



Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2017 – 06:17 PM EDT

PDB ID : 5UTF
Title : Crystal Structure of a Stabilized DS-SOSIP.6mut BG505 gp140 HIV-1 Env Trimer, Containing Mutations I201C-P433C (DS), L154M, Y177W, N300M, N302M, T320L, I420M in Complex with Human Antibodies PGT122 and 35O22 at 4.3 Å
Authors : Pancera, M.; Chuang, G.-Y.; Xu, K.; Kwong, P.D.
Deposited on : 2017-02-14
Resolution : 3.50 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-20029077
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-20029077

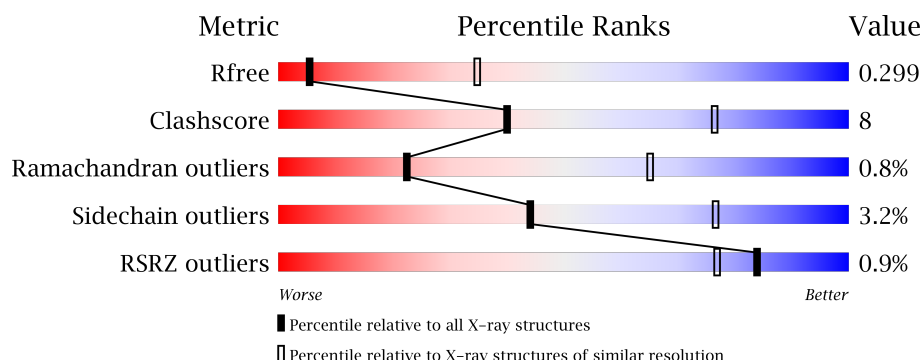
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	G	481	
2	B	153	
3	L	213	
4	H	235	
5	D	243	

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Mol	Chain	Length	Quality of chain
6	E	216	<div><div></div><div>2%</div><div>78%</div><div>20%</div><div></div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11964 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	439	Total	C	N	O	S	0	0	0
			3464	2179	609	642	34			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	154	MET	LEU	engineered mutation	UNP Q2N0S6
G	177	TRP	TYR	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6
G	300	MET	ASN	engineered mutation	UNP Q2N0S6
G	302	MET	ASN	engineered mutation	UNP Q2N0S6
G	320	LEU	THR	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	420	MET	ILE	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	GLU	engineered mutation	UNP Q2N0S6
G	510	ARG	LYS	engineered mutation	UNP Q2N0S6
G	512	ARG	ALA	engineered mutation	UNP Q2N0S6
G	513	ARG	VAL	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	0	0
			980	620	169	185	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

- Molecule 4 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

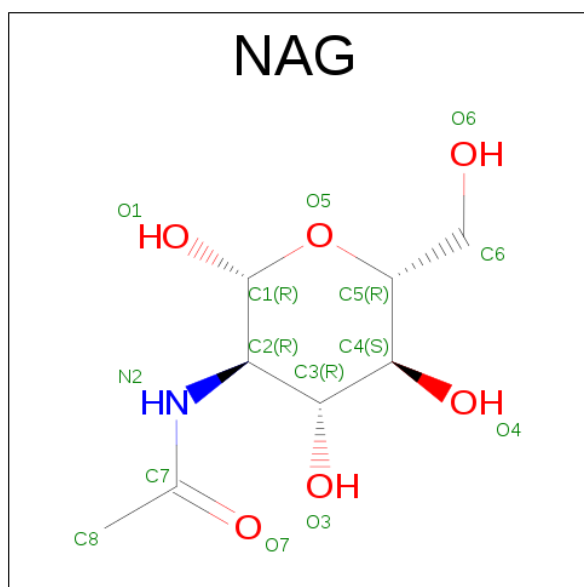
- Molecule 5 is a protein called 35022 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 6 is a protein called 35022 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

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



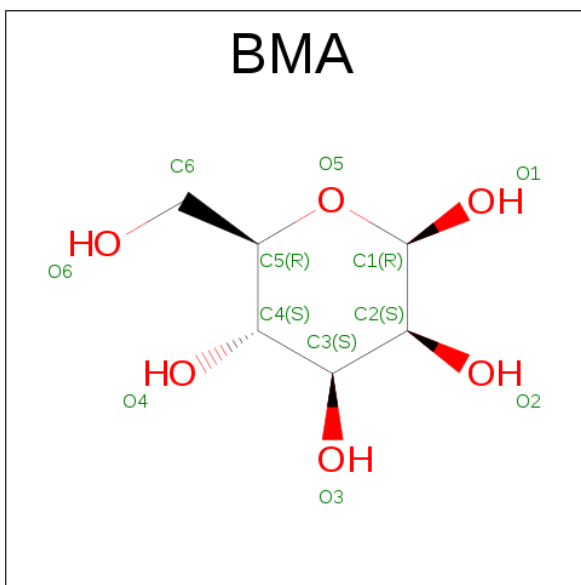
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1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

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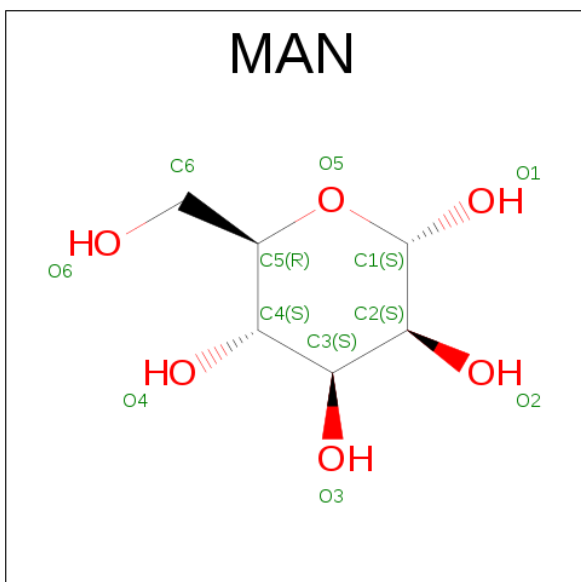
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1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

