



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2018 – 12:09 PM EST

PDB ID : 6BF4
Title : Crystal Structure of HIV-1 Clade AE Strain CNE55 gp120 Core in Complex with Neutralizing Antibody VRC-PG05 that Targets the Center of the Silent Face on the Outer Domain of gp120
Authors : Zhou, T.; Kwong, P.D.
Deposited on : 2017-10-25
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

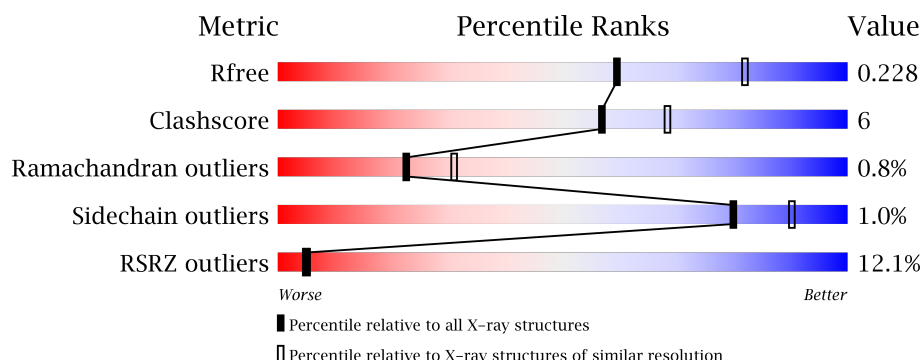
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	344	<div> <div>26%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
1	G	344	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
2	B	229	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
2	H	229	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
3	C	219	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	L	219	

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	NAG	A	501	-	-	-	X
4	NAG	A	523	-	-	-	X
4	NAG	G	525	-	-	-	X
5	MAN	A	533	-	-	-	X
5	MAN	G	536	-	-	-	X
6	EDO	B	301	-	-	-	X
6	EDO	G	537	-	-	-	X
6	EDO	L	302	-	-	-	X
6	EDO	L	303	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13124 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 HIV-1 clade AE gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2639	1656	460	503	20			
1	G	333	Total	C	N	O	S	0	0	0
			2607	1639	452	496	20			

- Molecule 2 is a protein called VRC-PG05 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1702	1077	290	326	9			
2	H	221	Total	C	N	O	S	0	0	0
			1676	1062	285	320	9			

- Molecule 3 is a protein called VRC-PG05 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1714	1077	291	340	6			
3	L	218	Total	C	N	O	S	0	0	0
			1707	1074	290	338	5			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



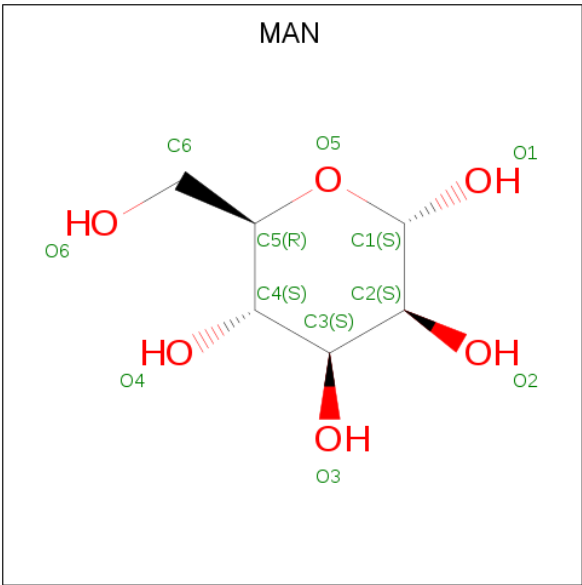
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

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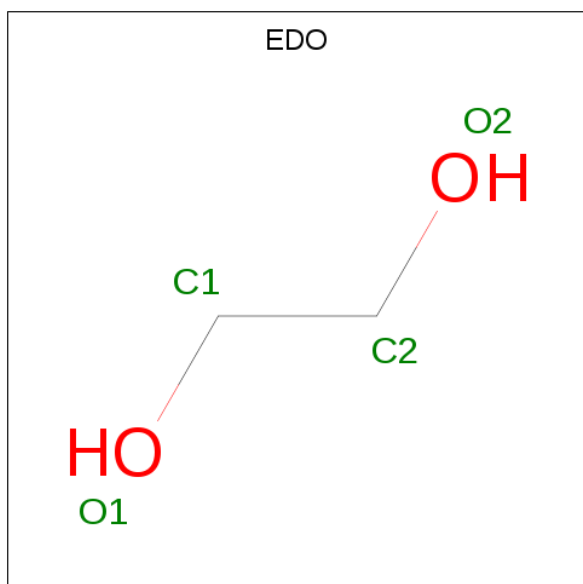
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



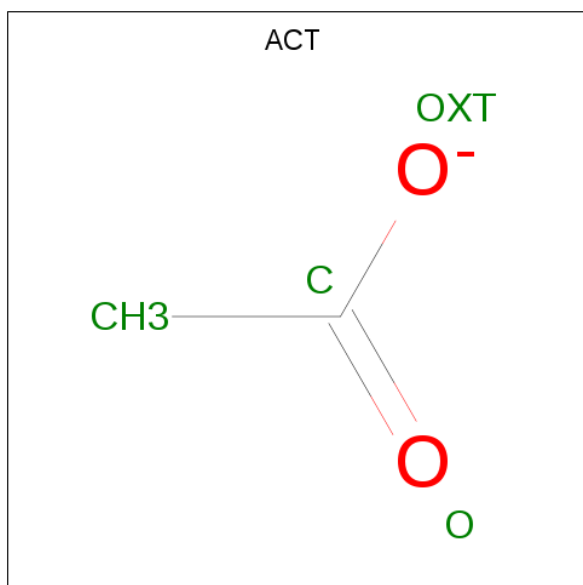
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

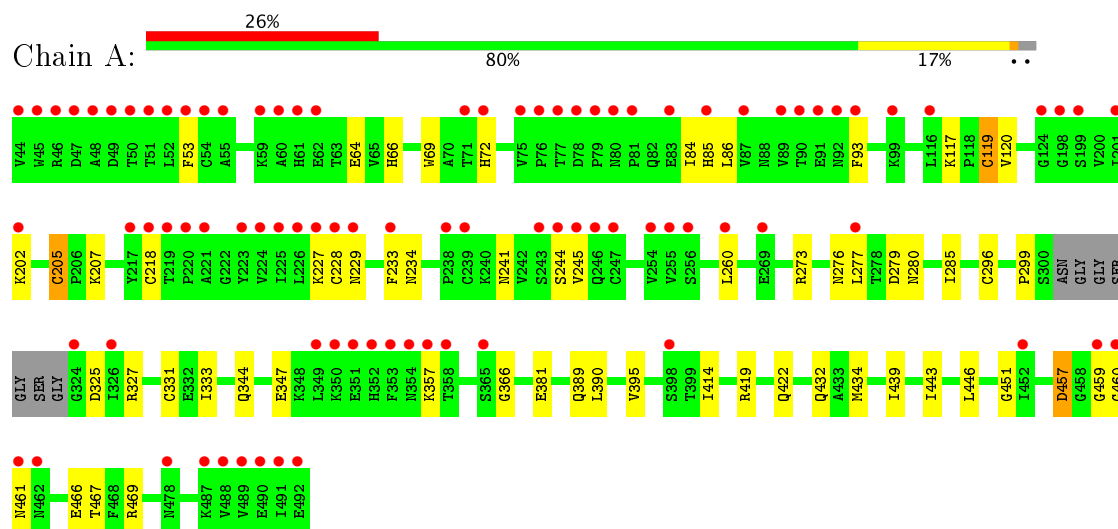
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	O	0	0
			7	7		
8	B	26	Total	O	0	0
			26	26		
8	C	30	Total	O	0	0
			30	30		
8	G	36	Total	O	0	0
			36	36		
8	H	38	Total	O	0	0
			38	38		
8	L	39	Total	O	0	0
			39	39		

