



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 6DFS / pdb_00006dfs
Title : mouse TCR I.29 in complex with IAg7-p8E9E6ss
Authors : Wang, Y.; Dai, S.
Deposited on : 2018-05-15
Resolution : 3.10 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

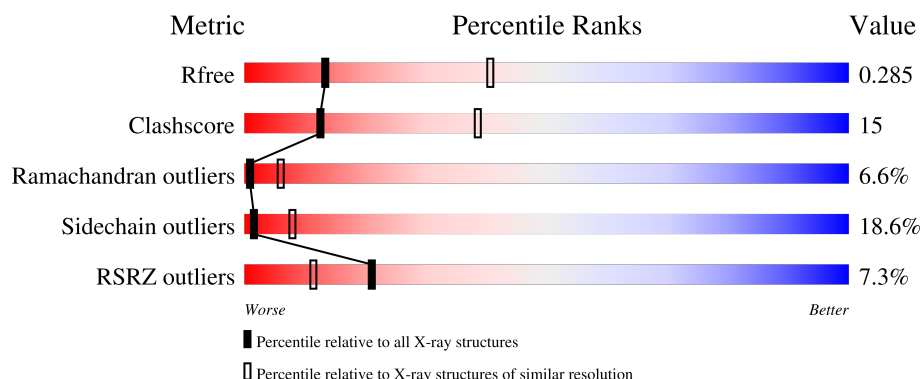
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	210	4% 51% 36% 9% ..
2	B	242	5% 56% 33% 9% .
3	C	183	8% 52% 32% 13% ..
4	D	215	10% 31% 32% 7% 30%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6260 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 mouse TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1606	1004	269	325	8			

- Molecule 2 is a protein called mouse TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1922	1217	335	361	9			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	181	Total	C	N	O	S	0	0	0
			1449	939	234	273	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	64	CYS	ASN	conflict	UNP P04228

- Molecule 4 is a protein called H2-Ab1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	150	Total	C	N	O	S	0	1	0
			1250	787	222	234	7			

There are 27 discrepancies between the modelled and reference sequences:

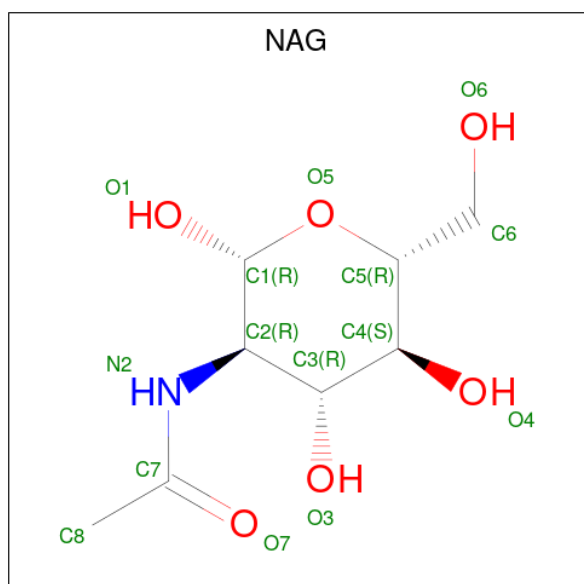
Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	HIS	-	expression tag	UNP Q31135
D	-27	LEU	-	expression tag	UNP Q31135
D	-26	VAL	-	expression tag	UNP Q31135

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-25	GLU	-	expression tag	UNP Q31135
D	-24	ARG	-	expression tag	UNP Q31135
D	-23	LEU	-	expression tag	UNP Q31135
D	-22	TYR	-	expression tag	UNP Q31135
D	-21	LEU	-	expression tag	UNP Q31135
D	-20	VAL	-	expression tag	UNP Q31135
D	-19	CYS	-	expression tag	UNP Q31135
D	-18	GLY	-	expression tag	UNP Q31135
D	-17	GLU	-	expression tag	UNP Q31135
D	-16	GLU	-	expression tag	UNP Q31135
D	-15	GLY	-	expression tag	UNP Q31135
D	-14	ALA	-	expression tag	UNP Q31135
D	-8	GLY	-	expression tag	UNP Q31135
D	-7	GLY	-	expression tag	UNP Q31135
D	-6	GLY	-	expression tag	UNP Q31135
D	-5	SER	-	expression tag	UNP Q31135
D	-4	LEU	-	expression tag	UNP Q31135
D	-3	VAL	-	expression tag	UNP Q31135
D	-2	GLY	-	expression tag	UNP Q31135
D	-1	GLY	-	expression tag	UNP Q31135
D	0	SER	-	expression tag	UNP Q31135
D	1	GLY	-	expression tag	UNP Q31135
D	2	GLY	-	expression tag	UNP Q31135
D	3	GLY	-	expression tag	UNP Q31135