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



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

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

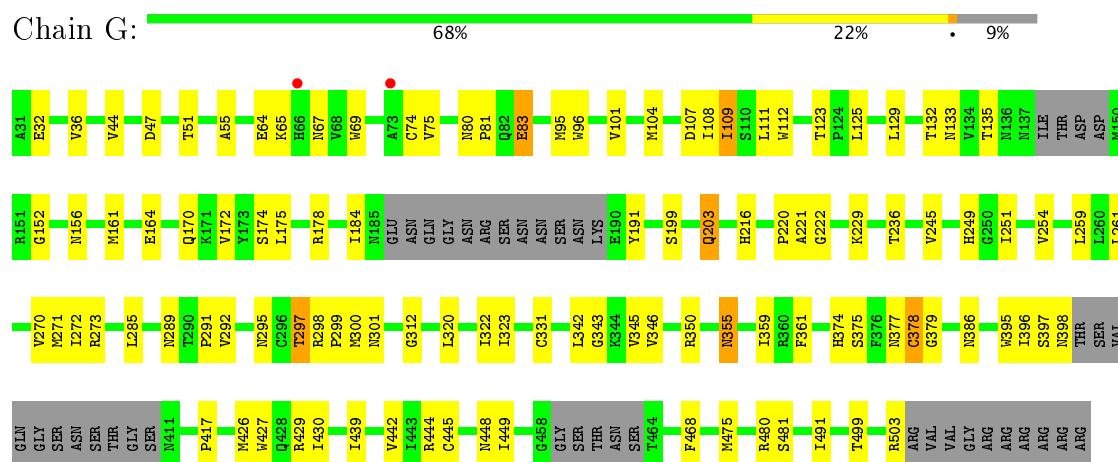


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9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

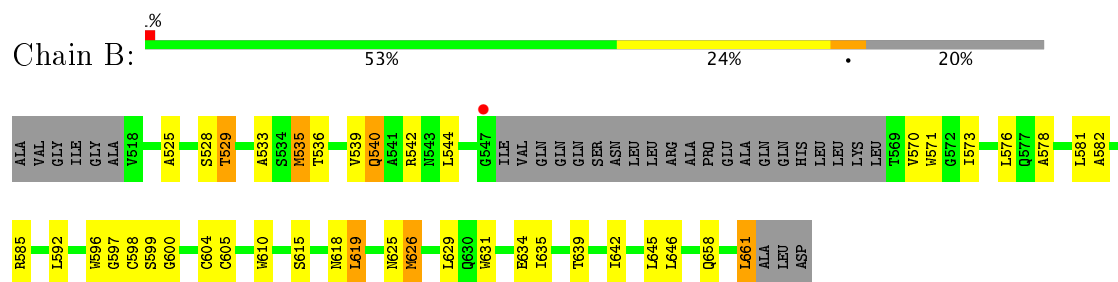
3 Residue-property plots [i](#)

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.

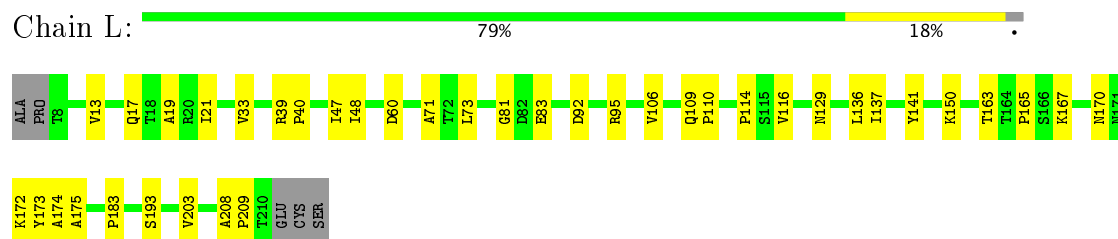
- Molecule 1: Envelope glycoprotein gp120



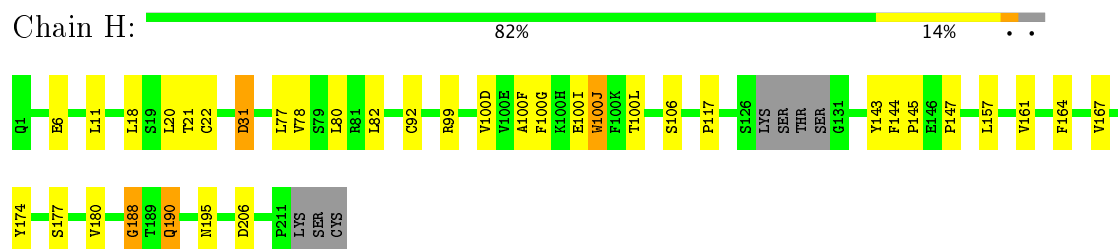
- Molecule 2: Envelope glycoprotein gp41



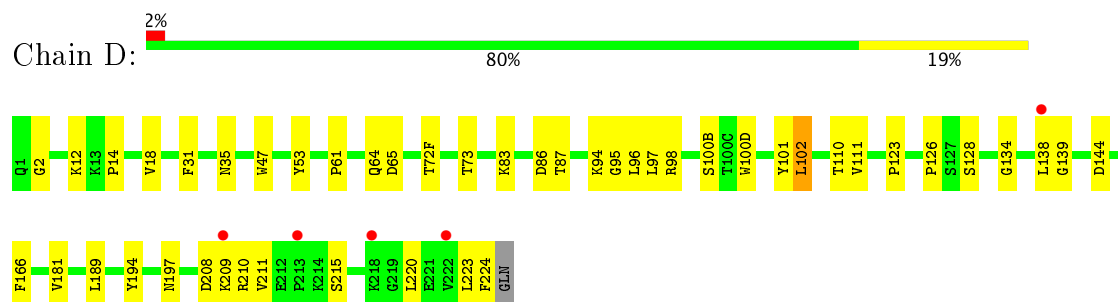
- Molecule 3: PGT122 Light chain



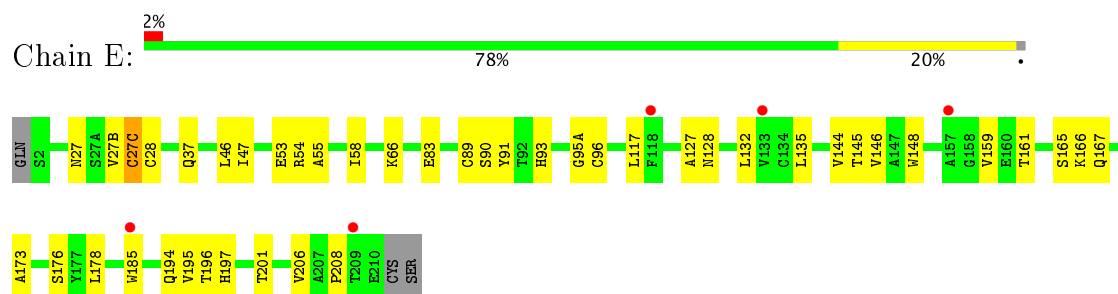
- Molecule 4: PGT122 Heavy chain



• Molecule 5: 35022 Heavy chain



• Molecule 6: 35022 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	128.38Å 128.38Å 313.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.98 – 3.50 38.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	50.8 (38.98-3.50) 50.8 (38.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.215 , 0.299 0.214 , 0.299	Depositor DCC
R_{free} test set	948 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 12.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.156 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11964	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: BMA, NAG, 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	G	0.28	0/3537	0.47	0/4796
2	B	0.26	0/998	0.45	0/1353
3	L	0.27	0/1619	0.47	0/2217
4	H	0.26	0/1789	0.47	0/2443
5	D	0.25	0/1880	0.46	0/2560
6	E	0.25	0/1659	0.45	0/2269
All	All	0.26	0/11482	0.46	0/15638