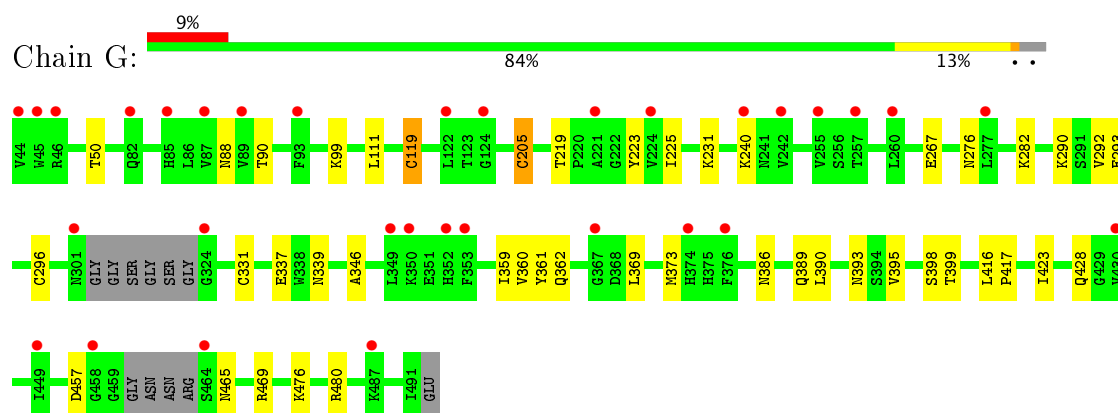
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

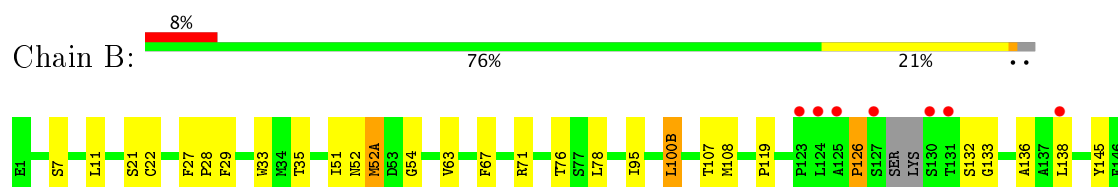
- Molecule 1: HIV-1 clade AE gp120 core

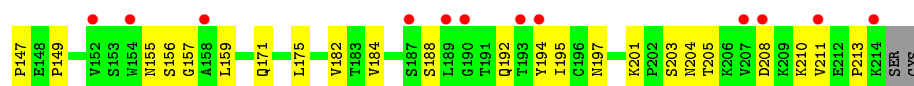


- Molecule 1: HIV-1 clade AE gp120 core

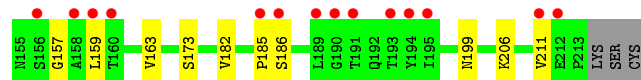
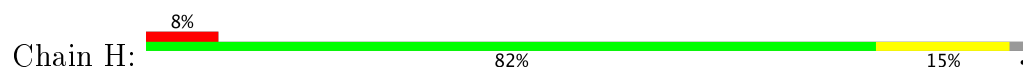


- Molecule 2: VRC-PG05 Fab heavy chain

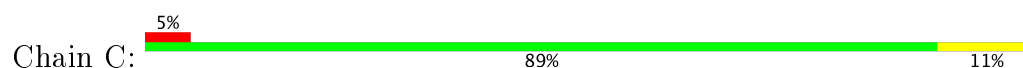




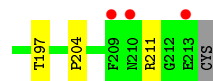
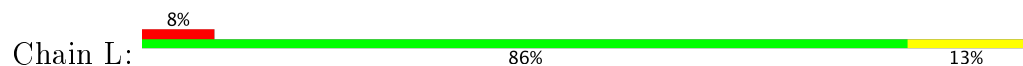
- Molecule 2: VRC-PG05 Fab heavy chain



- Molecule 3: VRC-PG05 Fab light chain



- Molecule 3: VRC-PG05 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	231.44Å 89.25Å 123.41Å 90.00° 119.15° 90.00°	Depositor
Resolution (Å)	39.85 – 2.38 39.85 – 2.38	Depositor EDS
% Data completeness (in resolution range)	88.5 (39.85-2.38) 88.5 (39.85-2.38)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.192 , 0.228 0.191 , 0.228	Depositor DCC
R_{free} test set	3883 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.758	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13124	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ACT, NAG, EDO, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2696	0.43	0/3661
1	G	0.25	0/2663	0.44	0/3616
2	B	0.25	0/1743	0.49	0/2370
2	H	0.26	0/1717	0.49	0/2336
3	C	0.25	0/1755	0.45	0/2383
3	L	0.26	0/1748	0.47	0/2375
All	All	0.25	0/12322	0.46	0/16741

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2639	0	2569	39	0
1	G	2607	0	2540	27	0
2	B	1702	0	1677	29	0
2	H	1676	0	1649	16	0
3	C	1714	0	1647	17	0
3	L	1707	0	1642	18	0
4	A	196	0	175	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	14	0	13	0	0
4	G	196	0	174	1	0
4	L	14	0	13	0	0
5	A	209	0	174	0	0
5	G	242	0	202	0	0
6	A	4	0	6	0	0
6	B	8	0	12	3	0
6	G	4	0	6	2	0
6	H	4	0	6	0	0
6	L	8	0	12	0	0
7	B	4	0	3	0	0
8	A	7	0	0	0	0
8	B	26	0	0	0	0
8	C	30	0	0	0	0
8	G	36	0	0	0	0
8	H	38	0	0	0	0
8	L	39	0	0	1	0
All	All	13124	0	12520	146	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 6.

