



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:44 AM UTC

PDB ID : 8SZY / pdb_00008szy
Title : Crystal Structure of Heterotrimeric Anti-TIGIT Fabs in complex with human TIGIT
Authors : Diong, S.J.; Lee, P.S.
Deposited on : 2023-05-30
Resolution : 2.31 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

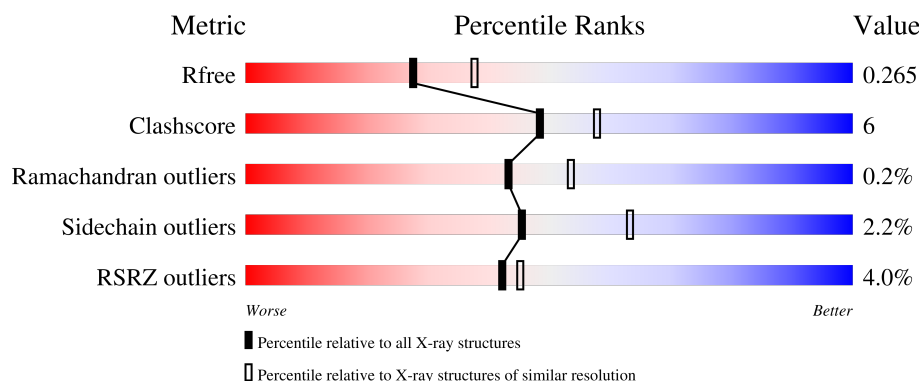
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.



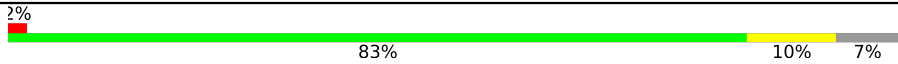
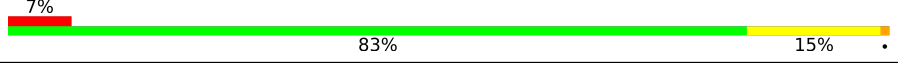
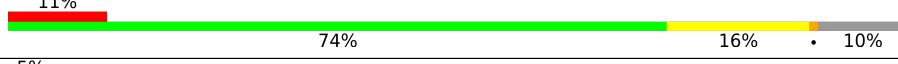
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	228	3% 81% 11% 7%
1	C	228	4% 79% 12% 7%
2	B	219	2% 83% 15% ..
2	D	219	3% 86% 12% ..
3	H	241	0% 83% 9% 7%

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Mol	Chain	Length	Quality of chain
3	I	241	
4	L	216	
4	M	216	
5	T	114	
5	U	114	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29201 atoms, of which 14310 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 CHA.9.543 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	211	Total	C	H	N	O	S	0	0	0
			3130	1003	1548	261	311	7			
1	C	211	Total	C	H	N	O	S	0	0	0
			3107	998	1534	258	310	7			

- Molecule 2 is a protein called CHA.9.543 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	216	Total	C	H	N	O	S	0	0	0
			3293	1053	1620	279	335	6			
2	D	216	Total	C	H	N	O	S	0	0	0
			3266	1048	1603	275	334	6			

- Molecule 3 is a protein called BMS-986207 Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	224	Total	C	H	N	O	S	0	0	0
			3339	1087	1640	272	336	4			
3	I	223	Total	C	H	N	O	S	0	0	0
			3329	1084	1636	271	334	4			

- Molecule 4 is a protein called BMS-986207 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	L	215	Total	C	H	N	O	S	0	0	0
			3249	1037	1599	277	332	4			
4	M	215	Total	C	H	N	O	S	0	0	0
			3241	1035	1595	277	330	4			

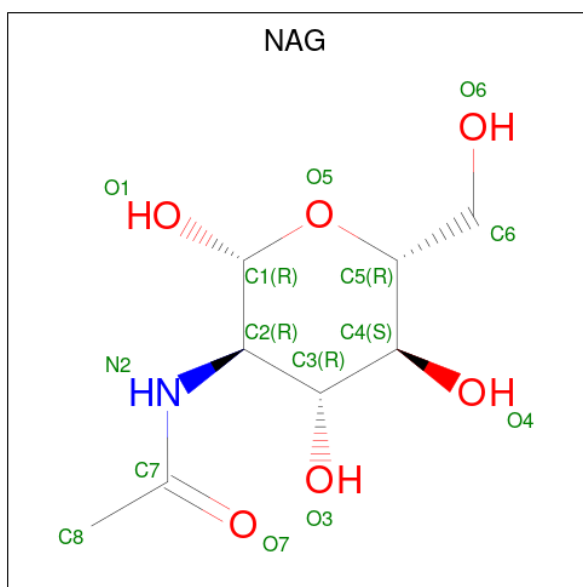
- Molecule 5 is a protein called T-cell immunoreceptor with Ig and ITIM domains.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	T	103	Total	C	H	N	O	S	0	0	0
			1537	496	752	130	157	2			
5	U	103	Total	C	H	N	O	S	0	0	0
			1544	497	757	130	158	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	47	SER	CYS	engineered mutation	UNP Q495A1
T	107	GLY	-	expression tag	UNP Q495A1
T	108	GLY	-	expression tag	UNP Q495A1
T	109	HIS	-	expression tag	UNP Q495A1
T	110	HIS	-	expression tag	UNP Q495A1
T	111	HIS	-	expression tag	UNP Q495A1
T	112	HIS	-	expression tag	UNP Q495A1
T	113	HIS	-	expression tag	UNP Q495A1
T	114	HIS	-	expression tag	UNP Q495A1
U	47	SER	CYS	engineered mutation	UNP Q495A1
U	107	GLY	-	expression tag	UNP Q495A1
U	108	GLY	-	expression tag	UNP Q495A1
U	109	HIS	-	expression tag	UNP Q495A1
U	110	HIS	-	expression tag	UNP Q495A1
U	111	HIS	-	expression tag	UNP Q495A1
U	112	HIS	-	expression tag	UNP Q495A1
U	113	HIS	-	expression tag	UNP Q495A1
U	114	HIS	-	expression tag	UNP Q495A1