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	G	3464	0	3394	68	0
2	B	980	0	955	27	0
3	L	1577	0	1518	25	0
4	H	1742	0	1716	26	0
5	D	1832	0	1806	30	0
6	E	1615	0	1542	31	0
7	B	42	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	448	0	397	14	0
8	G	55	0	42	1	0
9	G	209	0	179	4	0
All	All	11964	0	11588	195	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 8.

All (195) 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:163:THR:HG22	4:H:167:VAL:HB	1.58	0.84
7:G:648:NAG:H2	4:H:100(D):VAL:HA	1.59	0.82
1:G:350:ARG:NH2	1:G:396:ILE:O	2.13	0.81
7:B:702:NAG:H83	6:E:54:ARG:HH21	1.52	0.73
2:B:536:THR:O	2:B:540:GLN:NE2	2.23	0.72
1:G:221:ALA:HB3	2:B:582:ALA:HB1	1.73	0.71
1:G:291:PRO:HG3	7:G:631:NAG:H61	1.73	0.70
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.75	0.67
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.58	0.67
3:L:137:ILE:HB	3:L:175:ALA:HB3	1.78	0.66
6:E:37:GLN:HB2	6:E:47:ILE:HD11	1.77	0.65
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.77	0.65
3:L:39:ARG:NH1	3:L:81:GLY:O	2.30	0.65
1:G:298:ARG:NH2	1:G:439:ILE:O	2.30	0.65
3:L:116:VAL:HG12	3:L:137:ILE:HG23	1.80	0.64
5:D:12:LYS:HG3	5:D:18:VAL:HB	1.80	0.63
5:D:72(F):THR:HG1	5:D:73:THR:HG1	1.47	0.63
1:G:175:LEU:HB3	1:G:320:LEU:HB2	1.80	0.63
2:B:539:VAL:HG13	2:B:542:ARG:HH22	1.63	0.63
3:L:170:ASN:HB3	3:L:172:LYS:H	1.63	0.63
4:H:11:LEU:HB2	4:H:145:PRO:HG3	1.83	0.61
5:D:72(F):THR:OG1	5:D:73:THR:OG1	2.20	0.59
2:B:625:ASN:HB2	5:D:97:LEU:HD22	1.84	0.59
4:H:100(D):VAL:O	4:H:100(F):ALA:N	2.34	0.58
1:G:426:MET:HB3	1:G:427:TRP:CE3	2.39	0.58
7:G:602:NAG:H3	7:G:602:NAG:H83	1.86	0.58
1:G:109:ILE:HG12	1:G:430:ILE:HG21	1.85	0.58
2:B:525:ALA:HB1	2:B:528:SER:HB2	1.86	0.58
7:G:622:NAG:H83	7:G:622:NAG:H3	1.86	0.57
5:D:35:ASN:HD21	5:D:100(D):TRP:HE3	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:VAL:HB	1:G:449:ILE:HB	1.86	0.57
1:G:261:LEU:HD11	1:G:374:HIS:CE1	2.39	0.56
7:G:640:NAG:H83	7:G:640:NAG:H3	1.87	0.56
3:L:13:VAL:HG21	3:L:19:ALA:HA	1.88	0.56
6:E:165:SER:O	6:E:173:ALA:N	2.37	0.55
1:G:261:LEU:HD11	1:G:374:HIS:HE1	1.71	0.55
1:G:379:GLY:N	7:G:617:NAG:O6	2.39	0.55
4:H:188:GLY:HA3	4:H:190:GLN:N	2.21	0.55
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.89	0.55
5:D:126:PRO:HB2	5:D:215:SER:HB2	1.89	0.54
1:G:297:THR:HG23	1:G:444:ARG:HG3	1.88	0.54
1:G:83:GLU:HG2	1:G:245:VAL:HG22	1.90	0.54
3:L:33:VAL:HG11	3:L:71:ALA:HB1	1.90	0.54
2:B:598:CYS:O	2:B:600:GLY:N	2.40	0.54
1:G:132:THR:HA	7:G:633:NAG:H82	1.89	0.54
1:G:108:ILE:HD13	1:G:111:LEU:HD12	1.90	0.54
1:G:503:ARG:HD2	2:B:605:CYS:O	2.07	0.54
6:E:145:THR:OG1	6:E:196:THR:HB	2.08	0.54
9:G:610:MAN:H5	6:E:93:HIS:NE2	2.23	0.54
4:H:20:LEU:HB2	4:H:80:LEU:HB3	1.89	0.53
1:G:503:ARG:NH1	2:B:597:GLY:HA3	2.23	0.53
4:H:99:ARG:HD3	4:H:100(J):TRP:CZ3	2.43	0.53
1:G:270:VAL:HG12	1:G:289:ASN:H	1.74	0.53
4:H:21:THR:HG23	4:H:77:LEU:HD13	1.90	0.53
3:L:92:ASP:HB3	3:L:95:ARG:HB2	1.90	0.53
6:E:127:ALA:N	6:E:128:ASN:HA	2.24	0.53
1:G:396:ILE:HG22	1:G:397:SER:H	1.73	0.53
4:H:157:LEU:HD21	4:H:180:VAL:HG11	1.90	0.53
4:H:22:CYS:HB3	4:H:78:VAL:HB	1.91	0.52
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.91	0.52
1:G:96:TRP:HH2	1:G:285:LEU:HG	1.74	0.52
3:L:150:LYS:HB2	3:L:193:SER:HB2	1.90	0.52
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.92	0.52
2:B:634:GLU:HA	7:B:703:NAG:H82	1.91	0.51
3:L:39:ARG:HG3	3:L:40:PRO:HD2	1.91	0.51
7:B:702:NAG:H62	6:E:53:GLU:HG2	1.93	0.51
6:E:54:ARG:HD2	6:E:58:ILE:HG22	1.93	0.51
4:H:117:PRO:HB3	4:H:143:TYR:HB3	1.92	0.51
1:G:272:ILE:HD11	1:G:345:VAL:HG13	1.92	0.51
4:H:31:ASP:OD1	4:H:31:ASP:N	2.43	0.51
5:D:2:GLY:H	5:D:102:LEU:HD11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:96:LEU:HD13	5:D:101:TYR:HB2	1.94	0.50
1:G:295:ASN:O	1:G:331:CYS:HA	2.11	0.50
1:G:222:GLY:HA3	2:B:585:ARG:HD3	1.94	0.50
6:E:144:VAL:HG12	6:E:197:HIS:HB2	1.92	0.50
4:H:161:VAL:HG22	4:H:180:VAL:HG22	1.93	0.49
6:E:185:TRP:CZ3	6:E:208:PRO:HG3	2.47	0.49
1:G:448:ASN:HD22	7:G:631:NAG:H83	1.76	0.49
5:D:134:GLY:HA2	5:D:223:LEU:HD13	1.94	0.49
2:B:529:THR:O	2:B:533:ALA:N	2.40	0.49
6:E:46:LEU:HG	6:E:55:ALA:HB2	1.96	0.48
1:G:174:SER:OG	1:G:175:LEU:N	2.46	0.48
1:G:254:VAL:HG11	1:G:261:LEU:HB2	1.95	0.48
9:G:608:MAN:H2	6:E:93:HIS:CG	2.49	0.47
1:G:350:ARG:HD3	1:G:355:ASN:O	2.14	0.47
6:E:27(C):CYS:HA	6:E:28:CYS:HA	1.65	0.47
1:G:95:MET:SD	1:G:273:ARG:HD3	2.53	0.47
3:L:167:LYS:HB3	3:L:173:TYR:CZ	2.49	0.47
2:B:618:ASN:OD1	2:B:619:LEU:N	2.44	0.47
4:H:106:SER:HB3	4:H:147:PRO:HD3	1.96	0.47
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.96	0.47
4:H:6:GLU:N	4:H:6:GLU:OE1	2.47	0.47
7:G:601:NAG:O6	5:D:31:PHE:HA	2.15	0.46
5:D:47:TRP:CZ3	6:E:95(A):GLY:HA3	2.50	0.46
1:G:51:THR:HB	2:B:578:ALA:HB2	1.97	0.46
4:H:100(D):VAL:HG21	4:H:100(G):PHE:HD2	1.80	0.46
2:B:529:THR:HG22	2:B:626:MET:H	1.79	0.46
6:E:132:LEU:HD12	6:E:178:LEU:HD23	1.96	0.46
