1
3	C	1822	0	1703	45	1
4	A	49	0	43	3	0
5	A	1	0	0	0	0
5	B	2	0	0	1	0
5	C	2	0	0	0	0
6	A	60	0	80	11	0
6	B	72	0	96	13	0
6	C	12	0	16	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	3	0	0	1	0
8	B	4	0	0	8	0
9	B	28	0	25	0	0
10	A	98	0	0	1	0
10	B	92	0	0	4	0
10	C	17	0	0	0	0
All	All	14474	0	14147	254	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 9.

All (254) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:ASN:ND2	8:B:2679:IOD:I	2.35	1.25
8:B:2679:IOD:I	10:B:2007:HOH:O	2.24	1.25
2:B:1032:GLU:HG3	8:B:2678:IOD:I	2.26	1.04
2:B:1010:CYS:HB3	2:B:1013:GLU:HB2	1.43	0.99
2:B:1105:LYS:HD2	8:B:2681:IOD:I	2.45	0.87
2:B:1032:GLU:CG	8:B:2678:IOD:I	3.03	0.77
3:C:49:THR:HG22	3:C:69:LYS:HG3	1.69	0.75
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.68	0.73
1:A:448:THR:HG21	1:A:453:ASN:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:NZ	1:A:460:VAL:O	2.21	0.72
3:C:99:ILE:HA	3:C:108:ILE:HG22	1.73	0.70
3:C:225:SER:OG	3:C:226:TYR:N	2.22	0.69
2:B:873:CYS:HB2	2:B:901:VAL:HB	1.74	0.69
3:C:98:ASP:HB3	3:C:109:THR:HG23	1.74	0.68
1:A:471:LEU:HB3	1:A:521:ILE:HD11	1.77	0.67
2:B:1211:LEU:O	2:B:1217:LYS:NZ	2.25	0.67
2:B:875:LEU:O	2:B:880:ARG:NH1	2.29	0.66
2:B:766:GLU:OE2	3:C:90:ARG:NH1	2.30	0.65
2:B:1635:ASP:OD1	2:B:1636:GLU:N	2.29	0.65
1:A:571:GLU:HG3	1:A:573:ARG:H	1.62	0.64
1:A:99:GLU:HA	1:A:100:LYS:C	2.18	0.64
2:B:1258:GLU:OE2	2:B:1260:ARG:NH2	2.31	0.64
1:A:42:MET:HB3	1:A:86:VAL:HG23	1.79	0.63
1:A:366:PRO:HB3	1:A:416:SER:H	1.62	0.63
1:A:304:ARG:H	6:A:1668:GOL:H2	1.64	0.63
3:C:206:CYS:HB3	3:C:254:TRP:CZ2	2.34	0.63
1:A:176:LYS:NZ	1:A:178:ASP:OD2	2.28	0.63
2:B:941:THR:HG23	2:B:1345:VAL:HG22	1.80	0.63
2:B:1072:ARG:NH1	6:B:2668:GOL:O3	2.31	0.63
2:B:1391:ARG:NH1	2:B:1453:HIS:O	2.32	0.62
1:A:225:LYS:HG3	6:A:1669:GOL:H2	1.82	0.62
2:B:996:ASP:HB3	2:B:999:ARG:HG3	1.82	0.62
3:C:149:GLN:HG2	3:C:150:LEU:H	1.65	0.61
2:B:1528:THR:HG23	2:B:1531:GLU:H	1.66	0.61
2:B:1499:ASP:N	2:B:1499:ASP:OD1	2.31	0.60
4:A:1063:NAG:H62	4:A:1064:NAG:N2	2.17	0.60
1:A:569:GLN:HG3	1:A:582:THR:H	1.68	0.59
3:C:230:VAL:HG23	3:C:246:SER:HB2	1.84	0.59
1:A:475:PHE:HE1	1:A:517:LEU:HB3	1.67	0.59
2:B:1152:GLN:OE1	6:B:2666:GOL:O3	2.20	0.59
1:A:427:LYS:HG3	6:A:1667:GOL:H32	1.85	0.59
3:C:22:THR:OG1	3:C:23:ILE:N	2.35	0.59
1:A:388:PRO:HB2	1:A:427:LYS:HB3	1.85	0.58
3:C:244:SER:OG	3:C:245:SER:N	2.35	0.58
2:B:1091:ASN:N	2:B:1091:ASN:OD1	2.34	0.58
3:C:227:ASN:ND2	3:C:227:ASN:O	2.36	0.58
1:A:120:VAL:HG11	2:B:1039:LEU:HD12	1.86	0.58
2:B:1505:LEU:HD12	6:B:2674:GOL:H31	1.86	0.58
2:B:758:GLU:OE1	2:B:881:ARG:NH2	2.36	0.58
2:B:1127:GLN:O	2:B:1130:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:OE2	1:A:258:ARG:NH1	2.38	0.57
1:A:37:GLU:OE2	1:A:212:ASN:ND2	2.27	0.57
1:A:25:MET:SD	1:A:544:ARG:HG2	2.44	0.57
2:B:971:VAL:O	2:B:974:THR:OG1	2.18	0.57
2:B:1566:GLU:OE2	2:B:1601:HIS:NE2	2.38	0.57
3:C:71:THR:HG23	3:C:73:THR:H	1.68	0.57
3:C:206:CYS:HB3	3:C:254:TRP:HZ2	1.69	0.56