All (146) 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)
3:L:189:HIS:O	3:L:211:ARG:NH1	2.05	0.90
2:H:9:GLY:HA2	2:H:18:LEU:HD21	1.55	0.86
1:A:357:LYS:NZ	1:A:461:ASN:O	2.07	0.86
1:G:50:THR:O	1:G:99:LYS:NZ	2.10	0.84
1:G:389:GLN:HB3	4:G:527:NAG:H61	1.62	0.82
3:C:187:GLU:O	3:C:211:ARG:NH1	2.15	0.80
1:A:432:GLN:HG2	1:G:423:ILE:HD11	1.69	0.75
2:B:201:LYS:HD2	6:B:302:EDO:H11	1.75	0.69
1:A:227:LYS:HE3	1:A:245:VAL:HG11	1.75	0.68
3:L:126:LYS:O	3:L:128:GLY:N	2.28	0.67
3:C:54:ARG:NH1	3:C:62:PHE:O	2.26	0.67
1:G:361:TYR:N	1:G:393:ASN:OD1	2.24	0.66
1:G:292:VAL:HG13	6:G:537:EDO:H11	1.78	0.65
1:A:461:ASN:ND2	1:A:466:GLU:OE2	2.31	0.63
1:G:339:ASN:HD22	1:G:395:VAL:HB	1.65	0.62
2:B:197:ASN:ND2	2:B:208:ASP:OD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.82	0.60
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.82	0.60
3:L:126:LYS:HG3	3:L:127:SER:H	1.66	0.59
1:G:390:LEU:HD13	1:G:416:LEU:HD21	1.83	0.59
1:G:119:CYS:N	1:G:205:CYS:SG	2.76	0.59
4:A:525:NAG:HN2	2:B:100(B):LEU:HB2	1.69	0.57
1:A:64:GLU:OE2	1:A:66:HIS:HD2	1.87	0.57
2:B:52:ASN:O	2:B:71:ARG:NH2	2.37	0.57
2:B:188:SER:HB3	2:B:192:GLN:HB3	1.85	0.57
3:C:61:ARG:HH12	3:C:82:ASP:CG	2.05	0.57
1:G:293:GLU:H	6:G:537:EDO:H12	1.69	0.57
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.85	0.57
3:L:83:VAL:HB	3:L:106:ILE:HD13	1.85	0.57
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.87	0.56
3:L:149:LYS:HG2	3:L:154:LEU:HD23	1.88	0.56
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.88	0.56
3:C:61:ARG:NH1	3:C:82:ASP:OD1	2.25	0.55
2:H:135:THR:HA	2:H:185:PRO:HA	1.89	0.55
2:H:138:LEU:HD13	2:H:211:VAL:HG21	1.87	0.55
1:G:290:LYS:NZ	1:G:337:GLU:HG3	2.22	0.55
2:B:35:THR:HB	2:B:95:ILE:HD11	1.88	0.54
2:B:136:ALA:N	2:B:184:VAL:O	2.33	0.54
1:A:277:LEU:HD11	4:A:501:NAG:H83	1.88	0.54
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.89	0.54
1:G:90:THR:HG22	1:G:240:LYS:HA	1.90	0.54
2:H:199:ASN:ND2	2:H:206:LYS:HE2	2.23	0.53
3:C:147:GLN:HB3	3:C:195:GLU:HB3	1.90	0.53
1:A:229:ASN:HB2	1:A:241:ASN:HB3	1.90	0.53
2:B:107:THR:HG22	6:B:302:EDO:H12	1.91	0.53
2:B:159:LEU:HD13	2:B:182:VAL:HG21	1.91	0.52
1:A:389:GLN:HB3	4:A:523:NAG:H61	1.91	0.52
3:C:27(B):VAL:HG21	3:C:33:VAL:HG23	1.90	0.52
1:A:459:GLY:O	1:A:461:ASN:N	2.43	0.52
1:A:347:GLU:HG2	4:A:514:NAG:H83	1.92	0.52
3:L:118:PHE:HB2	3:L:133:VAL:HB	1.91	0.52
3:C:190:LYS:NZ	3:C:190:LYS:HB2	2.24	0.52
1:G:369:LEU:HD22	1:G:373:MET:HE2	1.92	0.52
1:G:386:ASN:HB3	1:G:417:PRO:HG2	1.91	0.52
1:A:327:ARG:NH1	1:A:422:GLN:OE1	2.43	0.51
2:B:203:SER:O	2:B:205:THR:N	2.43	0.51
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:186:TYR:O	3:L:192:TYR:OH	2.27	0.51
3:L:197:THR:HG22	3:L:204:PRO:HB3	1.93	0.51
3:L:129:THR:HA	3:L:182:SER:HA	1.94	0.50
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.94	0.50
1:G:290:LYS:HZ1	1:G:337:GLU:HG3	1.77	0.50
2:H:159:LEU:HD21	2:H:182:VAL:HG11	1.93	0.50
2:B:108:MET:HB3	2:B:149:PRO:HD3	1.94	0.49
3:C:108:ARG:HD2	3:C:171:SER:HB2	1.93	0.49
1:G:398:SER:OG	1:G:399:THR:N	2.45	0.49
1:A:381:GLU:OE2	1:A:439:ILE:HG23	2.12	0.49
3:C:3:VAL:H	3:C:26:SER:HB3	1.78	0.49
3:L:30:ARG:HD2	3:L:50:TRP:CE3	2.48	0.49
1:A:446:LEU:HD22	4:A:515:NAG:H82	1.95	0.48
2:B:171:GLN:HG2	2:B:175:LEU:O	2.13	0.48
3:C:108:ARG:NH1	3:C:109:THR:O	2.46	0.48
3:C:163:VAL:HG22	3:C:175:LEU:HD12	1.96	0.48
3:C:140:TYR:CG	3:C:141:PRO:HA	2.49	0.47
3:C:61:ARG:NH1	3:C:82:ASP:OD2	2.47	0.47
2:B:126:PRO:HG3	2:B:138:LEU:HD23	1.94	0.47
1:G:219:THR:OG1	1:G:225:ILE:HG13	2.14	0.47
1:G:231:LYS:HG2	1:G:267:GLU:OE2	2.15	0.47
3:L:1:ASP:HB2	8:L:414:HOH:O	2.14	0.47
3:C:61:ARG:NH1	3:C:82:ASP:CG	2.67	0.47
2:H:35:THR:HB	2:H:95:ILE:HD11	1.96	0.46
2:H:51:ILE:HD11	2:H:54:GLY:HA2	1.98	0.46
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.51	0.46
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.97	0.46
2:H:108:MET:HB3	2:H:149:PRO:HD3	1.96	0.46
1:A:119:CYS:N	1:A:205:CYS:SG	2.89	0.46
2:H:163:VAL:HG22	2:H:182:VAL:HG22	1.98	0.46
2:B:132:SER:OG	2:B:133:GLY:N	2.49	0.45
2:B:155:ASN:O	2:B:157:GLY:N	2.49	0.45
1:A:296:CYS:HA	1:A:331:CYS:HA	1.98	0.45
1:A:53:PHE:CE1	1:A:218:CYS:HB2	2.51	0.45
1:A:395:VAL:HG13	1:A:414:ILE:HD11	1.99	0.45
1:A:64:GLU:OE2	1:A:66:HIS:CD2	2.69	0.45
3:L:124:GLN:O	3:L:127:SER:OG	2.30	0.45
3:L:145:LYS:HB3	3:L:145:LYS:HE3	1.87	0.45
1:A:325:ASP:OD2	1:A:419:ARG:NH1	2.50	0.45
1:A:344:GLN:HA	4:A:514:NAG:H81	1.97	0.44
2:B:33:TRP:HB2	2:B:95:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:HE2	1:A:202:LYS:HB3	1.69	0.44
2:B:138:LEU:HD21	2:B:194:TYR:CD2	2.53	0.44
3:L:13:VAL:HB	3:L:78:LEU:HD22	1.99	0.44
1:A:84:ILE:O	1:A:86:LEU:N	2.50	0.44
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.18	0.44
3:C:149:LYS:HG2	3:C:154:LEU:HD13	2.00	0.44
1:G:476:LYS:O	1:G:480:ARG:HG3	2.17	0.44
2:H:12:VAL:HG11	2:H:82(C):LEU:HD12	2.00	0.43
3:L:140:TYR:CG	3:L:141:PRO:HA	2.53	0.43
1:G:362:GLN:O	1:G:469:ARG:HG2	2.17	0.43
2:H:12:VAL:HG21	2:H:18:LEU:HD22	2.00	0.43
1:G:360:VAL:HG21	1:G:465:ASN:HD22	1.82	0.43
3:L:81:GLU:HG3	3:L:81:GLU:H	1.42	0.43
1:A:457:ASP:OD2	1:A:469:ARG:NE	2.38	0.43
1:G:296:CYS:HA	1:G:331:CYS:HA	2.00	0.43
2:B:52(A):MET:N	2:B:52(A):MET:SD	2.82	0.43
1:A:69:TRP:HA	1:A:72:HIS:CE1	2.53	0.43
1:A:84:ILE:HB	1:A:244:SER:HB2	2.00	0.43
2:B:51:ILE:HD11	2:B:54:GLY:HA2	2.00	0.43
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.99	0.43
3:L:151:ASP:OD2	3:L:189:HIS:HB3	2.18	0.43
1:A:120:VAL:HB	1:A:434:MET:HE3	2.00	0.42
2:H:30:ASN:HB3	2:H:73:ASN:HB3	2.01	0.42
2:H:34:MET:HB3	2:H:78:LEU:HD22	2.01	0.42
1:A:117:LYS:HB2	1:A:117:LYS:HE3	1.83	0.42
6:B:301:EDO:H21	3:C:98:PHE:H	1.84	0.42
1:G:282:LYS:HD3	1:G:282:LYS:HA	1.90	0.42
1:G:428:GLN:OE1	1:G:428:GLN:N	2.38	0.41
1:A:234:ASN:HD22	4:A:501:NAG:C7	2.32	0.41
1:G:346:ALA:O	1:G:359:ILE:HG13	2.20	0.41
1:A:276:ASN:ND2	1:A:279:ASP:HB2	2.34	0.41
1:G:339:ASN:ND2	1:G:395:VAL:HB	2.34	0.41
2:B:11:LEU:HB2	2:B:147:PRO:HG3	2.01	0.41
1:G:219:THR:HG21	1:G:223:TYR:C	2.41	0.41
2:B:7:SER:HB3	2:B:21:SER:OG	2.20	0.41
1:A:273:ARG:HB2	1:A:285:ILE:HB	2.02	0.41
1:A:333:ILE:HG21	1:A:390:LEU:HD21	2.03	0.41
2:B:126:PRO:HD2	2:B:213:PRO:HA	2.03	0.41
2:B:138:LEU:HB2	2:B:211:VAL:HG11	2.03	0.41
2:B:27:PHE:O	2:B:29:PHE:N	2.54	0.41
4:A:513:NAG:H62	4:A:514:NAG:N2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:CE1	1:A:228:CYS:HB2	2.55	0.40
2:B:29:PHE:CD1	2:B:76:THR:HA	2.56	0.40
1:A:207:LYS:HG3	1:A:439:ILE:HG22	2.03	0.40
2:B:195:ILE:HG22	2:B:210:LYS:HA	2.02	0.40
1:A:457:ASP:HB2	1:A:467:THR:HB	2.03	0.40
1:G:457:ASP:OD1	1:G:469:ARG:NH2	2.55	0.40
2:H:80:LEU:HD23	2:H:82:MET:HE2	2.03	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	333/344 (97%)	303 (91%)	25 (8%)	5 (2%)	12	15
1	G	327/344 (95%)	312 (95%)	14 (4%)	1 (0%)	44	59
2	B	221/229 (96%)	200 (90%)	17 (8%)	4 (2%)	10	11
2	H	217/229 (95%)	203 (94%)	12 (6%)	2 (1%)	20	27
3	C	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
3	L	216/219 (99%)	207 (96%)	8 (4%)	1 (0%)	32	44
All	All	1531/1584 (97%)	1432 (94%)	86 (6%)	13 (1%)	22	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
3	L	127	SER
1	A	460	GLY
2	B	126	PRO
1	A	85	HIS