3:L:129:ASN:HA	3:L:183:PRO:HG2	1.98	0.46
6:E:27(B):VAL:O	6:E:90:SER:OG	2.19	0.46
6:E:165:SER:N	6:E:173:ALA:O	2.33	0.46
1:G:361:PHE:HE2	1:G:395:TRP:CD1	2.33	0.46
1:G:152:GLY:C	1:G:178:ARG:HH21	2.19	0.45
1:G:271:MET:HG2	1:G:273:ARG:CZ	2.46	0.45
1:G:427:TRP:CD1	1:G:475:MET:HG3	2.51	0.45
1:G:36:VAL:HG12	2:B:610:TRP:CE3	2.45	0.45
5:D:138:LEU:HD13	5:D:211:VAL:HG11	1.97	0.45
5:D:194:TYR:O	5:D:210:ARG:HD2	2.16	0.45
5:D:61:PRO:HA	5:D:64:GLN:HB2	1.97	0.45
1:G:164:GLU:HG3	1:G:312:GLY:HA3	1.99	0.45
1:G:270:VAL:HG12	1:G:289:ASN:N	2.31	0.45
1:G:74:CYS:SG	1:G:75:VAL:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:167:LYS:HB3	3:L:173:TYR:CE2	2.52	0.45
7:G:614:NAG:H62	7:G:615:NAG:C7	2.47	0.45
1:G:377:ASN:OD1	1:G:378:CYS:N	2.50	0.45
3:L:165:PRO:HA	3:L:174:ALA:O	2.17	0.45
3:L:60:ASP:N	3:L:60:ASP:OD1	2.50	0.45
6:E:196:THR:HA	6:E:201:THR:HA	1.98	0.45
5:D:14:PRO:HG3	5:D:111:VAL:HG12	2.00	0.44
1:G:161:MET:HB3	1:G:170:GLN:HB3	2.00	0.44
4:H:195:ASN:ND2	4:H:206:ASP:OD1	2.48	0.44
4:H:157:LEU:O	4:H:161:VAL:HG21	2.18	0.44
2:B:642:ILE:O	2:B:646:LEU:HD12	2.18	0.44
5:D:100(B):SER:OG	6:E:91:TYR:OH	2.28	0.44
5:D:139:GLY:HA3	5:D:181:VAL:HA	1.98	0.44
6:E:117:LEU:HD23	6:E:206:VAL:HG13	1.99	0.44
2:B:570:VAL:HG12	2:B:571:TRP:H	1.83	0.44
1:G:132:THR:OG1	1:G:133:ASN:N	2.51	0.44
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.53	0.44
8:G:603:BMA:H61	9:G:604:MAN:H2	1.42	0.44
6:E:148:TRP:CD1	6:E:159:VAL:HG13	2.53	0.43
6:E:83:GLU:O	6:E:166:LYS:NZ	2.40	0.43
1:G:343:GLY:HA2	1:G:346:VAL:HG12	1.99	0.43
1:G:156:ASN:HA	1:G:175:LEU:HD12	2.00	0.43
1:G:299:PRO:HA	1:G:442:VAL:HG22	2.00	0.43
1:G:491:ILE:O	2:B:585:ARG:NH2	2.43	0.43
3:L:109:GLN:HG3	3:L:141:TYR:CZ	2.52	0.43
1:G:259:LEU:HD12	1:G:374:HIS:CD2	2.54	0.43
4:H:188:GLY:HA3	4:H:190:GLN:H	1.83	0.43
4:H:18:LEU:HB3	4:H:82:LEU:HB3	2.00	0.43
5:D:100(D):TRP:CZ2	6:E:91:TYR:HB2	2.54	0.43
6:E:27:ASN:HA	6:E:27(C):CYS:O	2.19	0.43
1:G:359:ILE:HD12	1:G:468:PHE:HE2	1.84	0.42
1:G:44:VAL:HA	2:B:629:LEU:HD23	2.00	0.42
1:G:203:GLN:HE21	1:G:203:GLN:HB3	1.59	0.42
3:L:174:ALA:HB1	4:H:164:PHE:CD2	2.54	0.42
9:G:652:MAN:H2	9:G:656:MAN:H2	1.71	0.42
2:B:529:THR:HG23	5:D:98:ARG:HD2	2.00	0.42
6:E:167:GLN:OE1	6:E:173:ALA:HB2	2.19	0.42
3:L:114:PRO:HG2	3:L:203:VAL:HG21	2.02	0.42
5:D:94:LYS:HD3	5:D:102:LEU:HB2	2.02	0.42
7:G:627:NAG:H61	7:G:628:NAG:N2	2.35	0.42
4:H:6:GLU:OE2	4:H:92:CYS:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:87:THR:HG23	5:D:110:THR:HA	2.02	0.42
5:D:220:LEU:HD12	5:D:223:LEU:HD12	2.02	0.42
1:G:107:ASP:O	1:G:111:LEU:HG	2.20	0.42
1:G:221:ALA:HB1	2:B:544:LEU:O	2.20	0.42
6:E:146:VAL:HG22	6:E:195:VAL:HG22	2.01	0.42
3:L:95:ARG:HD3	3:L:95:ARG:HA	1.77	0.42
1:G:300:MET:HE2	1:G:322:ILE:HG21	2.02	0.41
1:G:503:ARG:HH12	2:B:597:GLY:HA3	1.84	0.41
6:E:146:VAL:HA	6:E:194:GLN:O	2.20	0.41
3:L:208:ALA:HA	3:L:209:PRO:HD3	1.94	0.41
1:G:301:ASN:HB3	1:G:323:ILE:O	2.19	0.41
4:H:144:PHE:HA	4:H:145:PRO:HA	1.86	0.41
5:D:197:ASN:ND2	5:D:208:ASP:OD1	2.50	0.41
5:D:166:PHE:CZ	6:E:135:LEU:HB3	2.55	0.41
6:E:161:THR:HG23	6:E:176:SER:HB2	2.01	0.41
3:L:83:GLU:HB2	3:L:106:VAL:HG23	2.01	0.41
1:G:109:ILE:HG23	1:G:430:ILE:HG12	2.03	0.41
1:G:261:LEU:HA	1:G:448:ASN:O	2.20	0.41
7:G:629:NAG:H4	7:G:630:NAG:N2	2.35	0.41
2:B:535:MET:H	2:B:535:MET:HG2	1.65	0.41
2:B:592:LEU:HD22	2:B:596:TRP:CZ2	2.55	0.41
1:G:64:GLU:HG3	1:G:65:LYS:H	1.86	0.41
1:G:108:ILE:HG22	1:G:427:TRP:CZ2	2.55	0.41
1:G:112:TRP:CG	1:G:427:TRP:HZ3	2.38	0.41
5:D:83:LYS:N	5:D:86:ASP:OD2	2.52	0.41
5:D:189:LEU:HD21	5:D:224:PHE:HE1	1.86	0.41
6:E:28:CYS:HB3	6:E:66:LYS:HD2	2.03	0.41
1:G:170:GLN:HG2	1:G:172:VAL:HG13	2.03	0.41
1:G:249:HIS:O	1:G:251:ILE:HG13	2.21	0.41
4:H:100(D):VAL:HG22	4:H:100(I):GLU:OE1	2.20	0.41
4:H:167:VAL:O	4:H:174:TYR:HA	2.21	0.41
1:G:104:MET:O	1:G:108:ILE:HG12	2.21	0.41
1:G:129:LEU:O	1:G:191:TYR:N	2.51	0.41
1:G:101:VAL:HG21	1:G:480:ARG:HG2	2.03	0.41
1:G:83:GLU:OE1	1:G:229:LYS:HD3	2.20	0.41
7:G:601:NAG:H5	5:D:53:TYR:CD2	2.56	0.41
2:B:661:LEU:HA	2:B:661:LEU:HD13	1.82	0.40
5:D:94:LYS:HG2	5:D:95:GLY:O	2.21	0.40
6:E:161:THR:HA	6:E:176:SER:HA	2.03	0.40
3:L:13:VAL:HG13	3:L:17:GLN:HB2	2.03	0.40
1:G:445:CYS:HB3	7:G:617:NAG:H61	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:136:LEU:HD11	4:H:177:SER:HB2	2.02	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	G	429/481 (89%)	371 (86%)	52 (12%)	6 (1%)	13	53
2	B	119/153 (78%)	105 (88%)	12 (10%)	2 (2%)	11	49
3	L	206/213 (97%)	187 (91%)	18 (9%)	1 (0%)	32	73
4	H	224/235 (95%)	207 (92%)	15 (7%)	2 (1%)	20	63
5	D	240/243 (99%)	223 (93%)	16 (7%)	1 (0%)	38	77
6	E	211/216 (98%)	191 (90%)	20 (10%)	0	100	100
All	All	1429/1541 (93%)	1284 (90%)	133 (9%)	12 (1%)	22	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	81	PRO
2	B	599	SER
3	L	110	PRO
4	H	190	GLN
1	G	67	ASN
1	G	69	TRP
2	B	615	SER
1	G	80	ASN
1	G	135	THR
4	H	188	GLY
5	D	144	ASP
1	G	220	PRO