2:B:1641:GLU:N	2:B:1642:ASN:HA	2.19	0.56
3:C:77:LEU:HB2	6:C:1260:GOL:H32	1.87	0.56
2:B:1414:ASP:HB3	2:B:1417:ASP:HB2	1.87	0.56
1:A:32:ASN:HA	1:A:645:THR:HG23	1.88	0.56
1:A:45:GLU:OE1	1:A:534:TYR:OH	2.15	0.56
2:B:989:GLN:H	2:B:1289:HIS:HA	1.72	0.55
2:B:1515:GLU:H	6:B:2674:GOL:H2	1.71	0.55
1:A:496:ASN:OD1	1:A:497:LYS:HE2	2.06	0.55
2:B:1633:GLU:O	2:B:1637:CYS:N	2.35	0.55
2:B:1587:PRO:HG2	6:B:2674:GOL:H12	1.88	0.54
2:B:1128:GLU:HG2	2:B:1129:MET:N	2.21	0.54
8:B:2679:IOD:I	3:C:60:LYS:HE2	2.78	0.54
3:C:159:HIS:O	3:C:160:ASN:ND2	2.38	0.54
1:A:28:ILE:HG22	1:A:44:LEU:HD23	1.88	0.54
2:B:1113:LYS:NZ	2:B:1119:GLN:OE1	2.41	0.54
1:A:44:LEU:HD13	1:A:55:VAL:HG21	1.89	0.54
2:B:1597:GLU:HB2	2:B:1600:LYS:HG3	1.90	0.54
1:A:119:LYS:HD3	1:A:647:THR:OG1	2.09	0.53
3:C:215:TYR:O	3:C:216:LEU:HB2	2.07	0.53
1:A:82:HIS:HE1	1:A:488:ARG:HH22	1.57	0.53
3:C:182:LEU:HD12	3:C:201:CYS:HB3	1.90	0.53
2:B:934:GLU:H	2:B:934:GLU:CD	2.11	0.53
1:A:646:PHE:H	1:A:654:THR:HG23	1.75	0.52
3:C:154:ILE:HG13	3:C:199:PRO:O	2.10	0.52
2:B:1148:LEU:O	2:B:1152:GLN:HG2	2.09	0.52
2:B:1581:GLN:O	2:B:1582:ARG:NH1	2.40	0.52
2:B:1031:THR:HG22	2:B:1283:GLN:HG3	1.92	0.52
2:B:1399:THR:OG1	2:B:1400:MET:N	2.43	0.52
2:B:978:THR:HB	2:B:1324:THR:HG23	1.92	0.52
2:B:754:ASP:OD2	2:B:918:HIS:ND1	2.28	0.52
2:B:875:LEU:HD12	2:B:882:HIS:NE2	2.24	0.52
1:A:311:VAL:HG11	1:A:319:LEU:HD21	1.91	0.52
5:B:2676:CL:CL	10:B:2001:HOH:O	2.56	0.52
2:B:1032:GLU:HA	8:B:2678:IOD:I	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:HIS:HA	3:C:174:TYR:HA	1.91	0.51
3:C:45:ASN:N	3:C:48:ASP:OD2	2.37	0.51
1:A:503:ALA:HB3	4:A:1062:FUC:H5	1.93	0.51
2:B:1442:ASN:N	2:B:1442:ASN:OD1	2.40	0.51
1:A:433:GLU:OE2	6:A:1667:GOL:O3	2.28	0.51
1:A:54:PRO:HA	1:A:75:VAL:HG22	1.93	0.51
1:A:528:SER:HA	1:A:555:VAL:HG23	1.93	0.51
2:B:874:SER:HB2	2:B:900:ILE:HG22	1.92	0.51
1:A:37:GLU:HG2	1:A:92:ALA:HA	1.93	0.51
2:B:1035:GLU:HA	2:B:1039:LEU:CD2	2.41	0.51
3:C:73:THR:OG1	3:C:73:THR:O	2.22	0.51
2:B:1522:LYS:HB2	2:B:1523:SER:HB3	1.94	0.50
3:C:159:HIS:ND1	3:C:160:ASN:O	2.45	0.50
1:A:221:GLU:OE2	6:A:1673:GOL:O1	2.30	0.50
1:A:391:VAL:HG23	1:A:409:LEU:HD13	1.94	0.50
2:B:891:LYS:HB3	6:B:2664:GOL:H31	1.92	0.50
1:A:248:GLU:O	6:A:1668:GOL:O2	2.26	0.49
1:A:580:GLN:HG2	6:A:1671:GOL:H2	1.95	0.49
1:A:355:ILE:HD13	1:A:424:VAL:HG12	1.94	0.49
1:A:396:THR:OG1	1:A:397:VAL:N	2.45	0.49
2:B:1217:LYS:HE3	2:B:1248:PHE:CZ	2.46	0.49
1:A:46:ALA:O	1:A:82:HIS:HD2	1.95	0.48
1:A:43:VAL:HG22	4:A:1062:FUC:H62	1.94	0.48
2:B:766:GLU:OE2	3:C:90:ARG:HG2	2.13	0.48
1:A:261:TYR:HB2	2:B:826:MET:HG2	1.95	0.48
1:A:104:LYS:HA	1:A:104:LYS:HD3	1.59	0.48
1:A:500:LEU:HD21	1:A:644:LEU:HD21	1.96	0.48
2:B:874:SER:OG	2:B:875:LEU:N	2.46	0.48
1:A:221:GLU:HG3	6:A:1673:GOL:H32	1.96	0.48
2:B:1237:LEU:HD23	2:B:1278:ALA:HB1	1.95	0.48
2:B:948:ASP:OD2	2:B:951:ARG:NH2	2.46	0.48
1:A:391:VAL:HB	1:A:397:VAL:HG11	1.95	0.48
3:C:121:GLU:HG3	3:C:138:PRO:HB2	1.94	0.48