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Mol	Chain	Res	Type
1	A	280	ASN
2	B	156	SER
1	A	299	PRO
1	G	276	ASN
2	H	157	GLY
2	H	186	SER
2	B	28	PRO
1	A	366	GLY

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	299/302 (99%)	296 (99%)	3 (1%)	80	90
1	G	296/302 (98%)	292 (99%)	4 (1%)	71	85
2	B	189/193 (98%)	187 (99%)	2 (1%)	78	89
2	H	186/193 (96%)	183 (98%)	3 (2%)	68	82
3	C	193/193 (100%)	193 (100%)	0	100	100
3	L	192/193 (100%)	191 (100%)	1 (0%)	91	96
All	All	1355/1376 (98%)	1342 (99%)	13 (1%)	80	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	CYS
1	A	205	CYS
1	A	457	ASP
2	B	52(A)	MET
2	B	100(B)	LEU
1	G	88	ASN
1	G	111	LEU
1	G	119	CYS
1	G	205	CYS
2	H	7	SER

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Mol	Chain	Res	Type
2	H	100(B)	LEU
2	H	173	SER
3	L	81	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	124	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

79 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	501	1	14,14,15	0.24	0	15,19,21	0.48	0
4	NAG	A	502	1,4	14,14,15	0.33	0	15,19,21	0.56	0
4	NAG	A	503	5,4	14,14,15	0.31	0	15,19,21	0.54	0
5	MAN	A	504	5,4	11,11,12	0.72	0	13,15,17	1.05	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	505	5	11,11,12	0.54	0	13,15,17	1.25	2 (15%)
5	MAN	A	506	5	11,11,12	0.72	0	13,15,17	1.36	2 (15%)
5	MAN	A	507	5	11,11,12	0.71	0	13,15,17	1.52	2 (15%)
5	MAN	A	508	5	11,11,12	0.64	0	13,15,17	1.23	1 (7%)
5	MAN	A	509	5	11,11,12	0.65	0	13,15,17	1.47	2 (15%)
5	MAN	A	510	5	11,11,12	0.66	0	13,15,17	1.16	2 (15%)
5	MAN	A	511	5	11,11,12	0.69	0	13,15,17	1.05	2 (15%)
4	NAG	A	512	1	14,14,15	0.19	0	15,19,21	0.60	0
4	NAG	A	513	1,4	14,14,15	0.22	0	15,19,21	0.66	0
4	NAG	A	514	4	14,14,15	0.25	0	15,19,21	0.57	0
4	NAG	A	515	1,4	14,14,15	0.25	0	15,19,21	0.52	0
4	NAG	A	516	5,4	14,14,15	0.29	0	15,19,21	0.61	0
5	MAN	A	517	5,4	11,11,12	0.77	0	13,15,17	1.03	1 (7%)
5	MAN	A	518	5	11,11,12	0.65	0	13,15,17	1.20	1 (7%)
5	MAN	A	519	5	11,11,12	0.72	0	13,15,17	1.09	2 (15%)
5	MAN	A	520	5	11,11,12	0.72	0	13,15,17	1.15	2 (15%)
4	NAG	A	521	1	14,14,15	0.16	0	15,19,21	0.47	0
4	NAG	A	522	1	14,14,15	0.23	0	15,19,21	0.49	0
4	NAG	A	523	1	14,14,15	0.33	0	15,19,21	0.40	0
4	NAG	A	524	1	14,14,15	0.30	0	15,19,21	0.62	1 (6%)
4	NAG	A	525	1,4	14,14,15	0.16	0	15,19,21	0.68	0
4	NAG	A	526	5,4	14,14,15	0.27	0	15,19,21	0.54	0
5	MAN	A	527	5,4	11,11,12	0.74	0	13,15,17	1.07	2 (15%)
5	MAN	A	528	5	11,11,12	0.69	0	13,15,17	1.42	2 (15%)
5	MAN	A	529	5	11,11,12	0.62	0	13,15,17	1.13	2 (15%)
5	MAN	A	530	5	11,11,12	0.65	0	13,15,17	1.19	2 (15%)
5	MAN	A	531	5	11,11,12	1.11	1 (9%)	13,15,17	1.12	0
5	MAN	A	532	5	11,11,12	0.71	0	13,15,17	1.33	2 (15%)
5	MAN	A	533	5	11,11,12	0.75	0	13,15,17	1.04	2 (15%)
6	EDO	A	534	-	3,3,3	0.46	0	2,2,2	0.33	0
6	EDO	B	301	-	3,3,3	0.47	0	2,2,2	0.31	0
6	EDO	B	302	-	3,3,3	0.45	0	2,2,2	0.35	0
7	ACT	B	303	-	1,3,3	1.33	0	0,3,3	0.00	-
4	NAG	C	301	3	14,14,15	0.21	0	15,19,21	0.46	0
4	NAG	G	501	1	14,14,15	0.18	0	15,19,21	0.40	0
4	NAG	G	502	1	14,14,15	0.27	0	15,19,21	0.44	0
4	NAG	G	503	1,4	14,14,15	0.24	0	15,19,21	0.54	0
4	NAG	G	504	5,4	14,14,15	0.40	0	15,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	G	505	5,4	11,11,12	0.80	1 (9%)	13,15,17	1.38	2 (15%)
5	MAN	G	506	5	11,11,12	0.61	0	13,15,17	1.22	2 (15%)
5	MAN	G	507	5	11,11,12	0.83	0	13,15,17	1.05	1 (7%)
5	MAN	G	508	5	11,11,12	0.70	0	13,15,17	1.37	2 (15%)
5	MAN	G	509	5	11,11,12	0.65	0	13,15,17	1.15	2 (15%)
5	MAN	G	510	5	11,11,12	0.72	0	13,15,17	1.45	3 (23%)
5	MAN	G	511	5	11,11,12	0.66	0	13,15,17	1.10	2 (15%)
5	MAN	G	512	5	11,11,12	0.77	0	13,15,17	1.22	2 (15%)
5	MAN	G	513	5	11,11,12	0.70	0	13,15,17	1.33	2 (15%)
4	NAG	G	514	1	14,14,15	0.43	0	15,19,21	0.69	1 (6%)
4	NAG	G	515	1,4	14,14,15	0.20	0	15,19,21	0.43	0
4	NAG	G	516	5,4	14,14,15	0.23	0	15,19,21	0.68	0