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	G	392/429 (91%)	373 (95%)	19 (5%)	30	67
2	B	106/129 (82%)	93 (88%)	13 (12%)	5	27
3	L	177/181 (98%)	177 (100%)	0	100	100
4	H	198/205 (97%)	195 (98%)	3 (2%)	70	88
5	D	205/206 (100%)	203 (99%)	2 (1%)	80	91
6	E	186/189 (98%)	183 (98%)	3 (2%)	68	87
All	All	1264/1339 (94%)	1224 (97%)	40 (3%)	44	76

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	32	GLU
1	G	47	ASP
1	G	83	GLU
1	G	109	ILE
1	G	123	THR
1	G	125	LEU
1	G	184	ILE
1	G	199	SER
1	G	203	GLN
1	G	236	THR
1	G	297	THR
1	G	342	LEU
1	G	355	ASN
1	G	375	SER
1	G	378	CYS
1	G	398	ASN
1	G	429	ARG
1	G	481	SER
1	G	499	THR
2	B	529	THR
2	B	535	MET
2	B	540	GLN

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Mol	Chain	Res	Type
2	B	573	ILE
2	B	576	LEU
2	B	581	LEU
2	B	604	CYS
2	B	619	LEU
2	B	626	MET
2	B	639	THR
2	B	645	LEU
2	B	658	GLN
2	B	661	LEU
4	H	31	ASP
4	H	100(J)	TRP
4	H	100(L)	THR
5	D	65	ASP
5	D	102	LEU
6	E	27(C)	CYS
6	E	89	CYS
6	E	96	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	203	GLN
1	G	374	HIS
2	B	540	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