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	T	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
6	U	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

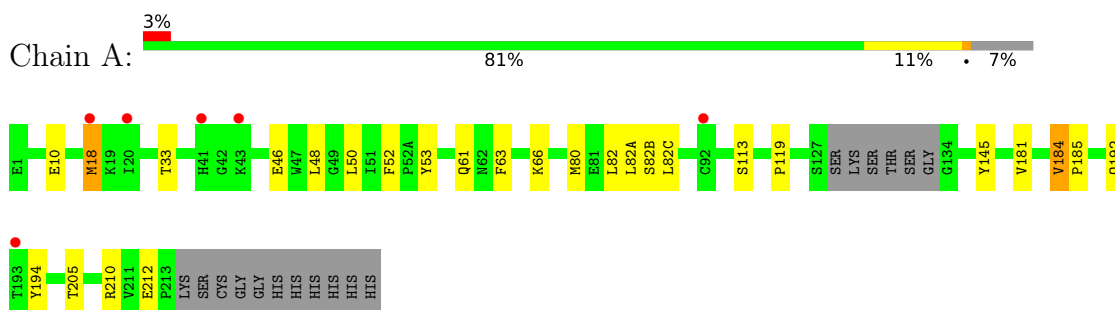
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	16	Total	O	0	0
			16	16		
7	H	13	Total	O	0	0
			13	13		
7	L	8	Total	O	0	0
			8	8		
7	T	9	Total	O	0	0
			9	9		
7	C	11	Total	O	0	0
			11	11		
7	D	15	Total	O	0	0
			15	15		
7	I	14	Total	O	0	0
			14	14		
7	M	11	Total	O	0	0
			11	11		
7	U	3	Total	O	0	0
			3	3		

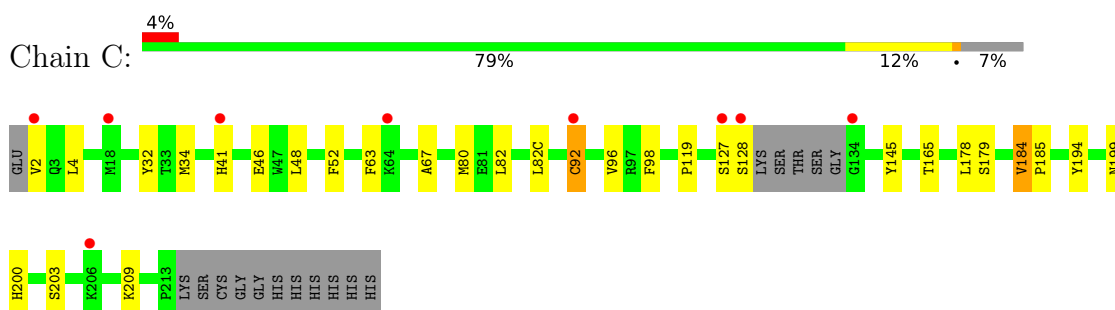
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