5	MAN	G	517	5,4	11,11,12	1.08	0	13,15,17	0.84	0
5	MAN	G	518	5	11,11,12	0.99	1 (9%)	13,15,17	1.33	2 (15%)
5	MAN	G	519	5	11,11,12	1.23	2 (18%)	13,15,17	1.52	2 (15%)
4	NAG	G	520	1,4	14,14,15	0.36	0	15,19,21	0.53	0
4	NAG	G	521	5,4	14,14,15	0.26	0	15,19,21	0.65	0
5	MAN	G	522	5,4	11,11,12	0.93	0	13,15,17	0.97	2 (15%)
5	MAN	G	523	5	11,11,12	0.67	0	13,15,17	1.19	2 (15%)
5	MAN	G	524	5	11,11,12	0.78	0	13,15,17	1.21	2 (15%)
4	NAG	G	525	1	14,14,15	0.50	0	15,19,21	0.49	0
4	NAG	G	526	1	14,14,15	0.21	0	15,19,21	0.51	0
4	NAG	G	527	1	14,14,15	0.37	0	15,19,21	0.40	0
4	NAG	G	528	1,4	14,14,15	0.42	0	15,19,21	0.63	0
4	NAG	G	529	5,4	14,14,15	0.29	0	15,19,21	0.55	0
5	MAN	G	530	5,4	11,11,12	0.77	0	13,15,17	1.23	2 (15%)
5	MAN	G	531	5	11,11,12	0.90	1 (9%)	13,15,17	1.09	1 (7%)
5	MAN	G	532	5	11,11,12	0.67	0	13,15,17	1.07	2 (15%)
5	MAN	G	533	5	11,11,12	0.77	0	13,15,17	0.98	1 (7%)
5	MAN	G	534	5	11,11,12	1.00	1 (9%)	13,15,17	0.97	0
5	MAN	G	535	5	11,11,12	0.82	0	13,15,17	1.29	2 (15%)
5	MAN	G	536	5	11,11,12	0.79	0	13,15,17	1.06	2 (15%)
6	EDO	G	537	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	H	301	-	3,3,3	0.46	0	2,2,2	0.46	0
4	NAG	L	301	3	14,14,15	0.27	0	15,19,21	0.47	0
6	EDO	L	302	-	3,3,3	0.49	0	2,2,2	0.31	0
6	EDO	L	303	-	3,3,3	0.48	0	2,2,2	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	503	5,4	-	0/6/23/26	0/1/1/1
5	MAN	A	504	5,4	-	0/2/19/22	1/1/1/1
5	MAN	A	505	5	-	0/2/19/22	0/1/1/1
5	MAN	A	506	5	-	0/2/19/22	0/1/1/1
5	MAN	A	507	5	-	0/2/19/22	0/1/1/1
5	MAN	A	508	5	-	0/2/19/22	0/1/1/1
5	MAN	A	509	5	-	0/2/19/22	0/1/1/1
5	MAN	A	510	5	-	0/2/19/22	0/1/1/1
5	MAN	A	511	5	-	0/2/19/22	0/1/1/1
4	NAG	A	512	1	-	0/6/23/26	0/1/1/1
4	NAG	A	513	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	514	4	-	0/6/23/26	0/1/1/1
4	NAG	A	515	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	516	5,4	-	0/6/23/26	0/1/1/1
5	MAN	A	517	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	518	5	-	0/2/19/22	0/1/1/1
5	MAN	A	519	5	-	0/2/19/22	0/1/1/1
5	MAN	A	520	5	-	0/2/19/22	0/1/1/1
4	NAG	A	521	1	-	0/6/23/26	0/1/1/1
4	NAG	A	522	1	-	0/6/23/26	0/1/1/1
4	NAG	A	523	1	-	0/6/23/26	0/1/1/1
4	NAG	A	524	1	-	0/6/23/26	0/1/1/1
4	NAG	A	525	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	526	5,4	-	0/6/23/26	0/1/1/1
5	MAN	A	527	5,4	-	0/2/19/22	1/1/1/1
5	MAN	A	528	5	-	0/2/19/22	0/1/1/1
5	MAN	A	529	5	-	0/2/19/22	0/1/1/1
5	MAN	A	530	5	-	0/2/19/22	0/1/1/1
5	MAN	A	531	5	-	0/2/19/22	0/1/1/1
5	MAN	A	532	5	-	0/2/19/22	0/1/1/1
5	MAN	A	533	5	-	0/2/19/22	0/1/1/1
6	EDO	A	534	-	-	0/1/1/1	0/0/0/0
6	EDO	B	301	-	-	0/1/1/1	0/0/0/0
6	EDO	B	302	-	-	0/1/1/1	0/0/0/0
7	ACT	B	303	-	-	0/0/0/0	0/0/0/0
4	NAG	C	301	3	-	0/6/23/26	0/1/1/1
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1
4	NAG	G	503	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	504	5,4	-	0/6/23/26	0/1/1/1
5	MAN	G	505	5,4	-	0/2/19/22	1/1/1/1
5	MAN	G	506	5	-	0/2/19/22	0/1/1/1
5	MAN	G	507	5	-	0/2/19/22	0/1/1/1
5	MAN	G	508	5	-	0/2/19/22	0/1/1/1
5	MAN	G	509	5	-	0/2/19/22	0/1/1/1
5	MAN	G	510	5	-	0/2/19/22	0/1/1/1
5	MAN	G	511	5	-	0/2/19/22	0/1/1/1
5	MAN	G	512	5	-	0/2/19/22	0/1/1/1
5	MAN	G	513	5	-	0/2/19/22	0/1/1/1
4	NAG	G	514	1	-	0/6/23/26	0/1/1/1
4	NAG	G	515	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	516	5,4	-	0/6/23/26	0/1/1/1
5	MAN	G	517	5,4	-	0/2/19/22	0/1/1/1
5	MAN	G	518	5	-	0/2/19/22	1/1/1/1
5	MAN	G	519	5	-	0/2/19/22	0/1/1/1
4	NAG	G	520	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	521	5,4	-	0/6/23/26	0/1/1/1
5	MAN	G	522	5,4	-	0/2/19/22	1/1/1/1
5	MAN	G	523	5	-	0/2/19/22	0/1/1/1
5	MAN	G	524	5	-	0/2/19/22	0/1/1/1
4	NAG	G	525	1	-	0/6/23/26	0/1/1/1
4	NAG	G	526	1	-	0/6/23/26	0/1/1/1
4	NAG	G	527	1	-	0/6/23/26	0/1/1/1
4	NAG	G	528	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	529	5,4	-	0/6/23/26	0/1/1/1
5	MAN	G	530	5,4	-	0/2/19/22	0/1/1/1