59 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$
7	NAG	B	701	2	14,14,15	0.32	0	15,19,21	0.63	0
7	NAG	B	702	2	14,14,15	0.32	0	15,19,21	0.40	0
7	NAG	B	703	2	14,14,15	0.45	0	15,19,21	0.42	0
7	NAG	G	601	1,7	14,14,15	0.16	0	15,19,21	0.78	1 (6%)
7	NAG	G	602	8,7	14,14,15	0.45	0	15,19,21	1.43	3 (20%)
8	BMA	G	603	9,7	11,11,12	0.79	0	13,15,17	0.91	0
9	MAN	G	604	9,8	11,11,12	1.33	1 (9%)	13,15,17	1.99	4 (30%)
9	MAN	G	605	9	11,11,12	0.86	0	13,15,17	1.36	1 (7%)
9	MAN	G	606	9	11,11,12	1.00	0	13,15,17	1.32	2 (15%)
9	MAN	G	607	9	11,11,12	0.72	0	13,15,17	1.43	2 (15%)
9	MAN	G	608	9,8	11,11,12	0.73	0	13,15,17	1.25	2 (15%)
9	MAN	G	609	9	11,11,12	0.75	0	13,15,17	0.92	0
9	MAN	G	610	9	11,11,12	0.69	0	13,15,17	1.53	2 (15%)
7	NAG	G	611	1,7	14,14,15	0.46	0	15,19,21	0.46	0
7	NAG	G	612	8,7	14,14,15	0.38	0	15,19,21	0.44	0
8	BMA	G	613	7	11,11,12	0.51	0	13,15,17	0.94	1 (7%)
7	NAG	G	614	1,7	14,14,15	0.29	0	15,19,21	0.49	0
7	NAG	G	615	7	14,14,15	0.34	0	15,19,21	0.59	0
7	NAG	G	616	1,7	14,14,15	0.30	0	15,19,21	0.56	0
7	NAG	G	617	8,7	14,14,15	0.41	0	15,19,21	0.51	0
8	BMA	G	618	9,7	11,11,12	0.93	0	13,15,17	0.93	0
9	MAN	G	619	8	11,11,12	0.79	0	13,15,17	1.11	2 (15%)
9	MAN	G	620	9,8	11,11,12	0.98	0	13,15,17	1.03	1 (7%)
9	MAN	G	621	9	11,11,12	0.89	1 (9%)	13,15,17	1.35	2 (15%)
7	NAG	G	622	1	14,14,15	0.59	0	15,19,21	1.28	1 (6%)
7	NAG	G	623	1	14,14,15	0.42	0	15,19,21	0.42	0
7	NAG	G	624	1	14,14,15	0.20	0	15,19,21	0.56	0
7	NAG	G	625	1,7	14,14,15	0.38	0	15,19,21	0.56	0
7	NAG	G	626	7	14,14,15	0.15	0	15,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	627	1,7	14,14,15	0.34	0	15,19,21	0.60	0
7	NAG	G	628	7	14,14,15	0.42	0	15,19,21	0.63	0
7	NAG	G	629	1,7	14,14,15	0.24	0	15,19,21	0.62	0
7	NAG	G	630	7	14,14,15	0.73	0	15,19,21	0.74	1 (6%)
7	NAG	G	631	1,7	14,14,15	0.18	0	15,19,21	0.59	0
7	NAG	G	632	7	14,14,15	0.21	0	15,19,21	0.49	0
7	NAG	G	633	1	14,14,15	0.45	0	15,19,21	0.69	1 (6%)
7	NAG	G	634	1,7	14,14,15	0.23	0	15,19,21	0.58	0
7	NAG	G	635	8,7	14,14,15	0.25	0	15,19,21	0.53	0
8	BMA	G	636	9,7	11,11,12	0.75	0	13,15,17	0.74	0
9	MAN	G	637	8	11,11,12	0.83	0	13,15,17	1.33	3 (23%)
9	MAN	G	638	8	11,11,12	0.66	0	13,15,17	1.62	3 (23%)
7	NAG	G	639	1,7	14,14,15	0.25	0	15,19,21	0.56	0
7	NAG	G	640	7	14,14,15	0.60	0	15,19,21	1.40	2 (13%)
7	NAG	G	641	1,7	14,14,15	0.17	0	15,19,21	0.48	0
7	NAG	G	642	7	14,14,15	0.32	0	15,19,21	0.52	0
7	NAG	G	643	1,7	14,14,15	0.31	0	15,19,21	0.57	0
7	NAG	G	644	7	14,14,15	0.20	0	15,19,21	0.46	0
7	NAG	G	645	1,7	14,14,15	0.38	0	15,19,21	0.35	0
7	NAG	G	646	7	14,14,15	0.15	0	15,19,21	0.57	0
7	NAG	G	647	1,7	14,14,15	0.39	0	15,19,21	0.45	0
7	NAG	G	648	8,7	14,14,15	0.30	0	15,19,21	0.78	0
8	BMA	G	649	9,7	11,11,12	1.05	0	13,15,17	1.32	3 (23%)
9	MAN	G	650	9,8	11,11,12	1.09	1 (9%)	13,15,17	0.86	1 (7%)
9	MAN	G	651	9	11,11,12	0.77	0	13,15,17	1.04	2 (15%)
9	MAN	G	652	9	11,11,12	0.75	0	13,15,17	1.11	2 (15%)
9	MAN	G	653	9,8	11,11,12	0.87	0	13,15,17	1.23	3 (23%)
9	MAN	G	654	9	11,11,12	0.76	0	13,15,17	1.33	2 (15%)
9	MAN	G	655	9	11,11,12	0.59	0	13,15,17	1.41	2 (15%)
9	MAN	G	656	9	11,11,12	0.91	0	13,15,17	1.26	2 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	701	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	0/6/23/26	0/1/1/1
7	NAG	B	703	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	602	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	603	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	604	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	605	9	-	0/2/19/22	0/1/1/1
9	MAN	G	606	9	-	0/2/19/22	0/1/1/1
9	MAN	G	607	9	-	0/2/19/22	0/1/1/1
9	MAN	G	608	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	609	9	-	0/2/19/22	0/1/1/1
9	MAN	G	610	9	-	0/2/19/22	0/1/1/1
7	NAG	G	611	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	612	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	613	7	-	0/2/19/22	0/1/1/1
7	NAG	G	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	615	7	-	0/6/23/26	0/1/1/1
7	NAG	G	616	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	617	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	618	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	619	8	-	0/2/19/22	0/1/1/1
9	MAN	G	620	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	621	9	-	0/2/19/22	1/1/1/1
7	NAG	G	622	1	-	0/6/23/26	0/1/1/1
7	NAG	G	623	1	-	0/6/23/26	0/1/1/1
7	NAG	G	624	1	-	0/6/23/26	0/1/1/1
7	NAG	G	625	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	626	7	-	0/6/23/26	0/1/1/1
7	NAG	G	627	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	628	7	-	0/6/23/26	0/1/1/1
7	NAG	G	629	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	630	7	-	0/6/23/26	0/1/1/1
7	NAG	G	631	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	632	7	-	0/6/23/26	0/1/1/1
7	NAG	G	633	1	-	0/6/23/26	0/1/1/1
7	NAG	G	634	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	635	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	636	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	637	8	-	0/2/19/22	0/1/1/1
9	MAN	G	638	8	-	0/2/19/22	0/1/1/1
7	NAG	G	639	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	640	7	-	0/6/23/26	0/1/1/1
7	NAG	G	641	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	642	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	643	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	644	7	-	0/6/23/26	0/1/1/1
7	NAG	G	645	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	646	7	-	0/6/23/26	0/1/1/1
7	NAG	G	647	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	648	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	649	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	650	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	651	9	-	0/2/19/22	0/1/1/1
9	MAN	G	652	9	-	0/2/19/22	0/1/1/1
9	MAN	G	653	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	654	9	-	0/2/19/22	0/1/1/1
9	MAN	G	655	9	-	0/2/19/22	0/1/1/1
9	MAN	G	656	9	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	650	MAN	O5-C1	-2.98	1.38	1.43
9	G	621	MAN	O5-C5	2.02	1.47	1.43
9	G	604	MAN	C1-C2	3.79	1.61	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	608	MAN	O2-C2-C3	-2.66	104.94	110.17
9	G	604	MAN	O2-C2-C3	-2.61	105.06	110.17
9	G	621	MAN	O2-C2-C3	-2.53	105.20	110.17
9	G	607	MAN	O2-C2-C3	-2.37	105.53	110.17
9	G	651	MAN	O2-C2-C3	-2.34	105.57	110.17
9	G	656	MAN	O2-C2-C3	-2.29	105.67	110.17
9	G	610	MAN	O2-C2-C3	-2.28	105.70	110.17
9	G	650	MAN	O2-C2-C3	-2.22	105.82	110.17
9	G	638	MAN	O2-C2-C3	-2.19	105.88	110.17
9	G	606	MAN	O2-C2-C3	-2.16	105.93	110.17
9	G	619	MAN	O2-C2-C3	-2.14	105.96	110.17
9	G	637	MAN	O2-C2-C3	-2.05	106.14	110.17
9	G	652	MAN	O2-C2-C3	-2.05	106.15	110.17
9	G	653	MAN	O2-C2-C3	-2.04	106.16	110.17
9	G	655	MAN	O2-C2-C3	-2.00	106.24	110.17
7	G	602	NAG	C1-O5-C5	2.02	114.96	112.17
7	G	602	NAG	C1-C2-N2	2.06	114.02	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	637	MAN	O5-C1-C2	2.07	114.03	110.79
8	G	649	BMA	C1-O5-C5	2.08	115.03	112.17
9	G	620	MAN	C1-O5-C5	2.11	115.07	112.17
7	G	640	NAG	C1-C2-N2	2.11	114.10	110.49
9	G	653	MAN	O5-C1-C2	2.14	114.15	110.79
9	G	651	MAN	C1-O5-C5	2.21	115.21	112.17
8	G	649	BMA	C1-C2-C3	2.26	112.52	109.65
9	G	654	MAN	O3-C3-C2	2.27	114.16	110.02
7	G	633	NAG	C1-O5-C5	2.28	115.31	112.17
9	G	619	MAN	C1-O5-C5	2.30	115.33	112.17
8	G	613	BMA	C1-O5-C5	2.34	115.39	112.17
7	G	601	NAG	C1-O5-C5	2.36	115.42	112.17
7	G	630	NAG	C1-O5-C5	2.45	115.54	112.17
8	G	649	BMA	O5-C1-C2	2.56	114.80	110.79
9	G	652	MAN	C1-O5-C5	2.62	115.78	112.17
9	G	653	MAN	C1-O5-C5	2.66	115.84	112.17
9	G	638	MAN	O5-C1-C2	2.76	115.12	110.79
9	G	608	MAN	C1-O5-C5	2.82	116.05	112.17
9	G	637	MAN	C1-O5-C5	2.84	116.08	112.17
9	G	654	MAN	C1-O5-C5	2.92	116.19	112.17
9	G	656	MAN	C1-O5-C5	3.07	116.40	112.17
9	G	606	MAN	C1-O5-C5	3.20	116.57	112.17
9	G	621	MAN	C1-O5-C5	3.37	116.81	112.17
9	G	604	MAN	O5-C1-C2	3.37	116.07	110.79
9	G	605	MAN	C1-O5-C5	3.44	116.91	112.17
9	G	604	MAN	C1-C2-C3	3.44	114.02	109.65
9	G	604	MAN	C1-O5-C5	3.54	117.05	112.17
9	G	607	MAN	C1-O5-C5	3.82	117.43	112.17
9	G	655	MAN	C1-O5-C5	3.82	117.43	112.17
9	G	638	MAN	C1-O5-C5	3.92	117.56	112.17
7	G	622	NAG	C2-N2-C7	4.14	128.98	122.94
7	G	602	NAG	C2-N2-C7	4.25	129.15	122.94
9	G	610	MAN	C1-O5-C5	4.25	118.03	112.17
7	G	640	NAG	C2-N2-C7	4.29	129.20	122.94