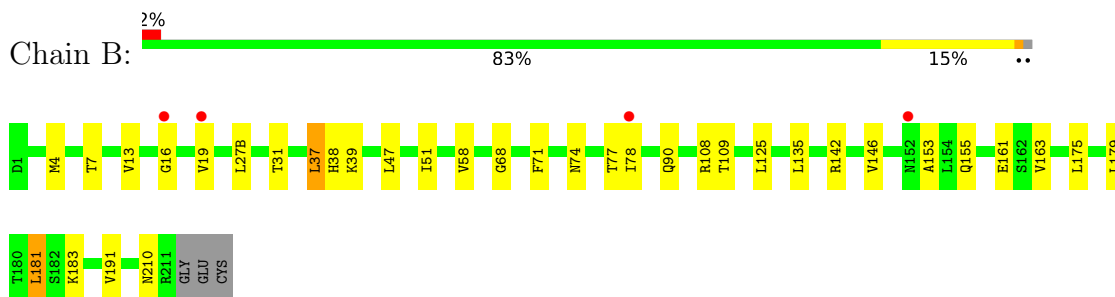
- Molecule 1: CHA.9.543 Fab heavy chain



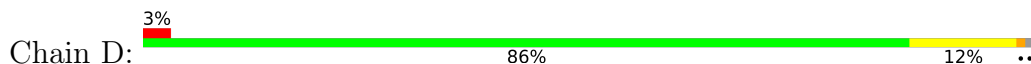
- Molecule 1: CHA.9.543 Fab heavy chain

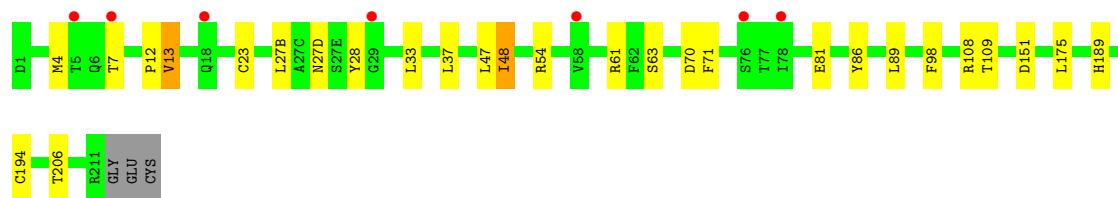


- Molecule 2: CHA.9.543 light chain

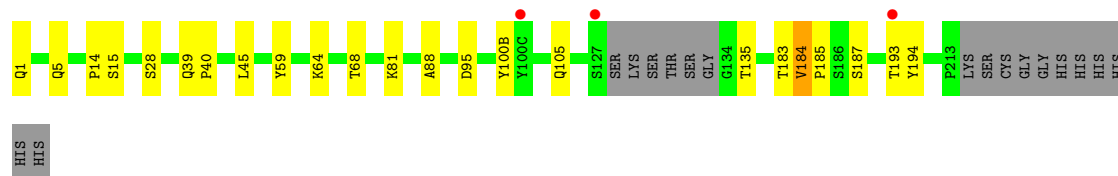
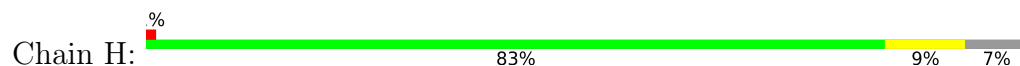


- Molecule 2: CHA.9.543 light chain

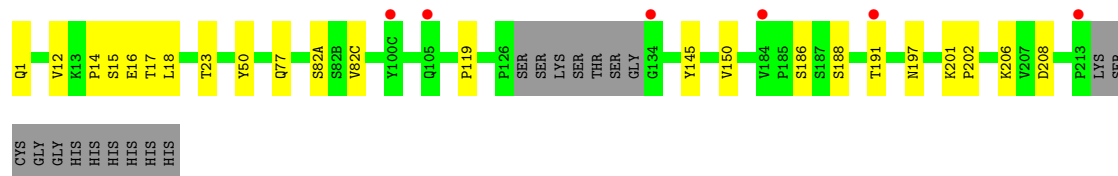
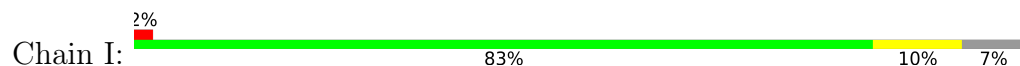




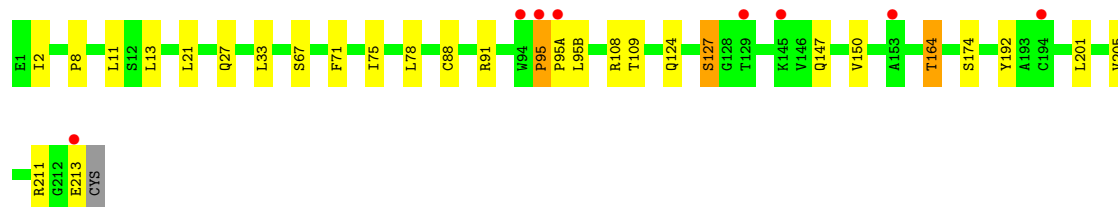
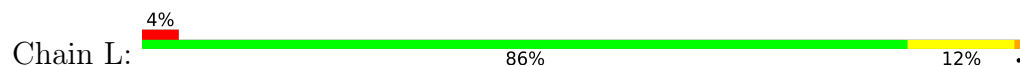
• Molecule 3: BMS-986207 Fab Heavy Chain



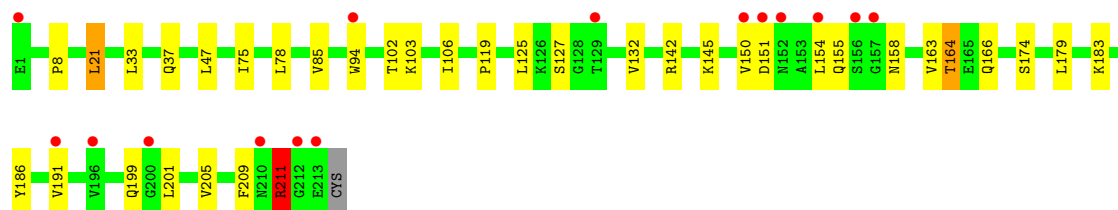
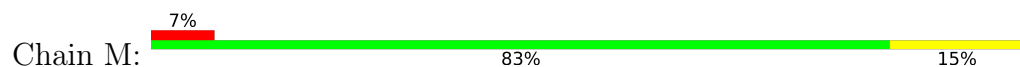
• Molecule 3: BMS-986207 Fab Heavy Chain