5	MAN	G	531	5	-	0/2/19/22	0/1/1/1
5	MAN	G	532	5	-	0/2/19/22	0/1/1/1
5	MAN	G	533	5	-	0/2/19/22	0/1/1/1
5	MAN	G	534	5	-	0/2/19/22	0/1/1/1
5	MAN	G	535	5	-	0/2/19/22	0/1/1/1
5	MAN	G	536	5	-	0/2/19/22	0/1/1/1
6	EDO	G	537	-	-	0/1/1/1	0/0/0/0
6	EDO	H	301	-	-	0/1/1/1	0/0/0/0
4	NAG	L	301	3	-	0/6/23/26	0/1/1/1
6	EDO	L	302	-	-	0/1/1/1	0/0/0/0
6	EDO	L	303	-	-	0/1/1/1	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	531	MAN	O5-C1	-2.29	1.40	1.43
5	G	534	MAN	O5-C1	-2.12	1.40	1.43
5	G	505	MAN	O5-C5	2.06	1.47	1.43
5	G	519	MAN	O5-C5	2.29	1.48	1.43
5	A	531	MAN	C2-C3	2.45	1.55	1.52
5	G	518	MAN	C1-C2	2.52	1.58	1.52
5	G	519	MAN	C4-C5	2.72	1.58	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	532	MAN	O2-C2-C3	-3.34	103.62	110.17
5	G	507	MAN	O2-C2-C3	-3.23	103.83	110.17
5	A	506	MAN	O2-C2-C3	-2.99	104.31	110.17
5	G	508	MAN	O2-C2-C3	-2.94	104.41	110.17
5	G	535	MAN	O2-C2-C3	-2.90	104.49	110.17
5	G	512	MAN	O2-C2-C3	-2.72	104.83	110.17
5	A	528	MAN	O2-C2-C3	-2.72	104.84	110.17
5	A	507	MAN	O2-C2-C3	-2.69	104.90	110.17
5	A	505	MAN	O2-C2-C3	-2.66	104.96	110.17
5	A	510	MAN	O2-C2-C3	-2.65	104.98	110.17
5	G	506	MAN	O2-C2-C3	-2.58	105.11	110.17
5	G	511	MAN	O2-C2-C3	-2.58	105.12	110.17
5	G	531	MAN	O2-C2-C3	-2.51	105.25	110.17
5	G	530	MAN	O2-C2-C3	-2.50	105.25	110.17
5	G	509	MAN	O2-C2-C3	-2.42	105.43	110.17
5	A	530	MAN	O2-C2-C3	-2.34	105.57	110.17
5	G	510	MAN	C1-C2-C3	-2.34	106.68	109.65
5	A	529	MAN	O2-C2-C3	-2.30	105.65	110.17
5	A	509	MAN	O2-C2-C3	-2.30	105.66	110.17
5	A	527	MAN	O2-C2-C3	-2.26	105.73	110.17
5	G	510	MAN	O2-C2-C3	-2.22	105.82	110.17
5	G	518	MAN	O2-C2-C3	-2.21	105.84	110.17
5	G	536	MAN	O2-C2-C3	-2.20	105.85	110.17
5	A	533	MAN	O2-C2-C3	-2.19	105.87	110.17
5	A	511	MAN	O2-C2-C3	-2.18	105.90	110.17
5	G	533	MAN	O2-C2-C3	-2.17	105.91	110.17
5	A	519	MAN	O2-C2-C3	-2.15	105.96	110.17
5	G	524	MAN	O2-C2-C3	-2.12	106.01	110.17
5	A	520	MAN	O2-C2-C3	-2.12	106.01	110.17
5	G	523	MAN	O2-C2-C3	-2.08	106.08	110.17
5	G	513	MAN	O2-C2-C3	-2.07	106.11	110.17
5	G	522	MAN	O2-C2-C3	-2.06	106.13	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	MAN	O2-C2-C3	-2.05	106.14	110.17
5	A	517	MAN	O2-C2-C3	-2.05	106.14	110.17
5	G	532	MAN	O2-C2-C3	-2.04	106.17	110.17
4	A	524	NAG	C1-O5-C5	2.00	114.93	112.17
4	G	514	NAG	C1-O5-C5	2.02	114.95	112.17
5	G	505	MAN	C1-C2-C3	2.12	112.34	109.65
5	G	522	MAN	C1-O5-C5	2.12	115.09	112.17
5	A	533	MAN	C1-O5-C5	2.28	115.31	112.17
5	G	511	MAN	C1-O5-C5	2.29	115.33	112.17
5	A	511	MAN	C1-O5-C5	2.44	115.53	112.17
5	A	527	MAN	C1-O5-C5	2.48	115.58	112.17
5	G	536	MAN	C1-O5-C5	2.48	115.58	112.17
5	A	510	MAN	C1-O5-C5	2.48	115.59	112.17
5	G	530	MAN	C1-O5-C5	2.54	115.67	112.17
5	A	504	MAN	C1-O5-C5	2.59	115.74	112.17
5	G	519	MAN	C3-C4-C5	2.64	114.87	110.22
5	G	532	MAN	C1-O5-C5	2.67	115.85	112.17
5	A	519	MAN	C1-O5-C5	2.68	115.86	112.17
5	G	512	MAN	C1-O5-C5	2.73	115.93	112.17
5	A	529	MAN	C1-O5-C5	2.73	115.94	112.17
5	G	509	MAN	C1-O5-C5	2.76	115.97	112.17
5	G	535	MAN	C1-O5-C5	2.77	115.99	112.17
5	G	506	MAN	C1-O5-C5	2.78	116.00	112.17
5	A	528	MAN	C1-O5-C5	2.83	116.07	112.17
5	A	520	MAN	C1-O5-C5	2.89	116.14	112.17
5	A	532	MAN	C1-O5-C5	2.95	116.23	112.17
5	A	508	MAN	C1-O5-C5	2.99	116.29	112.17
5	G	524	MAN	C1-O5-C5	3.02	116.32	112.17
5	A	530	MAN	C1-O5-C5	3.11	116.45	112.17
5	A	505	MAN	C1-O5-C5	3.15	116.51	112.17
5	A	518	MAN	C1-O5-C5	3.19	116.56	112.17
5	G	523	MAN	C1-O5-C5	3.25	116.64	112.17
5	A	506	MAN	C1-O5-C5	3.28	116.69	112.17
5	G	508	MAN	C1-O5-C5	3.43	116.89	112.17
5	G	510	MAN	C1-O5-C5	3.45	116.92	112.17
5	G	518	MAN	C1-O5-C5	3.52	117.01	112.17
5	G	505	MAN	C1-O5-C5	3.54	117.05	112.17
5	G	513	MAN	C1-O5-C5	3.68	117.23	112.17
5	G	519	MAN	C1-O5-C5	3.85	117.47	112.17
5	A	509	MAN	C1-O5-C5	4.19	117.95	112.17
5	A	507	MAN	C1-O5-C5	4.34	118.15	112.17