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

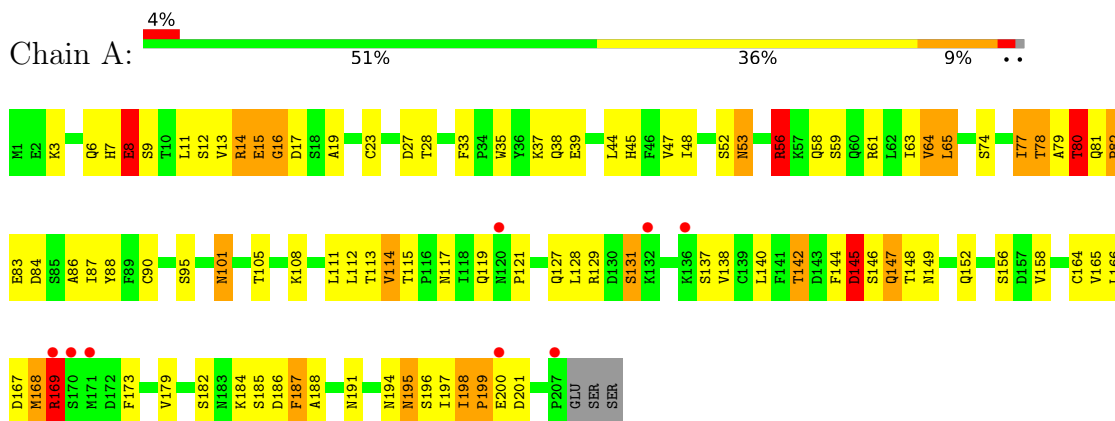
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	4	Total	O	0	0
			4	4		
6	C	6	Total	O	0	0
			6	6		
6	D	3	Total	O	0	0
			3	3		

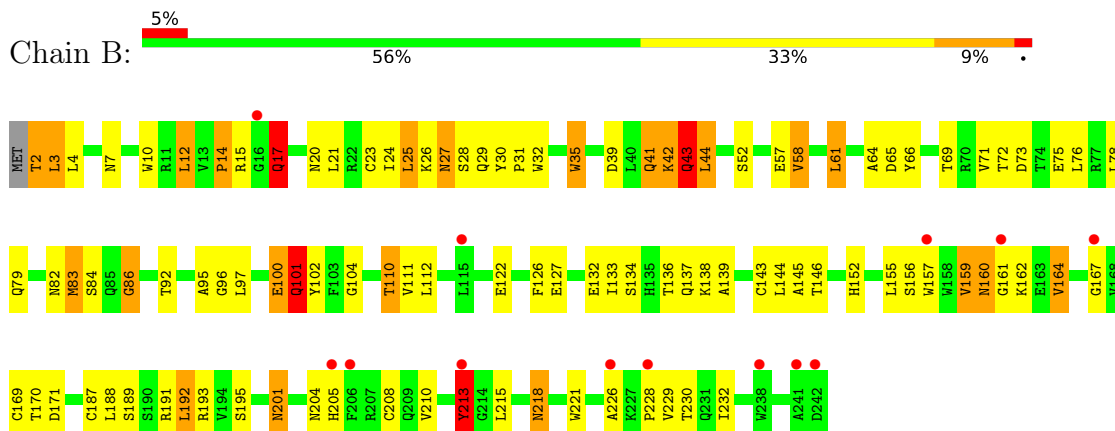
3 Residue-property plots

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.