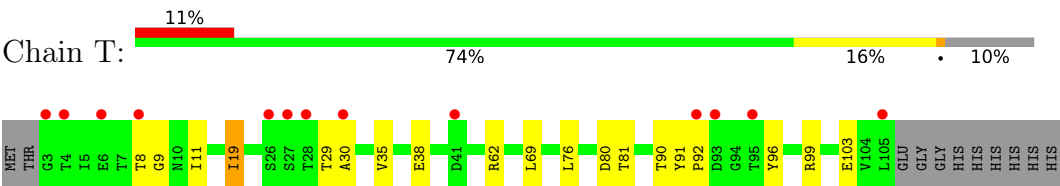
• Molecule 4: BMS-986207 light chain



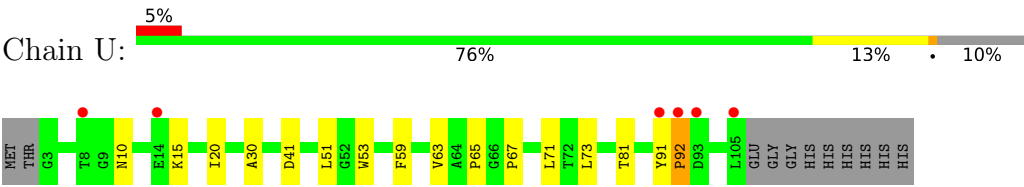
• Molecule 4: BMS-986207 light chain



• Molecule 5: T-cell immunoreceptor with Ig and ITIM domains



● Molecule 5: T-cell immunoreceptor with Ig and ITIM domains



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.85Å 216.91Å 109.45Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	45.60 – 2.31 45.60 – 2.31	Depositor EDS
% Data completeness (in resolution range)	70.2 (45.60-2.31) 70.5 (45.60-2.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.227 , 0.269 0.223 , 0.265	Depositor DCC
R_{free} test set	3195 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29201	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

5.1 Standard geometry

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

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	0.25	1/1621 (0.1%)	0.42	0/2209
1	C	0.27	0/1612	0.45	1/2198 (0.0%)
2	B	0.26	0/1713	0.48	0/2328
2	D	0.51	2/1703 (0.1%)	0.71	3/2316 (0.1%)
3	H	0.31	1/1740 (0.1%)	0.48	0/2385
3	I	0.25	0/1734	0.47	0/2377
4	L	0.33	0/1689	0.60	1/2300 (0.0%)
4	M	0.30	0/1685	0.44	0/2295
5	T	0.49	0/802	0.79	2/1095 (0.2%)
5	U	0.23	0/804	0.47	0/1098
All	All	0.33	4/15103 (0.0%)	0.53	7/20601 (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
2	D	0	3
4	L	0	1
4	M	0	1
5	T	0	2
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	13	VAL	C-N	10.08	1.48	1.33
3	H	185	PRO	C-O	-6.82	1.15	1.23
2	D	48	ILE	C-O	-5.49	1.18	1.23
1	A	185	PRO	C-O	-5.03	1.18	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	95	PRO	N-CA-C	10.16	123.10	110.70
2	D	12	PRO	CA-C-N	-9.58	109.19	123.27
2	D	12	PRO	C-N-CA	-9.58	109.19	123.27
2	D	12	PRO	O-C-N	6.68	130.59	123.10
1	C	92	CYS	N-CA-C	-6.41	100.13	110.32
5	T	96	TYR	N-CA-C	-6.32	99.51	109.50
5	T	9	GLY	CA-C-O	-5.35	117.17	121.77