There are no chirality outliers.

There are no torsion outliers.

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	518	MAN	C1-C2-C3-C4-C5-O5
5	A	527	MAN	C1-C2-C3-C4-C5-O5
5	G	522	MAN	C1-C2-C3-C4-C5-O5
5	G	505	MAN	C1-C2-C3-C4-C5-O5
5	A	504	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	2	0
4	A	513	NAG	1	0
4	A	514	NAG	3	0
4	A	515	NAG	1	0
4	A	523	NAG	1	0
4	A	525	NAG	1	0
6	B	301	EDO	1	0
6	B	302	EDO	2	0
4	G	527	NAG	1	0
6	G	537	EDO	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	337/344 (97%)	1.47	90 (26%) 1 1	66, 116, 187, 209	0
1	G	333/344 (96%)	0.57	32 (9%) 9 9	48, 93, 136, 171	0
2	B	225/229 (98%)	0.43	19 (8%) 12 12	48, 79, 148, 183	0
2	H	221/229 (96%)	0.45	19 (8%) 11 11	30, 63, 136, 171	0
3	C	219/219 (100%)	0.39	11 (5%) 30 32	37, 67, 140, 198	0
3	L	218/219 (99%)	0.42	17 (7%) 14 14	34, 63, 144, 181	0
All	All	1553/1584 (98%)	0.68	188 (12%) 5 5	30, 87, 158, 209	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	GLY	10.2
1	A	44	VAL	9.8
1	A	198	GLY	9.2
1	A	491	ILE	9.0
1	A	225	ILE	8.3
1	A	244	SER	8.1
1	A	223	TYR	7.5
1	A	89	VAL	7.4
1	A	45	TRP	7.4
2	B	138	LEU	7.2
2	H	189	LEU	7.1
1	A	217	TYR	6.6
1	A	91	GLU	6.2
1	A	90	THR	5.9
3	C	214	CYS	5.8
1	A	52	LEU	5.7
1	A	245	VAL	5.6
1	A	461	ASN	5.5
1	A	224	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	61	HIS	5.2
1	A	60	ALA	5.2
3	C	150	VAL	5.0
3	C	209	PHE	4.9
2	B	125	ALA	4.7
2	B	189	LEU	4.7
1	A	239	CYS	4.6
3	L	213	GLU	4.5
1	A	247	CYS	4.3
2	H	195	ILE	4.3
2	H	159	LEU	4.3
1	A	220	PRO	4.2
3	C	192	TYR	4.2
1	A	357	LYS	4.2
1	G	87	VAL	4.2
1	A	324	GLY	4.1
1	G	353	PHE	4.1
1	A	87	VAL	4.1
2	H	191	THR	4.1
3	L	191	VAL	4.0
1	A	221	ALA	4.0
1	A	254	VAL	4.0
1	A	488	VAL	3.9
1	A	492	GLU	3.9
1	A	80	ASN	3.9
1	A	462	ASN	3.9
1	A	489	VAL	3.9
1	A	246	GLN	3.9
3	L	209	PHE	3.8
1	A	93	PHE	3.8
2	B	130	SER	3.7
1	A	53	PHE	3.7
1	A	75	VAL	3.6
1	A	459	GLY	3.6
1	G	367	GLY	3.6
3	L	125	LEU	3.6
2	B	211	VAL	3.6
3	L	150	VAL	3.6
1	A	81	PRO	3.6
2	B	193	THR	3.6
1	A	352	HIS	3.5
2	H	154	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	156	SER	3.5
3	C	187	GLU	3.4
1	A	79	PRO	3.4
1	A	55	ALA	3.4
2	H	211	VAL	3.4
1	A	78	ASP	3.4
2	H	128	SER	3.4
2	B	131	THR	3.4
2	H	124	LEU	3.3
2	B	214	LYS	3.3
1	A	218	CYS	3.3
1	A	51	THR	3.3
1	A	227	LYS	3.3
1	A	83	GLU	3.3
1	A	59	LYS	3.3
1	A	48	ALA	3.2
1	G	277	LEU	3.2
3	L	192	TYR	3.2
1	A	219	THR	3.2
2	H	190	GLY	3.2
1	A	255	VAL	3.1
1	G	44	VAL	3.1
3	L	122	ASP	3.1
1	A	77	THR	3.1
1	A	350	LYS	3.1
1	G	124	GLY	3.1
1	G	430	VAL	3.1
2	B	194	TYR	3.1
2	B	158	ALA	3.0
3	C	152	ASN	3.0
1	A	46	ARG	3.0
2	H	138	LEU	2.9
2	H	194	TYR	2.9
1	A	238	PRO	2.9
1	A	349	LEU	2.9
1	A	50	THR	2.9
1	A	354	ASN	2.8
1	A	277	LEU	2.8
1	G	255	VAL	2.8
2	B	123	PRO	2.8
1	A	398	SER	2.7
2	H	186	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	458	GLY	2.7
3	L	118	PHE	2.7
1	A	201	ILE	2.7
3	C	183	LYS	2.7
3	L	190	LYS	2.7
1	G	324	GLY	2.7
1	A	226	LEU	2.7
1	G	122	LEU	2.7
1	G	242	VAL	2.6
1	A	351	GLU	2.6
3	C	184	ALA	2.6
1	A	269	GLU	2.6
1	G	221	ALA	2.6
1	A	353	PHE	2.5
1	A	199	SER	2.5
1	G	376	PHE	2.5
2	H	193	THR	2.5
1	A	85	HIS	2.5
3	L	88	CYS	2.5
1	A	490	GLU	2.5
1	A	72	HIS	2.5
3	L	210	ASN	2.5
1	A	202	LYS	2.4
2	H	185	PRO	2.4
1	G	352	HIS	2.4
1	A	452	ILE	2.4
1	A	243	SER	2.4
1	A	47	ASP	2.4
1	G	46	ARG	2.4
3	L	179	LEU	2.4
1	A	233	PHE	2.4
1	G	257	THR	2.4
1	A	229	ASN	2.4
1	G	349	LEU	2.4
1	A	54	CYS	2.4
3	C	126	LYS	2.3
1	A	358	THR	2.3
3	L	132	VAL	2.3
1	G	85	HIS	2.3
1	G	350	LYS	2.3
3	C	118	PHE	2.3
2	H	158	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	124	LEU	2.3
3	L	180	THR	2.3
1	G	89	VAL	2.3
1	G	464	SER	2.3
2	B	190	GLY	2.3
1	A	92	ASN	2.3
1	A	76	PRO	2.3
2	B	127	SER	2.3
3	L	186	TYR	2.2
2	B	208	ASP	2.2
3	L	151	ASP	2.2
2	B	207	VAL	2.2
1	G	240	LYS	2.2
1	A	49	ASP	2.2
1	A	260	LEU	2.2
2	H	212	GLU	2.2
1	A	99	LYS	2.2
1	A	487	LYS	2.2
1	A	71	THR	2.2
1	A	62	GLU	2.2
1	A	228	CYS	2.2
1	G	45	TRP	2.2
1	G	449	ILE	2.2
2	B	154	TRP	2.2
1	G	487	LYS	2.1
1	G	224	VAL	2.1
2	H	160	THR	2.1
1	A	326	ILE	2.1
3	C	122	ASP	2.1
1	A	256	SER	2.1
1	G	82	GLN	2.1
1	G	374	HIS	2.1
2	H	127	SER	2.1
1	A	365	SER	2.1
1	G	260	LEU	2.1
1	G	301	ASN	2.1
3	L	184	ALA	2.1
1	A	124	GLY	2.1
2	B	187	SER	2.0
1	G	93	PHE	2.0
1	A	116	LEU	2.0
1	A	478	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	152	VAL	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](#)