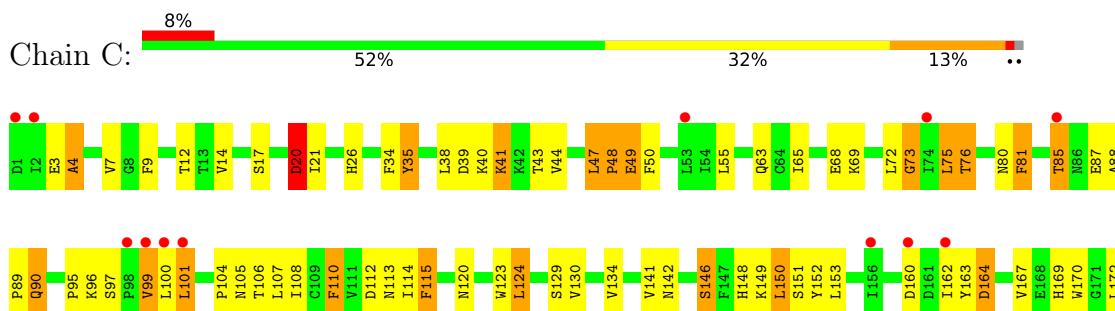
• Molecule 1: mouse TCR alpha chain

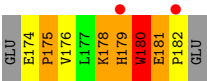


• Molecule 2: mouse TCR beta chain

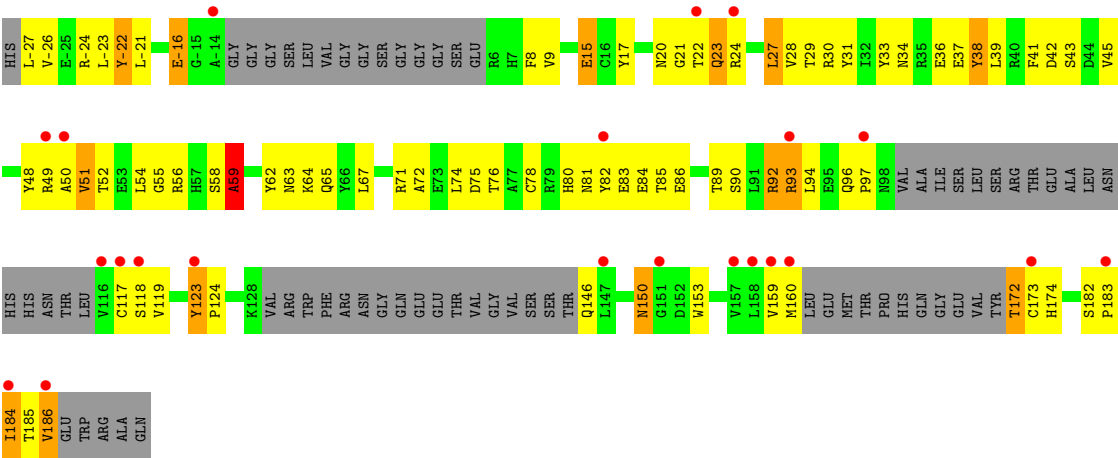
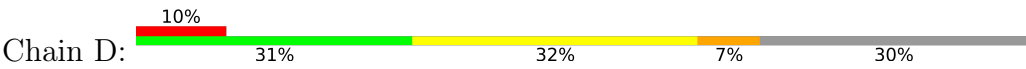


• Molecule 3: H-2 class II histocompatibility antigen, A-D alpha chain





● Molecule 4: H2-Ab1 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	269.52Å 269.52Å 45.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 3.10 50.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.01-3.10) 96.1 (50.01-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.240 , 0.285 0.244 , 0.285	Depositor DCC
R_{free} test set	1713 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6260	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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:
NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	4/1640 (0.2%)	1.38	11/2225 (0.5%)
2	B	1.07	2/1975 (0.1%)	1.24	10/2698 (0.4%)
3	C	1.10	1/1494 (0.1%)	1.26	13/2042 (0.6%)
4	D	1.16	0/1275	1.19	6/1722 (0.3%)
All	All	1.15	7/6384 (0.1%)	1.27	40/8687 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
3	C	0	2
4	D	0	3
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	GLN	N-CA	7.86	1.56	1.46
1	A	56	ARG	C-O	-5.74	1.16	1.23
3	C	180	TRP	CA-C	5.41	1.60	1.52
1	A	64	VAL	C-O	-5.19	1.18	1.24
1	A	52	SER	CA-C	5.10	1.59	1.52
1	A	33	PHE	C-O	-5.08	1.19	1.24
2	B	213	TYR	CA-CB	5.06	1.59	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	GLY	N-CA-C	9.15	122.86	110.69