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	13	VAL	Mainchain
2	D	54	ARG	Sidechain
2	D	61	ARG	Sidechain
4	L	211	ARG	Sidechain
4	M	211	ARG	Sidechain
5	T	62	ARG	Sidechain
5	T	91	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1582	1548	1548	19	0
1	C	1573	1534	1533	18	0
2	B	1673	1620	1620	27	0
2	D	1663	1603	1603	15	0
3	H	1699	1640	1640	11	0
3	I	1693	1636	1635	14	0
4	L	1650	1599	1599	19	0
4	M	1646	1595	1595	22	0
5	T	785	752	752	12	0
5	U	787	757	757	13	0
6	T	14	13	13	0	0
6	U	14	13	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	0	0	0
7	B	16	0	0	0	0
7	C	11	0	0	0	0
7	D	15	0	0	0	0
7	H	13	0	0	0	0
7	I	14	0	0	1	0
7	L	8	0	0	0	0
7	M	11	0	0	0	0
7	T	9	0	0	1	0
7	U	3	0	0	0	0
All	All	14891	14310	14308	160	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 (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:HD13	1:C:80:MET:HE1	1.55	0.88
2:B:4:MET:HE2	2:B:90:GLN:HB3	1.57	0.86
3:H:100(B):TYR:OH	5:T:38:GLU:OE2	1.95	0.83
2:B:4:MET:HE1	2:B:27(B):LEU:HD11	1.65	0.75
1:A:48:LEU:HD13	1:A:80:MET:HE1	1.67	0.75
5:U:63:VAL:HG12	5:U:73:LEU:HD23	1.67	0.75
2:B:179:LEU:CD2	2:B:181:LEU:HD11	2.20	0.71
1:C:184:VAL:HG22	1:C:185:PRO:HD2	1.73	0.70
1:C:82:LEU:HB3	1:C:82(C):LEU:HD21	1.73	0.70
2:B:37:LEU:HD11	2:B:39:LYS:HG3	1.74	0.69
2:D:37:LEU:HB2	2:D:47:LEU:HD11	1.76	0.68
3:I:12:VAL:HG21	3:I:18:LEU:HD23	1.74	0.68
1:A:210:ARG:NE	1:A:212:GLU:OE2	2.26	0.68
2:D:108:ARG:NH1	2:D:109:THR:O	2.27	0.68
4:M:164:THR:HG22	4:M:174:SER:H	1.60	0.67
2:B:142:ARG:NH2	2:B:163:VAL:HG21	2.09	0.67
3:H:68:THR:HG23	3:H:81:LYS:HB2	1.76	0.66
3:I:14:PRO:O	3:I:15:SER:OG	2.13	0.66
5:U:91:TYR:HB3	5:U:92:PRO:HD3	1.79	0.65
5:T:29:THR:HG23	3:I:186:SER:HB2	1.80	0.63
1:C:127:SER:OG	1:C:128:SER:N	2.33	0.62
2:B:153:ALA:O	2:B:155:GLN:NE2	2.32	0.61
4:L:164:THR:HG22	4:L:174:SER:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:VAL:HG23	2:B:78:ILE:HD11	1.83	0.61
2:B:31:THR:HB	2:B:51:ILE:HD11	1.80	0.61
2:D:27(B):LEU:CD1	2:D:33:LEU:HD12	2.32	0.59
5:U:63:VAL:CG1	5:U:73:LEU:HD23	2.33	0.59
1:C:200:HIS:ND1	1:C:203:SER:OG	2.31	0.59
5:T:29:THR:HG22	5:T:29:THR:O	2.03	0.58
3:H:5:GLN:NE2	3:H:105:GLN:OE1	2.33	0.58
3:I:197:ASN:ND2	3:I:208:ASP:OD1	2.37	0.57
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.87	0.57
4:L:150:VAL:HG22	4:L:192:TYR:CD2	2.40	0.57
2:B:78:ILE:HD12	2:B:78:ILE:H	1.70	0.56
4:M:142:ARG:HH21	4:M:163:VAL:HG11	1.71	0.55
5:T:103:GLU:OE2	7:T:301:HOH:O	2.18	0.55
5:U:20:ILE:HD12	5:U:67:PRO:HD3	1.89	0.55
1:C:46:GLU:HG2	1:C:63:PHE:CZ	2.43	0.54
4:L:201:LEU:HD13	4:L:205:VAL:HG23	1.90	0.53
2:B:179:LEU:HD23	2:B:181:LEU:HD11	1.91	0.53
5:U:30:ALA:HB1	5:U:92:PRO:HD2	1.91	0.53
5:T:30:ALA:HB1	5:T:90:THR:HB	1.92	0.52
2:B:16:GLY:HA2	2:B:77:THR:HG23	1.92	0.52
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.92	0.52
1:A:52:PHE:CE2	5:T:81:THR:HB	2.45	0.52
1:C:34:MET:HE2	1:C:92:CYS:SG	2.50	0.51
1:A:82:LEU:HB3	1:A:82(C):LEU:HD21	1.92	0.51
2:B:108:ARG:NH1	2:B:109:THR:O	2.43	0.51
3:H:14:PRO:O	3:H:15:SER:OG	2.28	0.51