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	G	656	MAN	C1-C2-C3-C4-C5-O5
9	G	621	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	702	NAG	2	0
7	B	703	NAG	1	0
7	G	601	NAG	2	0
7	G	602	NAG	1	0
8	G	603	BMA	1	0
9	G	604	MAN	1	0
9	G	608	MAN	1	0
9	G	610	MAN	1	0
7	G	614	NAG	1	0
7	G	615	NAG	1	0
7	G	617	NAG	2	0
7	G	622	NAG	1	0
7	G	627	NAG	1	0
7	G	628	NAG	1	0
7	G	629	NAG	1	0
7	G	630	NAG	1	0
7	G	631	NAG	2	0
7	G	633	NAG	1	0
7	G	640	NAG	1	0
7	G	648	NAG	1	0
9	G	652	MAN	1	0
9	G	656	MAN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	G	439/481 (91%)	-0.43	2 (0%) 90 86	23, 80, 145, 229	0
2	B	123/153 (80%)	-0.32	1 (0%) 86 79	32, 69, 128, 181	0
3	L	208/213 (97%)	-0.53	0 100 100	52, 105, 158, 211	0
4	H	228/235 (97%)	-0.51	0 100 100	52, 124, 172, 217	0
5	D	242/243 (99%)	-0.22	5 (2%) 64 55	64, 135, 240, 310	0
6	E	213/216 (98%)	-0.32	5 (2%) 61 51	73, 152, 227, 271	0
All	All	1453/1541 (94%)	-0.40	13 (0%) 84 77	23, 106, 210, 310	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	547	GLY	6.8
5	D	213	PRO	5.5
5	D	222	VAL	4.8
6	E	209	THR	3.3
6	E	157	ALA	2.7
5	D	209	LYS	2.5
1	G	66	HIS	2.5
6	E	118	PHE	2.5
6	E	185	TRP	2.4
1	G	73	ALA	2.3
6	E	133	VAL	2.2
5	D	138	LEU	2.2
5	D	218	LYS	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 ⓘ