1:A:36:LEU:HG	1:A:125:LEU:HA	1.95	0.48
2:B:800:THR:OG1	2:B:801:THR:N	2.46	0.48
1:A:429:GLN:H	1:A:429:GLN:CD	2.16	0.47
3:C:149:GLN:HG2	3:C:150:LEU:N	2.26	0.47
3:C:33:LYS:HA	3:C:53:LEU:HD22	1.97	0.47
1:A:357:PHE:O	1:A:362:LYS:NZ	2.47	0.47
2:B:971:VAL:HB	2:B:974:THR:HG21	1.95	0.47
1:A:481:ARG:HA	1:A:484:GLU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1507:ARG:NE	2:B:1560:GLU:OE2	2.42	0.47
3:C:152:PRO:O	3:C:174:TYR:OH	2.17	0.47
2:B:1111:LYS:NZ	2:B:1121:ASP:OD2	2.37	0.47
2:B:1194:TYR:CE1	2:B:1238:LEU:HB3	2.50	0.47
2:B:1308:THR:HG22	2:B:1310:ARG:HD3	1.97	0.47
2:B:949:PRO:HA	2:B:958:GLN:HB2	1.97	0.47
2:B:1246:PHE:O	2:B:1250:PRO:HD3	2.14	0.46
2:B:784:ASN:HB2	2:B:785:GLY:H	1.48	0.46
3:C:253:THR:C	3:C:254:TRP:HD1	2.19	0.46
2:B:1217:LYS:HE3	2:B:1248:PHE:HZ	1.79	0.46
2:B:974:THR:HA	6:B:2667:GOL:H11	1.98	0.46
1:A:334:SER:N	6:A:1674:GOL:O1	2.48	0.46
1:A:402:GLN:OE1	1:A:463:THR:HA	2.16	0.46
2:B:967:LEU:HB3	2:B:970:GLN:HB2	1.98	0.46
1:A:159:VAL:HG13	1:A:161:ARG:HG3	1.97	0.46
1:A:131:PHE:CZ	1:A:616:ILE:HG23	2.50	0.46
1:A:281:ARG:NH1	1:A:342:GLU:OE2	2.40	0.45
1:A:481:ARG:NH1	1:A:484:GLU:HG3	2.31	0.45
3:C:103:ASP:OD1	3:C:106:SER:OG	2.31	0.45
1:A:113:GLY:O	1:A:114:THR:HG22	2.17	0.45
1:A:292:PRO:HD2	6:A:1675:GOL:H12	1.98	0.45
2:B:1310:ARG:HG3	3:C:162:TYR:CD1	2.51	0.45
2:B:846:GLU:OE2	2:B:1406:SER:OG	2.24	0.45
1:A:385:TYR:CD1	1:A:403:GLY:HA2	2.52	0.45
1:A:148:ARG:CZ	1:A:594:VAL:HB	2.46	0.45
1:A:81:ASN:OD1	1:A:81:ASN:N	2.47	0.45
1:A:26:TYR:CD2	1:A:115:GLN:HG2	2.52	0.45
1:A:490:TYR:HE2	1:A:515:VAL:HG21	1.82	0.45
1:A:32:ASN:HB2	1:A:643:GLY:C	2.37	0.45
1:A:122:LEU:HD12	1:A:123:VAL:H	1.81	0.45
2:B:926:ARG:NH1	10:B:2009:HOH:O	2.49	0.45
1:A:496:ASN:ND2	1:A:525:PHE:HA	2.32	0.45
3:C:241:SER:HA	3:C:242:GLY:HA2	1.64	0.45
2:B:1029:ASP:OD1	2:B:1034:TRP:NE1	2.43	0.45
1:A:198:LEU:O	2:B:979:ARG:NH2	2.50	0.45
2:B:1040:GLU:H	2:B:1040:GLU:HG3	1.43	0.44
1:A:102:ARG:HA	1:A:103:ASN:HA	1.67	0.44
1:A:66:LYS:HB2	1:A:67:LEU:HD23	1.99	0.44
2:B:1026:HIS:CG	2:B:1088:LEU:HD21	2.53	0.44
1:A:102:ARG:HB3	1:A:103:ASN:CG	2.38	0.44
2:B:1238:LEU:HD11	2:B:1277:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:231:ASP:OD1	3:C:245:SER:OG	2.30	0.44
3:C:75:TRP:HB3	6:C:1260:GOL:H12	2.00	0.44
1:A:148:ARG:HG3	2:B:773:TRP:CZ2	2.52	0.44
1:A:484:GLU:CG	1:A:508:ARG:HH22	2.31	0.44
2:B:1577:GLN:HB3	2:B:1578:VAL:H	1.53	0.44
1:A:331:ILE:HG12	1:A:338:MET:HE2	2.01	0.43
2:B:1069:PHE:CD2	6:B:2668:GOL:H31	2.54	0.43
2:B:961:ASP:OD1	2:B:1331:THR:OG1	2.35	0.43
2:B:841:ARG:HD3	2:B:905:THR:HG23	2.00	0.43
2:B:999:ARG:NH2	10:B:2044:HOH:O	2.50	0.43
3:C:183:ILE:HA	3:C:183:ILE:HD13	1.73	0.43
2:B:753:GLU:HB2	2:B:754:ASP:H	1.53	0.43
2:B:829:PHE:HA	2:B:852:TYR:O	2.18	0.43
2:B:1035:GLU:HA	2:B:1039:LEU:HD21	2.01	0.43
2:B:1152:GLN:OE1	6:B:2666:GOL:O2	2.31	0.43
2:B:1214:ALA:HB2	2:B:1220:TRP:CZ2	2.54	0.43
2:B:1441:ARG:HD2	2:B:1441:ARG:HA	1.77	0.43