1:C:184:VAL:HG21	1:C:194:TYR:CZ	2.46	0.51
5:U:41:ASP:OD1	5:U:41:ASP:N	2.44	0.51
2:D:4:MET:HE3	2:D:23:CYS:SG	2.51	0.51
2:B:13:VAL:HG21	2:B:19:VAL:HG22	1.92	0.51
5:T:11:ILE:HG21	5:T:19:ILE:HD11	1.93	0.51
3:H:95:ASP:OD2	4:L:91:ARG:NH2	2.43	0.50
4:M:142:ARG:NH2	4:M:163:VAL:HG11	2.27	0.50
3:I:17:THR:HG22	3:I:82(A):SER:HA	1.93	0.50
5:T:80:ASP:O	5:T:81:THR:C	2.55	0.50
2:D:27(B):LEU:HD12	2:D:33:LEU:HD12	1.93	0.50
4:L:108:ARG:HG3	4:L:109:THR:O	2.12	0.50
1:C:46:GLU:HG2	1:C:63:PHE:CE2	2.46	0.50
2:B:181:LEU:HD12	2:B:181:LEU:N	2.27	0.50
2:D:27(D):ASN:HB3	2:D:28:TYR:H	1.77	0.49
1:A:66:LYS:HE3	1:A:82(A):LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:GLU:N	2:D:81:GLU:OE1	2.45	0.49
5:U:20:ILE:HD12	5:U:67:PRO:CD	2.43	0.49
2:B:37:LEU:HB2	2:B:47:LEU:HD11	1.94	0.48
3:I:188:SER:O	3:I:191:THR:N	2.39	0.48
4:M:150:VAL:O	4:M:150:VAL:HG23	2.12	0.48
3:I:23:THR:HG23	3:I:77:GLN:HG2	1.95	0.48
4:M:154:LEU:HD23	4:M:155:GLN:N	2.29	0.48
3:H:95:ASP:CG	4:L:91:ARG:HH22	2.21	0.48
4:L:33:LEU:HD22	4:L:71:PHE:CG	2.49	0.48
4:M:154:LEU:HD23	4:M:154:LEU:C	2.39	0.48
1:A:52:PHE:CE2	1:A:53:TYR:HB3	2.49	0.47
1:A:119:PRO:HD2	1:A:205:THR:HG21	1.95	0.47
4:M:85:VAL:HG22	4:M:103:LYS:HD3	1.97	0.47
2:D:89:LEU:HD13	2:D:98:PHE:CE1	2.49	0.47
2:D:89:LEU:HD13	2:D:98:PHE:CZ	2.50	0.47
3:I:201:LYS:N	3:I:202:PRO:CD	2.78	0.47
5:U:71:LEU:C	5:U:71:LEU:HD12	2.40	0.46
1:A:10:GLU:HG3	1:A:18:MET:HE1	1.97	0.46
4:L:2:ILE:CD1	4:L:27:GLN:HG3	2.46	0.46
2:D:37:LEU:HB3	2:D:47:LEU:HD21	1.97	0.46
4:M:37:GLN:HB2	4:M:47:LEU:HD11	1.96	0.46
5:U:59:PHE:O	5:U:63:VAL:HG22	2.16	0.46
1:A:33:THR:HB	1:A:50:LEU:HD13	1.98	0.46
2:D:151:ASP:OD2	2:D:189:HIS:ND1	2.44	0.46
5:U:53:TRP:CD2	5:U:65:PRO:HB3	2.50	0.46
4:L:95:PRO:HB2	4:L:95(A):PRO:HD3	1.97	0.46
4:L:124:GLN:O	4:L:124:GLN:HG2	2.16	0.46
1:A:50:LEU:HD12	1:A:50:LEU:C	2.41	0.46
2:B:13:VAL:HG21	2:B:19:VAL:CG2	2.46	0.46
1:A:46:GLU:HG2	1:A:63:PHE:CZ	2.52	0.45
1:A:48:LEU:CD1	1:A:80:MET:HE1	2.41	0.45
2:B:27(B):LEU:HD12	2:B:71:PHE:CE1	2.51	0.45
2:B:179:LEU:HD21	2:B:181:LEU:HD11	1.95	0.45
3:H:28:SER:HB3	5:T:92:PRO:HB2	1.98	0.45
2:B:37:LEU:HD22	2:B:38:HIS:N	2.32	0.45
4:L:108:ARG:NH1	4:L:109:THR:O	2.47	0.45
3:I:18:LEU:CD2	7:I:302:HOH:O	2.65	0.45
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.17	0.45
4:M:125:LEU:O	4:M:183:LYS:CE	2.65	0.45
3:I:145:TYR:CE1	3:I:150:VAL:HG23	2.53	0.44
4:M:8:PRO:O	4:M:102:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:40:PRO:HA	3:H:88:ALA:HA	1.99	0.44
1:C:178:LEU:HD23	1:C:179:SER:N	2.32	0.44
4:M:106:ILE:O	4:M:166:GLN:NE2	2.49	0.44
1:C:165:THR:HG23	1:C:178:LEU:HD21	1.99	0.44
1:A:181:VAL:HG11	2:B:135:LEU:HD22	1.99	0.44
1:C:41:HIS:O	1:C:41:HIS:ND1	2.50	0.43
1:A:113:SER:O	1:A:113:SER:OG	2.33	0.43
1:A:184:VAL:HG21	1:A:194:TYR:CZ	2.53	0.43
4:L:75:ILE:HG21	4:L:78:LEU:HD23	2.00	0.43
2:B:19:VAL:HG23	2:B:78:ILE:CD1	2.47	0.43
4:L:2:ILE:HD13	4:L:27:GLN:HG3	1.98	0.43
4:L:13:LEU:HB2	4:L:78:LEU:HD12	2.00	0.43
4:L:124:GLN:O	4:L:127:SER:HB3	2.18	0.43
2:B:146:VAL:HG12	2:B:161:GLU:OE2	2.19	0.43