3	C	88	ALA	CA-C-N	8.19	130.08	119.84
3	C	88	ALA	C-N-CA	8.19	130.08	119.84
1	A	95	SER	N-CA-C	-7.23	104.44	113.18
1	A	3	LYS	N-CA-C	-6.83	98.10	109.24
4	D	159	VAL	N-CA-C	6.76	118.64	106.61
1	A	168	MET	CA-C-N	6.68	133.72	121.70
1	A	168	MET	C-N-CA	6.68	133.72	121.70
1	A	198	ILE	CA-C-N	6.45	127.90	119.84
1	A	198	ILE	C-N-CA	6.45	127.90	119.84
3	C	35	TYR	N-CA-C	-6.42	99.28	109.23
2	B	122	GLU	N-CA-C	-6.38	99.42	109.50
4	D	38	TYR	N-CA-C	6.26	118.19	111.36
4	D	59	ALA	N-CA-C	6.19	120.39	112.34
4	D	75	ASP	N-CA-C	-6.04	105.57	113.12
1	A	145	ASP	N-CA-C	-6.01	102.56	110.43
3	C	108	ILE	N-CA-C	5.95	116.58	107.77
2	B	101	GLN	N-CA-C	-5.85	100.75	110.17
2	B	134	SER	N-CA-C	5.81	119.84	112.87
2	B	139	ALA	N-CA-C	5.71	116.77	107.23
1	A	101	ASN	CB-CA-C	-5.62	99.24	110.42
3	C	163	TYR	N-CA-C	5.62	118.05	108.90
1	A	80	THR	N-CA-C	5.56	117.71	110.43
2	B	104	GLY	CA-C-N	5.45	126.49	120.45
2	B	104	GLY	C-N-CA	5.45	126.49	120.45
3	C	20	ASP	CB-CA-C	5.42	121.20	110.42
3	C	21	ILE	CA-C-N	-5.33	118.50	122.18
3	C	21	ILE	C-N-CA	-5.33	118.50	122.18
3	C	47	LEU	N-CA-C	5.25	118.19	109.79
1	A	199	PRO	N-CA-C	5.24	123.25	112.47
3	C	99	VAL	N-CA-C	5.21	116.30	109.21
1	A	169	ARG	N-CA-CB	5.21	119.35	110.50
2	B	71	VAL	CB-CA-C	5.16	118.44	111.94
4	D	-22	TYR	N-CA-C	5.12	117.77	109.06
4	D	123	TYR	C-N-CD	-5.09	109.41	120.60
3	C	129	SER	N-CA-C	5.09	116.77	108.63
2	B	52	SER	CA-C-N	-5.05	115.03	120.03
2	B	52	SER	C-N-CA	-5.05	115.03	120.03
3	C	130	VAL	N-CA-C	5.04	115.60	107.73
3	C	48	PRO	N-CA-C	5.02	122.81	112.47