2:B:1034:TRP:HB2	8:B:2678:IOD:I	2.88	0.43
3:C:59:ARG:HG2	3:C:84:ARG:HG2	1.99	0.43
1:A:94:ARG:HA	1:A:96:PHE:HE1	1.84	0.43
2:B:1436:LYS:HD2	2:B:1436:LYS:HA	1.80	0.43
2:B:756:ILE:O	6:B:2665:GOL:O1	2.30	0.43
1:A:431:LEU:HG	1:A:435:GLU:HB3	2.00	0.43
1:A:55:VAL:HA	1:A:111:THR:O	2.19	0.43
2:B:1199:MET:HG2	6:B:2666:GOL:O2	2.19	0.43
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.89	0.43
2:B:1199:MET:HB2	2:B:1199:MET:HE3	1.82	0.43
1:A:136:LYS:HB2	1:A:136:LYS:HE3	1.76	0.43
1:A:488:ARG:HG3	1:A:489:TYR:CD2	2.54	0.43
2:B:875:LEU:HD23	2:B:875:LEU:HA	1.65	0.43
2:B:918:HIS:C	2:B:919:HIS:HD1	2.18	0.43
1:A:459:SER:OG	1:A:474:ASN:HB2	2.19	0.42
3:C:190:CYS:HB2	3:C:195:TRP:CZ3	2.53	0.42
1:A:98:SER:O	1:A:99:GLU:HB2	2.19	0.42
2:B:1111:LYS:HA	2:B:1111:LYS:HD3	1.81	0.42
1:A:24:PRO:HA	1:A:47:HIS:O	2.20	0.42
1:A:96:PHE:CD1	1:A:96:PHE:N	2.85	0.42
2:B:942:VAL:N	2:B:1344:VAL:O	2.51	0.42
1:A:299:GLU:H	6:A:1675:GOL:H31	1.84	0.42
3:C:218:SER:O	3:C:230:VAL:HG12	2.20	0.42
1:A:29:ILE:HA	1:A:645:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1219:ARG:HD2	2:B:1255:TRP:CE2	2.55	0.42
2:B:1565:ILE:HD13	2:B:1576:VAL:HG11	2.00	0.42
3:C:230:VAL:CG2	3:C:246:SER:HB2	2.49	0.42
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.55	0.42
2:B:891:LYS:HD2	6:B:2664:GOL:H31	2.00	0.42
1:A:386:ARG:HH11	1:A:400:LEU:HD23	1.83	0.42
1:A:55:VAL:HG22	1:A:74:THR:O	2.19	0.42
3:C:142:ILE:HA	3:C:142:ILE:HD13	1.85	0.42
2:B:1314:GLU:OE1	2:B:1315:SER:N	2.52	0.42
2:B:1618:LEU:HD12	2:B:1619:SER:N	2.35	0.42
3:C:154:ILE:HA	3:C:154:ILE:HD13	1.62	0.42
1:A:26:TYR:H	1:A:649:SER:HG	1.68	0.41
2:B:1065:ALA:HB2	2:B:1106:TRP:CD2	2.55	0.41
2:B:1519:PHE:HB2	2:B:1622:ILE:HG22	2.01	0.41
2:B:1298:LEU:HB3	2:B:1332:VAL:HG22	2.02	0.41
1:A:102:ARG:HB3	1:A:103:ASN:ND2	2.35	0.41
2:B:1326:GLU:OE1	2:B:1326:GLU:N	2.46	0.41
2:B:1615:LYS:HE2	2:B:1618:LEU:HB3	2.01	0.41
1:A:136:LYS:NZ	10:A:2013:HOH:O	2.52	0.41
1:A:456:LEU:HB2	1:A:535:TYR:HE2	1.85	0.41
2:B:1265:GLY:N	6:B:2675:GOL:O2	2.53	0.41
2:B:780:GLU:HA	2:B:781:PRO:HD3	1.96	0.41
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.88	0.41
2:B:879:LYS:H	2:B:879:LYS:HG2	1.66	0.41
1:A:209:TYR:CD2	1:A:214:PRO:HA	2.55	0.41
2:B:1523:SER:HB2	2:B:1525:ASP:OD1	2.21	0.41
2:B:1535:LYS:O	2:B:1538:GLU:HB2	2.20	0.41
1:A:153:ASN:ND2	8:A:1677:IOD:I	3.24	0.41
2:B:1106:TRP:O	2:B:1110:GLU:HB2	2.21	0.41
2:B:831:ILE:HD13	2:B:912:VAL:HG12	2.03	0.40
3:C:21:CYS:HB2	3:C:22:THR:H	1.57	0.40
1:A:82:HIS:CD2	1:A:505:ARG:HH12	2.38	0.40
3:C:71:THR:HG22	3:C:74:GLY:O	2.21	0.40
3:C:71:THR:HG23	3:C:73:THR:N	2.34	0.40
1:A:398:GLN:HE22	1:A:400:LEU:HD13	1.86	0.40
2:B:1439:SER:HB2	2:B:1440:ASP:OD1	2.21	0.40
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.57	0.40
1:A:336:SER:HB2	2:B:834:ARG:HG3	2.04	0.40
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.92	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)
2:B:1600:LYS:NZ	3:C:73:THR:O[1_545]	2.09	0.11