There are no carbohydrates in this entry.

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, 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
7	NAG	B	702	14/15	0.86	0.28	1.25	120,125,132,132	0
7	NAG	G	611	14/15	0.81	0.24	1.18	77,115,139,154	0
7	NAG	G	614	14/15	0.90	0.20	0.53	78,91,119,126	0
7	NAG	G	617	14/15	0.96	0.18	0.31	64,81,99,108	0
7	NAG	G	633	14/15	0.82	0.25	0.24	120,140,153,155	0
7	NAG	G	616	14/15	0.96	0.21	0.20	35,46,74,81	0
9	MAN	G	606	11/12	0.90	0.20	0.02	114,128,136,141	0
7	NAG	G	641	14/15	0.80	0.19	-0.41	130,153,164,168	0
7	NAG	G	643	14/15	0.94	0.16	-0.49	66,84,105,119	0
7	NAG	B	701	14/15	0.83	0.22	-0.49	127,140,159,161	0
7	NAG	G	602	14/15	0.94	0.15	-1.08	51,87,102,114	0
7	NAG	G	601	14/15	0.95	0.17	-1.09	40,52,82,84	0
9	MAN	G	654	11/12	0.95	0.13	-1.29	52,70,81,84	0
7	NAG	G	634	14/15	0.96	0.16	-1.36	47,65,79,90	0
7	NAG	G	631	14/15	0.91	0.11	-1.46	95,113,133,145	0
9	MAN	G	605	11/12	0.92	0.11	-1.47	64,87,104,106	0
9	MAN	G	653	11/12	0.97	0.14	-1.48	58,74,87,89	0
7	NAG	G	647	14/15	0.97	0.13	-1.48	51,64,85,88	0
7	NAG	G	639	14/15	0.92	0.16	-1.48	77,94,120,139	0
8	BMA	G	603	11/12	0.96	0.13	-2.07	88,98,104,109	0
9	MAN	G	619	11/12	0.93	0.09	-	127,133,142,147	0
9	MAN	G	620	11/12	0.94	0.16	-	137,146,157,161	0
7	NAG	G	645	14/15	0.94	0.18	-	69,90,104,106	0
9	MAN	G	621	11/12	0.94	0.21	-	120,129,138,142	0
7	NAG	G	624	14/15	0.71	0.40	-	147,163,168,171	0
9	MAN	G	609	11/12	0.95	0.14	-	112,121,130,131	0
9	MAN	G	655	11/12	0.95	0.12	-	71,84,97,106	0
7	NAG	G	640	14/15	0.89	0.33	-	131,143,147,149	0
8	BMA	G	613	11/12	0.89	0.15	-	134,145,159,163	0
7	NAG	G	635	14/15	0.94	0.16	-	100,112,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	BMA	G	618	11/12	0.94	0.17	-	85,101,124,129	0
7	NAG	B	703	14/15	0.93	0.15	-	94,102,111,114	0
9	MAN	G	652	11/12	0.89	0.17	-	136,148,156,159	0
7	NAG	G	626	14/15	0.92	0.19	-	79,104,121,125	0
9	MAN	G	651	11/12	0.88	0.21	-	97,118,129,131	0
7	NAG	G	622	14/15	0.91	0.17	-	94,99,101,102	0
7	NAG	G	629	14/15	0.85	0.35	-	135,151,173,185	0
7	NAG	G	623	14/15	0.88	0.24	-	79,108,130,137	0
7	NAG	G	642	14/15	0.84	0.21	-	164,173,193,196	0
9	MAN	G	604	11/12	0.93	0.12	-	87,94,101,101	0
7	NAG	G	627	14/15	0.97	0.16	-	54,82,104,107	0
7	NAG	G	644	14/15	0.83	0.28	-	111,132,138,138	0
9	MAN	G	650	11/12	0.92	0.11	-	109,119,130,135	0
9	MAN	G	608	11/12	0.97	0.15	-	57,63,83,99	0
7	NAG	G	630	14/15	0.82	0.36	-	182,188,193,194	0
9	MAN	G	656	11/12	0.87	0.26	-	149,160,162,163	0
7	NAG	G	625	14/15	0.97	0.13	-	66,87,98,105	0
8	BMA	G	636	11/12	0.95	0.10	-	112,115,119,124	0
9	MAN	G	610	11/12	0.92	0.13	-	131,141,151,153	0
7	NAG	G	648	14/15	0.97	0.15	-	63,81,85,87	0
7	NAG	G	632	14/15	0.90	0.22	-	141,151,158,159	0
7	NAG	G	646	14/15	0.86	0.18	-	102,127,140,147	0
8	BMA	G	649	11/12	0.95	0.16	-	72,82,94,100	0
9	MAN	G	607	11/12	0.94	0.11	-	78,96,105,105	0
7	NAG	G	615	14/15	0.80	0.26	-	133,141,148,148	0
9	MAN	G	637	11/12	0.94	0.09	-	129,134,138,139	0
9	MAN	G	638	11/12	0.93	0.11	-	119,125,131,137	0
7	NAG	G	628	14/15	0.93	0.12	-	73,86,91,91	0
7	NAG	G	612	14/15	0.87	0.18	-	134,150,157,160	0

6.5 Other polymers ⓘ

There are no such residues in this entry.