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.01	0.43
1:C:67:ALA:CB	1:C:80:MET:HE2	2.49	0.43
2:D:175:LEU:C	2:D:175:LEU:HD23	2.44	0.43
4:M:150:VAL:HG13	4:M:155:GLN:CG	2.49	0.43
1:A:210:ARG:HE	1:A:212:GLU:CD	2.23	0.42
1:C:32:TYR:CD2	1:C:96:VAL:HG22	2.54	0.42
2:D:33:LEU:HD13	2:D:71:PHE:CD1	2.54	0.42
4:L:21:LEU:HD12	4:L:21:LEU:N	2.34	0.42
4:M:75:ILE:HG21	4:M:78:LEU:HD23	2.00	0.42
5:T:35:VAL:HG21	5:T:69:LEU:HD13	2.00	0.42
3:H:59:TYR:HB2	3:H:64:LYS:HG3	2.01	0.42
4:M:119:PRO:HB3	4:M:209:PHE:CE2	2.55	0.42
3:I:16:GLU:O	3:I:82(C):VAL:HG22	2.19	0.42
1:C:98:PHE:CZ	5:U:10:ASN:HB3	2.54	0.42
4:M:21:LEU:N	4:M:21:LEU:HD12	2.35	0.42
5:T:19:ILE:HB	5:T:76:LEU:HD11	2.02	0.42
4:M:201:LEU:HD13	4:M:205:VAL:HG23	2.01	0.41
2:B:47:LEU:HA	2:B:58:VAL:HG21	2.01	0.41
4:M:151:ASP:HA	4:M:191:VAL:HG12	2.01	0.41
1:C:119:PRO:HB3	1:C:145:TYR:HB3	2.02	0.41
3:I:119:PRO:HB3	3:I:145:TYR:HB3	2.01	0.41
4:L:8:PRO:HG2	4:L:11:LEU:HD21	2.02	0.41
1:C:52:PHE:CE2	5:U:81:THR:HB	2.55	0.41
2:D:194:CYS:O	2:D:206:THR:HA	2.20	0.41
1:A:61:GLN:HG3	5:T:99:ARG:NH2	2.36	0.41
3:I:50:TYR:CD1	3:I:50:TYR:C	2.99	0.41
4:M:150:VAL:O	4:M:150:VAL:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:201:LYS:NZ	3:I:206:LYS:HE3	2.36	0.41
2:D:37:LEU:HD13	2:D:86:TYR:CE1	2.55	0.41
4:M:94:TRP:HA	4:M:94:TRP:CE3	2.56	0.41
4:M:158:ASN:O	4:M:179:LEU:HD12	2.20	0.41
4:M:186:TYR:O	4:M:211:ARG:HD2	2.20	0.41
1:A:82(A):LEU:O	1:A:82(B):SER:C	2.64	0.41
4:L:108:ARG:HG3	4:L:108:ARG:HH11	1.85	0.41
5:U:20:ILE:HD13	5:U:20:ILE:HA	1.91	0.41
2:B:74:ASN:OD1	2:B:74:ASN:C	2.63	0.40
3:H:184:VAL:HG21	3:H:194:TYR:CE1	2.56	0.40
2:B:125:LEU:HD22	2:B:183:LYS:HG3	2.04	0.40
4:L:33:LEU:HD11	4:L:88:CYS:HB2	2.04	0.40
1:C:165:THR:CG2	1:C:178:LEU:HD21	2.51	0.40
4:M:94:TRP:HA	4:M:94:TRP:HE3	1.86	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	207/228 (91%)	204 (99%)	3 (1%)	0	100	100
1	C	207/228 (91%)	199 (96%)	8 (4%)	0	100	100
2	B	214/219 (98%)	209 (98%)	4 (2%)	1 (0%)	24	30
2	D	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
3	H	220/241 (91%)	212 (96%)	8 (4%)	0	100	100
3	I	219/241 (91%)	212 (97%)	7 (3%)	0	100	100
4	L	213/216 (99%)	202 (95%)	10 (5%)	1 (0%)	24	30
4	M	213/216 (99%)	205 (96%)	7 (3%)	1 (0%)	24	30
5	T	101/114 (89%)	97 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	U	101/114 (89%)	97 (96%)	3 (3%)	1 (1%)	12	14
All	All	1909/2036 (94%)	1845 (97%)	60 (3%)	4 (0%)	43	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	95(B)	LEU
4	M	211	ARG
5	U	92	PRO
2	B	68	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	179/193 (93%)	176 (98%)	3 (2%)	53	70
1	C	178/193 (92%)	173 (97%)	5 (3%)	38	55
2	B	193/195 (99%)	190 (98%)	3 (2%)	55	72
2	D	191/195 (98%)	187 (98%)	4 (2%)	47	65
3	H	193/207 (93%)	188 (97%)	5 (3%)	40	57
3	I	192/207 (93%)	192 (100%)	0	100	100
4	L	186/188 (99%)	181 (97%)	5 (3%)	39	56
4	M	185/188 (98%)	178 (96%)	7 (4%)	29	43
5	T	86/96 (90%)	84 (98%)	2 (2%)	44	62
5	U	87/96 (91%)	85 (98%)	2 (2%)	44	62
All	All	1670/1758 (95%)	1634 (98%)	36 (2%)	45	63