## 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	643/645 (100%)	625 (97%)	15 (2%)	3 (0%)	34	60
2	B	898/915 (98%)	875 (97%)	22 (2%)	1 (0%)	56	81
3	C	240/245 (98%)	218 (91%)	14 (6%)	8 (3%)	5	7
All	All	1781/1805 (99%)	1718 (96%)	51 (3%)	12 (1%)	26	51

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	21	CYS
3	C	240	LEU
3	C	256	PRO
1	A	82	HIS
3	C	22	THR
3	C	160	ASN
1	A	99	GLU
2	B	1010	CYS
3	C	257	GLU
3	C	216	LEU
3	C	255	GLN
1	A	102	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/567 (100%)	491 (87%)	75 (13%)	5	8
2	B	797/810 (98%)	722 (91%)	75 (9%)	11	20
3	C	205/215 (95%)	169 (82%)	36 (18%)	2	3
All	All	1568/1592 (98%)	1382 (88%)	186 (12%)	6	11

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	50	GLN
1	A	65	LYS
1	A	67	LEU
1	A	71	SER
1	A	72	GLU
1	A	73	LYS
1	A	74	THR
1	A	77	THR
1	A	80	THR
1	A	81	ASN
1	A	86	VAL
1	A	87	THR
1	A	90	ILE
1	A	96	PHE
1	A	109	GLN
1	A	111	THR
1	A	112	PHE
1	A	114	THR
1	A	117	VAL
1	A	126	GLN
1	A	155	LYS
1	A	159	VAL
1	A	161	ARG
1	A	176	LYS
1	A	186	LEU
1	A	189	LEU
1	A	200	ASN
1	A	205	LYS
1	A	213	SER
1	A	216	GLN