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ALA	Peptide
1	A	39	GLU	Peptide
1	A	65	LEU	Peptide
3	C	178	LYS	Peptide
3	C	20	ASP	Peptide
4	D	21	GLY	Peptide
4	D	49	ARG	Peptide
4	D	92	ARG	Peptide

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	1606	0	1527	47	0
2	B	1922	0	1823	63	0
3	C	1449	0	1372	47	0
4	D	1250	0	1188	43	0
5	C	14	0	13	0	0
6	A	6	0	0	1	0
6	B	4	0	0	0	0
6	C	6	0	0	0	0
6	D	3	0	0	0	0
All	All	6260	0	5923	186	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 15.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:HG2	1:A:23:CYS:SG	2.19	0.82
3:C:87:GLU:HB3	3:C:113:ASN:HD21	1.47	0.78
1:A:56:ARG:NH1	1:A:58:GLN:OE1	2.18	0.77
4:D:30:ARG:NH1	4:D:37:GLU:OE1	2.17	0.75
4:D:50:ALA:HB2	4:D:55:GLY:O	1.88	0.74
4:D:123:TYR:CD1	4:D:124:PRO:HA	2.26	0.70
4:D:64:LYS:O	4:D:65:GLN:HG2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ASN:C	2:B:218:ASN:HD22	2.01	0.68
1:A:14:ARG:O	1:A:15:GLU:O	2.12	0.66
3:C:149:LYS:O	3:C:150:LEU:HD12	1.95	0.66
4:D:81:ASN:O	4:D:85:THR:OG1	2.14	0.65
4:D:-24:ARG:NH1	4:D:86:GLU:OE2	2.30	0.65
1:A:77:ILE:HD11	1:A:88:TYR:CE2	2.31	0.64
1:A:140:LEU:HD22	1:A:142:THR:OG1	1.99	0.62
2:B:3:LEU:HD11	2:B:30:TYR:CD2	2.34	0.62
1:A:7:HIS:O	1:A:8:GLU:HG2	1.99	0.62
1:A:61:ARG:O	1:A:78:THR:HB	2.00	0.62
2:B:27:ASN:OD1	2:B:27:ASN:C	2.43	0.61
3:C:38:LEU:HD13	3:C:65:ILE:HG13	1.83	0.61
4:D:174:HIS:HA	4:D:185:THR:HG22	1.83	0.60
2:B:215:LEU:HD12	2:B:229:VAL:HA	1.81	0.60
4:D:43:SER:HB2	4:D:74:LEU:HD12	1.83	0.59
4:D:64:LYS:O	4:D:65:GLN:CG	2.50	0.59
1:A:173:PHE:CE2	2:B:138:LYS:HE3	2.38	0.59
3:C:20:ASP:OD1	3:C:20:ASP:O	2.19	0.59
2:B:110:THR:OG1	2:B:152:HIS:NE2	2.37	0.58
2:B:14:PRO:O	2:B:17:GLN:HB2	2.03	0.57
1:A:53:ASN:OD1	1:A:53:ASN:N	2.37	0.57
2:B:41:GLN:C	2:B:42:LYS:O	2.47	0.57
1:A:13:VAL:O	1:A:114:VAL:HA	2.04	0.57
2:B:213:TYR:HA	2:B:230:THR:HG23	1.85	0.56
2:B:35:TRP:CE2	2:B:78:LEU:HB2	2.41	0.56
2:B:155:LEU:HD12	2:B:210:VAL:HG22	1.86	0.56
3:C:112:ASP:OD1	3:C:113:ASN:N	2.37	0.55
3:C:181:GLU:CB	3:C:182:PRO:CD	2.85	0.55
4:D:94:LEU:HD22	4:D:124:PRO:HD2	1.89	0.55
3:C:169:HIS:CG	3:C:170:TRP:H	2.25	0.55
2:B:157:TRP:CE3	2:B:192:LEU:HD23	2.42	0.54
2:B:35:TRP:CE2	2:B:76:LEU:HD23	2.43	0.54
1:A:198:ILE:HB	1:A:199:PRO:HD2	1.89	0.54
3:C:174:GLU:N	3:C:175:PRO:HD2	2.23	0.54
1:A:138:VAL:HG13	2:B:126:PHE:CE2	2.43	0.53
3:C:142:ASN:HB2	3:C:146:SER:OG	2.08	0.53
2:B:4:LEU:HD22	2:B:23:CYS:SG	2.49	0.53
1:A:45:HIS:HB2	6:A:306:HOH:O	2.08	0.53
1:A:7:HIS:O	1:A:8:GLU:CG	2.56	0.53
3:C:7:VAL:HG22	4:D:17:TYR:HD1	1.74	0.53
4:D:36:GLU:HG2	4:D:52:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:TYR:CE2	3:C:44:VAL:HG11	2.45	0.52
3:C:87:GLU:CB	3:C:113:ASN:HD21	2.20	0.52
3:C:38:LEU:CD1	3:C:65:ILE:HG13	2.40	0.52
2:B:83:MET:HE1	2:B:86:GLY:HA2	1.92	0.52
4:D:27:LEU:HD12	4:D:78:CYS:SG	2.49	0.52
3:C:80:ASN:O	3:C:81:PHE:HB2	2.09	0.52