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	184	VAL

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Mol	Chain	Res	Type
1	A	192	GLN
2	B	7	THR
2	B	37	LEU
2	B	181	LEU
3	H	135	THR
3	H	183	THR
3	H	184	VAL
3	H	187	SER
3	H	193	THR
4	L	67	SER
4	L	127	SER
4	L	147	GLN
4	L	164	THR
4	L	213	GLU
5	T	8	THR
5	T	19	ILE
1	C	2	VAL
1	C	4	LEU
1	C	184	VAL
1	C	199	ASN
1	C	209	LYS
2	D	7	THR
2	D	48	ILE
2	D	63	SER
2	D	70	ASP
4	M	21	LEU
4	M	33	LEU
4	M	127	SER
4	M	132	VAL
4	M	145	LYS
4	M	164	THR
4	M	199	GLN
5	U	15	LYS
5	U	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	18	GLN
2	B	189	HIS
3	H	39	GLN
4	L	37	GLN

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Mol	Chain	Res	Type
4	L	38	GLN
1	C	39	GLN
2	D	30	ASN
5	U	89	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	PCA	I	1	3	7,8,9	2.28	2 (28%)	9,10,12	2.24	5 (55%)
3	PCA	H	1	3	7,8,9	2.30	2 (28%)	9,10,12	2.26	5 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	I	1	3	-	0/0/11/13	0/1/1/1
3	PCA	H	1	3	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	PCA	CD-N	5.03	1.47	1.34
3	I	1	PCA	CD-N	5.00	1.46	1.34
3	H	1	PCA	CA-N	3.26	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	PCA	CA-N	3.22	1.50	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	PCA	CA-N-CD	-3.47	101.68	113.58
3	I	1	PCA	CA-N-CD	-3.28	102.36	113.58
3	I	1	PCA	OE-CD-CG	-2.99	121.38	126.72
3	H	1	PCA	OE-CD-CG	-2.86	121.62	126.72
3	H	1	PCA	CB-CA-N	2.80	110.95	103.24
3	I	1	PCA	CB-CA-N	2.72	110.72	103.24
3	I	1	PCA	CB-CA-C	-2.71	108.94	112.66
3	I	1	PCA	CG-CD-N	2.60	114.75	108.39
3	H	1	PCA	CG-CD-N	2.58	114.71	108.39
3	H	1	PCA	CB-CA-C	-2.57	109.12	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
6	NAG	U	201	-	14,14,15	0.33	0	17,19,21	0.39	0
6	NAG	T	201	-	14,14,15	0.23	0	17,19,21	0.55	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	NAG	U	201	-	-	2/6/23/26	0/1/1/1
6	NAG	T	201	-	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	201	NAG	C4-C5-C6-O6
6	T	201	NAG	O5-C5-C6-O6
6	U	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	211/228 (92%)	0.16	6 (2%) 55 57	24, 35, 52, 72	0
1	C	211/228 (92%)	0.34	9 (4%) 40 42	26, 37, 56, 85	0
2	B	216/219 (98%)	0.35	4 (1%) 66 68	23, 38, 55, 74	0
2	D	216/219 (98%)	0.40	7 (3%) 50 53	24, 40, 58, 79	0
3	H	223/241 (92%)	0.20	3 (1%) 75 76	20, 33, 52, 73	0
3	I	222/241 (92%)	0.22	6 (2%) 56 59	21, 33, 65, 99	0
4	L	215/216 (99%)	0.33	8 (3%) 45 48	19, 33, 66, 91	0
4	M	215/216 (99%)	0.46	15 (6%) 22 25	18, 34, 77, 102	0
5	T	103/114 (90%)	0.65	13 (12%) 8 9	24, 38, 75, 101	0
5	U	103/114 (90%)	0.43	6 (5%) 29 31	22, 37, 62, 96	0
All	All	1935/2036 (95%)	0.33	77 (3%) 42 45	18, 36, 64, 102	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	U	91	TYR	5.5
4	L	95	PRO	4.7
4	L	94	TRP	4.5
4	M	157	GLY	4.4
5	T	41	ASP	4.0
5	T	30	ALA	4.0
4	M	212	GLY	3.9
5	T	93	ASP	3.8
3	I	191	THR	3.8
5	T	8	THR	3.6
1	C	92	CYS	3.6
1	A	18	MET	3.5
5	U	105	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
4	M	94	TRP	3.3
4	M	213	GLU	3.3
4	M	210	ASN	3.3
4	L	153	ALA	3.1
3	H	100(C)	TYR	3.1
2	B	16	GLY	3.1
4	M	154	LEU	3.1
1	C	64	LYS	3.1
3	I	100(C)	TYR	3.1
5	T	4	THR	3.1
5	U	8	THR	3.1
3	I	105	GLN	3.1
5	U	93	ASP	3.0
2	D	29	GLY	2.9
1	A	41	HIS	2.9
5	U	14	GLU	2.9
5	T	92	PRO	2.9
1	C	206	LYS	2.8
3	I	134	GLY	2.7
1	C	127	SER	2.7
3	H	127	SER	2.7
4	M	191	VAL	2.6
5	T	28	THR	2.6
1	A	43	LYS	2.6
2	D	5	THR	2.6
5	T	3	GLY	2.6
2	D	7	THR	2.5
1	A	20	ILE	2.5
4	L	194	CYS	2.5
3	H	193	THR	2.5
1	C	41	HIS	2.5
2	B	152	ASN	2.5
4	M	152	ASN	2.4
5	T	105	LEU	2.4
4	M	1	GLU	2.4
1	C	2	VAL	2.4
2	B	78	ILE	2.4
4	L	95(A)	PRO	2.3
1	A	193	THR	2.3
4	M	156	SER	2.3
1	C	18	MET	2.3
1	A	92	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	18	GLN	2.3
4	L	145	LYS	2.3
5	T	27	SER	2.3
2	B	19	VAL	2.3
3	I	184	VAL	2.3
5	U	92	PRO	2.3
2	D	76	SER	2.3
4	L	213	GLU	2.2
5	T	6	GLU	2.2
4	M	129	THR	2.2
5	T	95	THR	2.2
4	M	196	VAL	2.2
3	I	213	PRO	2.2
1	C	128	SER	2.2
5	T	26	SER	2.2
2	D	58	VAL	2.1
4	M	151	ASP	2.1
2	D	78	ILE	2.1
4	M	150	VAL	2.1
1	C	134	GLY	2.1
4	L	129	THR	2.0
4	M	200	GLY	2.0

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

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. 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	B-factors(Å ²)	Q<0.9
3	PCA	H	1	8/9	0.72	0.17	57,59,60,60	0
3	PCA	I	1	8/9	0.74	0.15	68,70,72,72	0

6.3 Carbohydrates

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
6	NAG	T	201	14/15	0.74	0.17	68,71,87,87	0
6	NAG	U	201	14/15	0.77	0.15	67,71,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.