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Mol	Chain	Res	Type
1	A	236	VAL
1	A	248	GLU
1	A	249	LYS
1	A	279	GLU
1	A	297	SER
1	A	340[A]	GLN
1	A	340[B]	GLN
1	A	347	PRO
1	A	360	THR
1	A	365	LYS
1	A	389	VAL
1	A	394	GLU
1	A	398	GLN
1	A	411	ILE
1	A	413	THR
1	A	420	LEU
1	A	427	LYS
1	A	431	LEU
1	A	433	GLU
1	A	435	GLU
1	A	449	VAL
1	A	451	ASN
1	A	461	LEU
1	A	463	THR
1	A	465	LEU
1	A	470	THR
1	A	471	LEU
1	A	477	LEU
1	A	478	ARG
1	A	484	GLU
1	A	493	LEU
1	A	499	ARG
1	A	502	LYS
1	A	507	VAL
1	A	515	VAL
1	A	537	LEU
1	A	543	GLN
1	A	551	VAL
1	A	572	ASP
1	A	600	LYS
1	A	605	LEU
1	A	634	ASP

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Mol	Chain	Res	Type
1	A	647	THR
1	A	649	SER
2	B	753	GLU
2	B	783	LYS
2	B	784	ASN
2	B	789	LYS
2	B	803	GLU
2	B	826	MET
2	B	845	VAL
2	B	874	SER
2	B	880	ARG
2	B	891	LYS
2	B	919	HIS
2	B	937	ARG
2	B	975	GLU
2	B	999	ARG
2	B	1006	THR
2	B	1032	GLU
2	B	1039	LEU
2	B	1040	GLU
2	B	1041	LYS
2	B	1043	GLN
2	B	1088	LEU
2	B	1090	VAL
2	B	1091	ASN
2	B	1133	LEU
2	B	1136	ASN
2	B	1159	GLU
2	B	1171	LYS
2	B	1206	LEU
2	B	1212	THR
2	B	1259	GLN
2	B	1275	VAL
2	B	1284	LYS
2	B	1288	ASP
2	B	1293	ASN
2	B	1298	LEU
2	B	1300	LEU
2	B	1302	SER
2	B	1304	SER
2	B	1307	ILE
2	B	1310	ARG

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Mol	Chain	Res	Type
2	B	1314	GLU
2	B	1324	THR
2	B	1347	MET
2	B	1348	TYR
2	B	1357	THR
2	B	1360	LYS
2	B	1383	THR
2	B	1415	THR
2	B	1438	PHE
2	B	1450	LYS
2	B	1455	GLU
2	B	1468	ASN
2	B	1497	LYS
2	B	1522	LYS
2	B	1526	LYS
2	B	1527	VAL
2	B	1531	GLU
2	B	1533	LEU
2	B	1537	CYS
2	B	1548	ARG
2	B	1554	LEU
2	B	1566	GLU
2	B	1577	GLN
2	B	1592	GLU
2	B	1596	LEU
2	B	1599	LYS
2	B	1614	GLU
2	B	1619	SER
2	B	1624	LYS
2	B	1634	GLU
2	B	1637	CYS
2	B	1638	GLN
2	B	1639	ASP
2	B	1640	GLU
2	B	1657	VAL
3	C	23	ILE
3	C	38	THR
3	C	53	LEU
3	C	59	ARG
3	C	60	LYS
3	C	66	ILE
3	C	73	THR

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Mol	Chain	Res	Type
3	C	88	SER
3	C	97	LEU
3	C	107	SER
3	C	109	THR
3	C	111	SER
3	C	119	ILE
3	C	122	TYR
3	C	128	LEU
3	C	130	SER
3	C	148	CYS
3	C	153	SER
3	C	154	ILE
3	C	158	ARG
3	C	159	HIS
3	C	162	TYR
3	C	165	PHE
3	C	173	THR
3	C	183	ILE
3	C	194	GLU
3	C	204	VAL
3	C	211	ILE
3	C	216	LEU
3	C	220	PHE
3	C	225	SER
3	C	229	ASN
3	C	240	LEU
3	C	243	SER
3	C	252	ASN
3	C	253	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	82	HIS
1	A	216	GLN
1	A	580	GLN
2	B	1277	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