1:A:80:THR:HB	1:A:114:VAL:HG21	1.91	0.52
1:A:173:PHE:CE2	2:B:138:LYS:CE	2.93	0.52
2:B:39:ASP:OD1	2:B:39:ASP:C	2.52	0.52
2:B:65:ASP:OD2	2:B:82:ASN:ND2	2.42	0.52
2:B:192:LEU:HD12	2:B:192:LEU:C	2.35	0.52
4:D:172:THR:HG22	4:D:186:VAL:C	2.35	0.52
3:C:134:VAL:HA	3:C:152:TYR:O	2.09	0.52
2:B:61:LEU:O	2:B:64:ALA:O	2.28	0.51
4:D:50:ALA:CB	4:D:55:GLY:O	2.58	0.51
1:A:127:GLN:C	1:A:128:LEU:HD12	2.35	0.51
4:D:42:ASP:HB3	4:D:45:VAL:HG23	1.93	0.51
3:C:114:ILE:O	3:C:115:PHE:HB2	2.11	0.50
2:B:42:LYS:O	2:B:43:GLN:CB	2.58	0.50
3:C:142:ASN:OD1	3:C:148:HIS:ND1	2.38	0.50
1:A:165:VAL:O	2:B:169:CYS:SG	2.70	0.50
2:B:2:THR:O	2:B:4:LEU:N	2.44	0.50
2:B:42:LYS:O	2:B:43:GLN:HB3	2.12	0.50
1:A:61:ARG:NH2	1:A:84:ASP:OD2	2.44	0.50
4:D:82:TYR:C	4:D:82:TYR:CD1	2.89	0.50
3:C:47:LEU:HD11	4:D:153:TRP:CD1	2.47	0.49
3:C:63:GLN:OE1	4:D:-22:TYR:OH	2.19	0.49
4:D:48:TYR:CD2	4:D:62:TYR:HB3	2.47	0.49
1:A:6:GLN:CG	1:A:23:CYS:SG	2.95	0.49
2:B:10:TRP:CZ3	2:B:213:TYR:CE1	3.00	0.49
2:B:41:GLN:O	2:B:42:LYS:O	2.30	0.49
1:A:35:TRP:CZ3	1:A:90:CYS:HB3	2.47	0.49
3:C:110:PHE:C	3:C:110:PHE:CD1	2.91	0.49
2:B:32:TRP:CH2	2:B:97:LEU:HD21	2.48	0.49
4:D:150:ASN:N	4:D:150:ASN:OD1	2.44	0.49
2:B:12:LEU:HD22	2:B:112:LEU:HD22	1.95	0.48
1:A:195:ASN:OD1	1:A:195:ASN:N	2.46	0.48
1:A:16:GLY:HA2	1:A:79:ALA:HA	1.96	0.48
2:B:201:ASN:HD21	2:B:204:ASN:ND2	2.12	0.48
2:B:159:VAL:HG23	2:B:164:VAL:HG11	1.96	0.48
1:A:168:MET:HA	1:A:169:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:TYR:HB2	4:D:39:LEU:HB3	1.95	0.47
3:C:76:THR:HA	4:D:33:TYR:OH	2.14	0.47
4:D:59:ALA:O	4:D:63:ASN:ND2	2.47	0.47
1:A:168:MET:CE	2:B:193:ARG:O	2.63	0.47
2:B:20:ASN:HB3	2:B:79:GLN:HA	1.96	0.47
3:C:167:VAL:HG12	3:C:167:VAL:O	2.15	0.47
3:C:34:PHE:CD2	3:C:43:THR:HG23	2.49	0.47
3:C:180:TRP:CD1	3:C:181:GLU:N	2.82	0.47
1:A:168:MET:HA	1:A:169:ARG:CB	2.45	0.46
4:D:63:ASN:HA	4:D:67:LEU:HB2	1.96	0.46
1:A:158:VAL:HG22	1:A:182:SER:HB2	1.96	0.46
3:C:123:TRP:CG	3:C:153:LEU:HD22	2.51	0.46
1:A:80:THR:CG2	1:A:114:VAL:HG21	2.45	0.46
2:B:100:GLU:HG3	2:B:102:TYR:CE1	2.51	0.45
2:B:26:LYS:O	2:B:27:ASN:HB2	2.16	0.45
3:C:114:ILE:HG22	3:C:115:PHE:N	2.31	0.45
4:D:97:PRO:HB3	4:D:119:VAL:HG22	1.98	0.45
2:B:10:TRP:CE3	2:B:213:TYR:CE1	3.04	0.45
2:B:221:TRP:CZ2	2:B:228:PRO:HD3	2.52	0.45
4:D:67:LEU:O	4:D:71:ARG:HG3	2.17	0.45
1:A:82:PRO:HA	1:A:114:VAL:HG12	1.99	0.45
1:A:145:ASP:C	1:A:145:ASP:OD1	2.59	0.45
2:B:92:THR:OG1	2:B:101:GLN:HG3	2.16	0.44
2:B:100:GLU:HG3	2:B:102:TYR:CZ	2.52	0.44
3:C:68:GLU:O	3:C:69:LYS:C	2.59	0.44
3:C:169:HIS:CG	3:C:170:TRP:N	2.86	0.44
4:D:72:ALA:O	4:D:76:THR:HG23	2.17	0.44
2:B:35:TRP:CE2	2:B:76:LEU:CD2	3.00	0.44
1:A:44:LEU:HD21	2:B:44:LEU:HD21	2.00	0.44
1:A:47:VAL:HG12	1:A:48:ILE:HG22	2.00	0.44
2:B:171:ASP:HB2	2:B:188:LEU:CD1	2.47	0.44
2:B:26:LYS:O	2:B:27:ASN:CB	2.63	0.44
2:B:27:ASN:OD1	2:B:28:SER:N	2.51	0.44
4:D:67:LEU:CD1	4:D:71:ARG:HD2	2.47	0.44