There are no carbohydrates in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	G	525	14/15	0.76	0.29	18.27	94,108,114,117	0
6	EDO	L	302	4/4	0.85	0.32	5.26	73,74,75,76	0
6	EDO	G	537	4/4	0.71	0.34	5.07	64,66,68,73	0
6	EDO	L	303	4/4	0.60	0.33	4.18	76,89,97,97	0
5	MAN	G	536	11/12	0.88	0.27	4.03	54,87,91,95	0
4	NAG	A	501	14/15	0.85	0.52	3.80	109,134,144,150	0
6	EDO	B	301	4/4	0.89	0.22	2.95	78,84,87,88	0
5	MAN	A	533	11/12	0.94	0.21	2.68	74,83,91,94	0
4	NAG	A	523	14/15	0.89	0.24	2.50	88,101,104,107	0
4	NAG	G	527	14/15	0.88	0.16	1.90	67,88,105,107	0
6	EDO	B	302	4/4	0.85	0.17	0.91	94,94,95,96	0
5	MAN	A	532	11/12	0.92	0.19	0.80	77,92,101,102	0
4	NAG	G	526	14/15	0.88	0.21	0.79	54,86,110,111	0
4	NAG	G	515	14/15	0.84	0.20	0.54	67,83,100,100	0
4	NAG	A	513	14/15	0.83	0.28	0.46	99,120,127,135	0
4	NAG	G	501	14/15	0.91	0.18	-0.00	81,98,119,122	0
4	NAG	G	503	14/15	0.96	0.19	-0.09	37,45,50,51	0
5	MAN	A	506	11/12	0.90	0.14	-0.26	65,69,75,78	0
4	NAG	G	528	14/15	0.93	0.16	-0.39	41,50,56,57	0
5	MAN	G	532	11/12	0.87	0.13	-0.43	72,79,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	G	504	14/15	0.96	0.14	-0.51	29,51,58,64	0
4	NAG	A	525	14/15	0.94	0.15	-0.60	42,64,73,78	0
5	MAN	G	507	11/12	0.96	0.13	-0.84	33,40,45,47	0
4	NAG	A	502	14/15	0.96	0.17	-0.86	44,59,83,89	0
4	NAG	C	301	14/15	0.97	0.10	-0.95	57,62,72,76	0
6	EDO	A	534	4/4	0.90	0.13	-0.96	99,99,101,103	0
4	NAG	A	515	14/15	0.92	0.12	-1.19	61,75,94,95	0
4	NAG	A	522	14/15	0.90	0.10	-1.22	67,76,82,89	0
4	NAG	G	520	14/15	0.87	0.13	-1.27	70,83,92,93	0
4	NAG	A	503	14/15	0.94	0.12	-1.33	64,68,76,82	0
5	MAN	G	512	11/12	0.94	0.11	-1.51	47,52,64,64	0
5	MAN	G	509	11/12	0.94	0.12	-1.51	68,75,86,93	0
4	NAG	L	301	14/15	0.97	0.10	-1.77	34,57,68,69	0
5	MAN	A	518	11/12	0.91	0.14	-	66,74,86,97	0
4	NAG	A	514	14/15	0.74	0.40	-	142,146,149,151	0
5	MAN	A	531	11/12	0.89	0.14	-	97,107,112,113	0
4	NAG	G	514	14/15	0.79	0.20	-	87,100,115,123	0
5	MAN	A	520	11/12	0.82	0.55	-	109,119,128,131	0
5	MAN	G	511	11/12	0.96	0.13	-	48,51,63,71	0
5	MAN	G	513	11/12	0.86	0.19	-	108,125,126,127	0
5	MAN	A	519	11/12	0.78	0.30	-	111,120,129,134	0
5	MAN	G	533	11/12	0.94	0.12	-	84,88,96,98	0
5	MAN	A	505	11/12	0.96	0.13	-	56,59,66,68	0
5	MAN	G	519	11/12	0.58	0.39	-	136,142,145,149	0
5	MAN	G	530	11/12	0.98	0.11	-	50,59,64,66	0
5	MAN	A	504	11/12	0.91	0.16	-	56,65,75,81	0
4	NAG	G	516	14/15	0.85	0.20	-	65,98,109,118	0
5	MAN	A	508	11/12	0.88	0.13	-	76,83,91,105	0
4	NAG	A	521	14/15	0.79	0.31	-	99,114,127,131	0
5	MAN	A	510	11/12	0.96	0.14	-	66,71,85,92	0
5	MAN	G	505	11/12	0.93	0.13	-	35,42,56,59	0
5	MAN	A	507	11/12	0.94	0.13	-	61,64,84,85	0
6	EDO	H	301	4/4	0.85	0.24	-	57,62,64,70	0
4	NAG	A	524	14/15	0.65	0.55	-	118,135,139,142	0
5	MAN	G	535	11/12	0.84	0.12	-	59,72,78,81	0
5	MAN	G	534	11/12	0.94	0.12	-	71,73,85,89	0
4	NAG	G	529	14/15	0.96	0.13	-	44,49,53,59	0
4	NAG	A	516	14/15	0.85	0.21	-	92,97,102,104	0
5	MAN	G	522	11/12	0.88	0.20	-	77,83,86,87	0
4	NAG	G	502	14/15	0.50	0.46	-	101,124,133,135	0
5	MAN	A	530	11/12	0.91	0.12	-	100,111,116,119	0
5	MAN	A	517	11/12	0.90	0.15	-	81,96,106,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MAN	A	509	11/12	0.86	0.19	-	119,124,129,130	0
5	MAN	G	506	11/12	0.95	0.16	-	36,38,43,46	0
4	NAG	A	512	14/15	0.81	0.36	-	103,120,126,128	0
5	MAN	G	518	11/12	0.82	0.38	-	132,136,138,139	0
5	MAN	A	527	11/12	0.91	0.12	-	66,78,85,87	0
5	MAN	A	529	11/12	0.92	0.13	-	82,91,95,96	0
4	NAG	A	526	14/15	0.94	0.13	-	57,72,83,89	0
5	MAN	G	510	11/12	0.83	0.13	-	82,89,105,119	0
5	MAN	G	508	11/12	0.97	0.16	-	44,48,53,54	0
5	MAN	A	528	11/12	0.87	0.12	-	66,86,93,101	0
5	MAN	G	517	11/12	0.71	0.37	-	128,134,140,145	0
5	MAN	G	523	11/12	0.90	0.14	-	50,71,78,91	0
5	MAN	A	511	11/12	0.90	0.17	-	86,91,96,99	0
7	ACT	B	303	4/4	0.89	0.18	-	82,88,90,90	0
5	MAN	G	531	11/12	0.94	0.10	-	54,57,72,75	0
4	NAG	G	521	14/15	0.85	0.18	-	76,89,97,98	0
5	MAN	G	524	11/12	0.75	0.40	-	88,101,109,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.