6 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$
4	FUC	A	1062	4	10,10,11	1.06	0	13,14,16	1.07	1 (7%)
4	NAG	A	1063	1,4	14,14,15	0.53	0	15,19,21	0.76	0
4	NAG	A	1064	4	14,14,15	0.58	0	15,19,21	0.76	0
4	BMA	A	1065	4	11,11,12	0.69	0	15,15,17	0.91	1 (6%)
9	NAG	B	1939	9,2	14,14,15	0.69	0	15,19,21	0.86	1 (6%)
9	NAG	B	1940	9	14,14,15	0.53	0	15,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	A	1062	4	-	0/0/17/20	0/1/1/1
4	NAG	A	1063	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1064	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1065	4	-	0/2/19/22	0/1/1/1
9	NAG	B	1939	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	1940	9	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1939	NAG	O5-C5-C4	-2.40	106.15	110.13
4	A	1065	BMA	O2-C2-C3	-2.31	105.53	110.19
4	A	1062	FUC	O5-C5-C4	2.22	113.43	109.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1063	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
4	A	1062	FUC	2	0
4	A	1063	NAG	1	0
4	A	1064	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 14 are monoatomic - leaving 24 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	$\# Z  > 2$
6	GOL	A	1666	-	5,5,5	0.36	0	5,5,5	0.23	0
6	GOL	A	1667	-	5,5,5	0.34	0	5,5,5	0.27	0
6	GOL	A	1668	-	5,5,5	0.36	0	5,5,5	0.28	0
6	GOL	A	1669	-	5,5,5	0.34	0	5,5,5	0.20	0
6	GOL	A	1670	-	5,5,5	0.33	0	5,5,5	0.27	0
6	GOL	A	1671	-	5,5,5	0.36	0	5,5,5	0.22	0
6	GOL	A	1672	-	5,5,5	0.34	0	5,5,5	0.26	0
6	GOL	A	1673	-	5,5,5	0.36	0	5,5,5	0.18	0
6	GOL	A	1674	-	5,5,5	0.35	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	1675	-	5,5,5	0.34	0	5,5,5	0.29	0
6	GOL	B	2664	-	5,5,5	0.37	0	5,5,5	0.19	0
6	GOL	B	2665	-	5,5,5	0.34	0	5,5,5	0.26	0
6	GOL	B	2666	-	5,5,5	0.36	0	5,5,5	0.34	0
6	GOL	B	2667	-	5,5,5	0.34	0	5,5,5	0.28	0
6	GOL	B	2668	-	5,5,5	0.33	0	5,5,5	0.23	0
6	GOL	B	2669	-	5,5,5	0.37	0	5,5,5	0.26	0
6	GOL	B	2670	-	5,5,5	0.35	0	5,5,5	0.20	0
6	GOL	B	2671	-	5,5,5	0.34	0	5,5,5	0.28	0
6	GOL	B	2672	-	5,5,5	0.37	0	5,5,5	0.23	0
6	GOL	B	2673	-	5,5,5	0.35	0	5,5,5	0.20	0
6	GOL	B	2674	-	5,5,5	0.38	0	5,5,5	0.30	0
6	GOL	B	2675	-	5,5,5	0.38	0	5,5,5	0.28	0
6	GOL	C	1259	-	5,5,5	0.35	0	5,5,5	0.22	0
6	GOL	C	1260	-	5,5,5	0.36	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
6	GOL	A	1666	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1667	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1668	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1669	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1670	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1671	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1672	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1673	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1674	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1675	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2664	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2665	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2666	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2667	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2668	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2669	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2670	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2671	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2672	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2673	-	-	0/4/4/4	0/0/0/0
6	GOL	B	2674	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	2675	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1259	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1260	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1667	GOL	2	0
6	A	1668	GOL	2	0
6	A	1669	GOL	1	0
6	A	1671	GOL	1	0
6	A	1673	GOL	2	0
6	A	1674	GOL	1	0
6	A	1675	GOL	2	0
6	B	2664	GOL	2	0
6	B	2665	GOL	1	0
6	B	2666	GOL	3	0
6	B	2667	GOL	1	0
6	B	2668	GOL	2	0
6	B	2674	GOL	3	0
6	B	2675	GOL	1	0
6	C	1260	GOL	2	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	642/645 (99%)	-0.12	8 (1%) 81 77	29, 73, 140, 195	0
2	B	902/915 (98%)	-0.09	17 (1%) 70 64	28, 74, 121, 174	0
3	C	240/245 (97%)	0.48	34 (14%) 4 2	44, 91, 171, 207	0
All	All	1784/1805 (98%)	-0.02	59 (3%) 50 43	28, 75, 142, 207	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	209	PRO	6.6
3	C	217	SER	6.0
3	C	243	SER	5.9
3	C	250	PRO	5.3
3	C	242	GLY	5.2
3	C	258	LEU	4.7
3	C	253	THR	4.4
3	C	211	ILE	4.3
3	C	236	TYR	4.1
3	C	244	SER	3.7
2	B	1298	LEU	3.6
2	B	1351	LYS	3.6
1	A	50	GLN	3.5
3	C	238	TYR	3.4
2	B	1354	ASP	3.4
3	C	254	TRP	3.3
2	B	1663	ASN	3.3
3	C	257	GLU	3.2
1	A	92	ALA	3.2
3	C	210	THR	3.1
3	C	165	PHE	3.1
3	C	245	SER	3.1
3	C	247	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	395	ASP	3.1
3	C	237	GLY	3.0
2	B	1307	ILE	3.0
3	C	202	GLN	3.0
1	A	570	SER	3.0
2	B	1524	ASP	3.0
3	C	233	THR	3.0
3	C	246	SER	2.9
1	A	52	ASP	2.9
3	C	255	GLN	2.8
2	B	1352	ALA	2.7
3	C	162	TYR	2.7
2	B	1576	VAL	2.6
3	C	180	TYR	2.6
3	C	206	CYS	2.6
1	A	97	LYS	2.6
2	B	1641	GLU	2.6
2	B	971	VAL	2.5
2	B	1206	LEU	2.5
1	A	98	SER	2.5
3	C	256	PRO	2.5
2	B	1353	LYS	2.5
2	B	1573	SER	2.5
1	A	572	ASP	2.4
3	C	184	GLY	2.4
3	C	251	GLY	2.3
3	C	214	GLY	2.2
2	B	1256	LEU	2.2
3	C	205	LYS	2.2
3	C	152	PRO	2.1
3	C	156	ASN	2.1
3	C	218	SER	2.1
2	B	1628	VAL	2.1
3	C	240	LEU	2.1
2	B	1304	SER	2.1
2	B	1291	GLU	2.0