1:A:147:GLN:HA	1:A:147:GLN:OE1	2.17	0.44
3:C:172:LEU:HD12	3:C:172:LEU:O	2.17	0.44
2:B:145:ALA:HB3	2:B:188:LEU:HB3	2.01	0.43
3:C:26:HIS:HB2	3:C:34:PHE:CE1	2.52	0.43
4:D:89:THR:OG1	4:D:90:SER:N	2.52	0.43
2:B:170:THR:HG22	2:B:171:ASP:N	2.34	0.43
3:C:181:GLU:CB	3:C:182:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:TRP:NE1	2:B:78:LEU:HB2	2.32	0.43
2:B:160:ASN:O	2:B:162:LYS:N	2.51	0.43
3:C:40:LYS:O	3:C:41:LYS:C	2.62	0.43
3:C:151:SER:C	3:C:152:TYR:HD1	2.27	0.43
2:B:58:VAL:HA	2:B:66:TYR:O	2.19	0.43
4:D:-26:VAL:HG11	4:D:84:GLU:O	2.19	0.43
2:B:12:LEU:HD22	2:B:112:LEU:HB2	2.01	0.42
2:B:171:ASP:HB2	2:B:188:LEU:HD12	2.00	0.42
3:C:9:PHE:CE1	4:D:15:GLU:HG3	2.54	0.42
1:A:131:SER:HB2	2:B:127:GLU:OE2	2.19	0.42
4:D:-23:LEU:HD12	4:D:80:HIS:CD2	2.54	0.42
2:B:25:LEU:HD21	2:B:30:TYR:O	2.19	0.42
3:C:124:LEU:HB2	3:C:164:ASP:HB3	2.00	0.42
2:B:189:SER:OG	2:B:191:ARG:NH2	2.47	0.42
1:A:81:GLN:O	1:A:82:PRO:C	2.62	0.42
3:C:110:PHE:C	3:C:110:PHE:HD1	2.28	0.42
1:A:119:GLN:C	1:A:121:PRO:HD3	2.44	0.42
1:A:80:THR:CB	1:A:114:VAL:HG21	2.50	0.42
2:B:143:CYS:SG	2:B:208:CYS:SG	3.17	0.42
3:C:174:GLU:N	3:C:175:PRO:CD	2.83	0.42
4:D:41:PHE:C	4:D:41:PHE:CD1	2.97	0.42
2:B:132:GLU:O	2:B:136:THR:OG1	2.31	0.41
2:B:31:PRO:HD2	2:B:95:ALA:HA	2.02	0.41
2:B:84:SER:O	2:B:111:VAL:HG21	2.20	0.41
3:C:178:LYS:C	3:C:179:HIS:O	2.62	0.41
1:A:44:LEU:HD12	1:A:44:LEU:N	2.35	0.41
3:C:142:ASN:ND2	3:C:146:SER:OG	2.38	0.41
4:D:72:ALA:C	4:D:76:THR:HG23	2.45	0.41
2:B:145:ALA:O	2:B:187:CYS:HA	2.21	0.41
4:D:93:ARG:NH1	4:D:153:TRP:HB3	2.36	0.41
1:A:38:GLN:O	1:A:86:ALA:HB1	2.20	0.41
1:A:167:ASP:O	2:B:167:GLY:N	2.53	0.41
4:D:-22:TYR:O	4:D:-22:TYR:CG	2.73	0.41
1:A:111:LEU:HD23	1:A:112:LEU:N	2.36	0.41
3:C:47:LEU:O	3:C:49:GLU:N	2.53	0.41
3:C:72:LEU:O	3:C:73:GLY:C	2.63	0.41
2:B:27:ASN:OD1	2:B:29:GLN:N	2.47	0.41
4:D:-16:GLU:OE1	4:D:58:SER:OG	2.38	0.41
3:C:105:ASN:OD1	3:C:106:THR:N	2.52	0.41
3:C:142:ASN:HB2	3:C:146:SER:HG	1.84	0.41
2:B:2:THR:HG23	2:B:3:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:ASN:HB3	4:D:23:GLN:HG3	2.03	0.41
1:A:186:ASP:O	1:A:187:PHE:C	2.64	0.40
1:A:191:ASN:O	1:A:194:ASN:HB2	2.21	0.40
1:A:19:ALA:CB	1:A:112:LEU:HD11	2.51	0.40
1:A:81:GLN:O	1:A:83:GLU:N	2.54	0.40
3:C:72:LEU:O	3:C:75:LEU:N	2.54	0.40
3:C:3:GLU:O	3:C:4:ALA:CB	2.69	0.40
1:A:15:GLU:O	1:A:17:ASP:N	2.55	0.40
3:C:75:LEU:HD11	4:D:38:TYR:CE1	2.57	0.40
3:C:150:LEU:HB3	3:C:152:TYR:HE1	1.86	0.40
1:A:144:PHE:CD2	1:A:148:THR:HG22	2.56	0.40
2:B:215:LEU:O	2:B:229:VAL:HG23	2.22	0.40
4:D:37:GLU:OE2	4:D:51:VAL:HG21	2.21	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	205/210 (98%)	170 (83%)	24 (12%)	11 (5%)	1	9
2	B	239/242 (99%)	200 (84%)	25 (10%)	14 (6%)	1	8
3	C	177/183 (97%)	135 (76%)	23 (13%)	19 (11%)	0	2
4	D	141/215 (66%)	110 (78%)	25 (18%)	6 (4%)	2	12
All	All	762/850 (90%)	615 (81%)	97 (13%)	50 (7%)	1	6