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

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

### 6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	FUC	A	1062	10/11	0.81	0.32	2.42	67,116,142,148	0
4	NAG	A	1063	14/15	0.72	0.26	-	98,124,145,149	0
4	NAG	A	1064	14/15	0.88	0.17	-	137,141,147,152	0
4	BMA	A	1065	11/12	0.52	0.29	-	148,156,159,161	0
9	NAG	B	1939	14/15	0.84	0.26	-	103,130,146,146	0
9	NAG	B	1940	14/15	0.73	0.54	-	153,160,164,164	0

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	C	1260	6/6	0.91	0.26	8.74	54,83,89,90	0
6	GOL	A	1668	6/6	0.72	0.35	8.11	98,106,111,118	0
5	CL	B	2682	1/1	0.53	0.30	6.04	66,66,66,66	0
6	GOL	A	1673	6/6	0.95	0.34	6.02	75,77,87,88	0
6	GOL	A	1671	6/6	0.83	0.23	6.01	75,92,96,98	0
7	NA	B	2677	1/1	0.88	0.42	4.94	85,85,85,85	0
6	GOL	A	1675	6/6	0.75	0.27	4.40	121,124,125,128	0
6	GOL	A	1674	6/6	0.86	0.26	2.68	74,100,109,110	0
6	GOL	B	2672	6/6	0.82	0.32	2.35	105,110,115,116	0
6	GOL	A	1672	6/6	0.81	0.19	2.07	81,86,89,94	0
6	GOL	C	1259	6/6	0.90	0.21	1.95	77,94,98,101	0
6	GOL	B	2670	6/6	0.78	0.20	1.42	87,99,105,107	0
7	NA	A	1676	1/1	0.79	0.17	1.20	55,55,55,55	0
6	GOL	A	1667	6/6	0.97	0.27	0.90	76,78,91,105	0
6	GOL	B	2665	6/6	0.91	0.18	0.73	59,64,71,77	0
6	GOL	A	1670	6/6	0.91	0.18	0.72	57,64,69,76	0
6	GOL	B	2667	6/6	0.87	0.20	0.53	75,80,86,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	B	2676	1/1	0.90	0.16	0.27	72,72,72,72	0
6	GOL	B	2674	6/6	0.85	0.15	0.24	72,77,85,87	0
8	IOD	A	1678	1/1	0.97	0.15	0.14	64,64,64,64	1
8	IOD	A	1677	1/1	0.96	0.19	0.10	55,55,55,55	1
8	IOD	B	2681	1/1	0.99	0.17	-0.38	75,75,75,75	1
8	IOD	B	2680	1/1	0.95	0.13	-1.68	68,68,68,68	1
8	IOD	B	2678	1/1	0.99	0.11	-7.42	83,83,83,83	1
6	GOL	B	2671	6/6	0.89	0.21	-	77,79,80,82	0
6	GOL	B	2664	6/6	0.91	0.27	-	79,83,87,90	0
6	GOL	B	2669	6/6	0.78	0.41	-	116,118,119,119	0
6	GOL	A	1666	6/6	0.91	0.16	-	76,92,95,99	0
8	IOD	B	2679	1/1	0.99	0.09	-	67,67,67,67	1
8	IOD	A	1679	1/1	0.99	0.14	-	65,65,65,65	1
5	CL	C	1262	1/1	0.98	0.11	-	60,60,60,60	0
5	CL	A	1665	1/1	0.90	0.08	-	87,87,87,87	0
6	GOL	B	2668	6/6	0.82	0.17	-	56,77,84,88	0
6	GOL	B	2666	6/6	0.95	0.13	-	52,55,64,70	0
6	GOL	A	1669	6/6	0.61	0.39	-	95,100,101,102	0
6	GOL	B	2675	6/6	0.88	0.17	-	76,84,85,88	0
6	GOL	B	2673	6/6	0.55	0.51	-	104,108,113,114	0
5	CL	C	1261	1/1	0.98	0.26	-	49,49,49,49	0

## 6.5 Other polymers

There are no such residues in this entry.