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	169	ARG
1	A	187	PHE
1	A	200	GLU
2	B	3	LEU
2	B	43	GLN
2	B	161	GLY
2	B	226	ALA
3	C	4	ALA
3	C	48	PRO
3	C	81	PHE
3	C	89	PRO
3	C	175	PRO
3	C	180	TRP
3	C	181	GLU
4	D	22	THR
4	D	24	ARG
4	D	183	PRO
1	A	16	GLY
1	A	152	GLN
2	B	27	ASN
2	B	42	LYS
2	B	73	ASP
2	B	86	GLY
2	B	137	GLN
3	C	95	PRO
3	C	101	LEU
3	C	146	SER
1	A	8	GLU
2	B	100	GLU
2	B	160	ASN
3	C	90	GLN
4	D	184	ILE
1	A	131	SER
1	A	184	LYS
2	B	17	GLN
3	C	20	ASP
3	C	41	LYS
3	C	115	PHE
4	D	59	ALA
3	C	12	THR
3	C	73	GLY
3	C	85	THR

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Mol	Chain	Res	Type
3	C	96	LYS
3	C	179	HIS
4	D	34	ASN
1	A	82	PRO
2	B	14	PRO
2	B	133	ILE

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	182/189 (96%)	141 (78%)	41 (22%)	1	4
2	B	205/213 (96%)	172 (84%)	33 (16%)	2	11
3	C	160/165 (97%)	134 (84%)	26 (16%)	2	11
4	D	136/188 (72%)	109 (80%)	27 (20%)	1	6
All	All	683/755 (90%)	556 (81%)	127 (19%)	1	8

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	SER
1	A	11	LEU
1	A	12	SER
1	A	14	ARG
1	A	27	ASP
1	A	28	THR
1	A	37	LYS
1	A	53	ASN
1	A	56	ARG
1	A	59	SER
1	A	63	ILE
1	A	64	VAL
1	A	65	LEU
1	A	74	SER

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Mol	Chain	Res	Type
1	A	77	ILE
1	A	78	THR
1	A	80	THR
1	A	87	ILE
1	A	105	THR
1	A	108	LYS
1	A	113	THR
1	A	114	VAL
1	A	115	THR
1	A	117	ASN
1	A	129	ARG
1	A	137	SER
1	A	142	THR
1	A	145	ASP
1	A	146	SER
1	A	147	GLN
1	A	149	ASN
1	A	156	SER
1	A	164	CYS
1	A	166	LEU
1	A	179	VAL
1	A	185	SER
1	A	195	ASN
1	A	196	SER
1	A	197	ILE
1	A	201	ASP
2	B	2	THR
2	B	7	ASN
2	B	12	LEU
2	B	15	ARG
2	B	17	GLN
2	B	21	LEU
2	B	24	ILE
2	B	25	LEU
2	B	35	TRP
2	B	41	GLN
2	B	43	GLN
2	B	44	LEU
2	B	57	GLU
2	B	58	VAL
2	B	61	LEU
2	B	69	THR

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Mol	Chain	Res	Type
2	B	72	THR
2	B	75	GLU
2	B	83	MET
2	B	101	GLN
2	B	110	THR
2	B	144	LEU
2	B	146	THR
2	B	156	SER
2	B	159	VAL
2	B	164	VAL
2	B	192	LEU
2	B	195	SER
2	B	201	ASN
2	B	205	HIS
2	B	213	TYR
2	B	218	ASN
2	B	232	ILE
3	C	14	VAL
3	C	17	SER
3	C	20	ASP
3	C	39	ASP
3	C	49	GLU
3	C	50	PHE
3	C	55	LEU
3	C	75	LEU
3	C	76	THR
3	C	85	THR
3	C	90	GLN
3	C	97	SER
3	C	99	VAL
3	C	100	LEU
3	C	101	LEU
3	C	104	PRO
3	C	107	LEU
3	C	110	PHE
3	C	120	ASN
3	C	124	LEU
3	C	141	VAL
3	C	150	LEU
3	C	160	ASP
3	C	162	ILE
3	C	164	ASP

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Mol	Chain	Res	Type
3	C	176	VAL
4	D	-27	LEU
4	D	-21	LEU
4	D	-16	GLU
4	D	8	PHE
4	D	9	VAL
4	D	15	GLU
4	D	23	GLN
4	D	27	LEU
4	D	28	VAL
4	D	29	THR
4	D	51	VAL
4	D	54	LEU
4	D	56	ARG
4	D	83	GLU
4	D	92	ARG
4	D	93	ARG
4	D	96	GLN
4	D	117	CYS
4	D	118	SER
4	D	146	GLN
4	D	150	ASN
4	D	160	MET
4	D	172	THR
4	D	173	CYS
4	D	182	SER
4	D	184	ILE
4	D	186	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	194	ASN
2	B	17	GLN
2	B	41	GLN
2	B	43	GLN
2	B	45	GLN
2	B	101	GLN
2	B	173	GLN
2	B	201	ASN
2	B	211	GLN

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Mol	Chain	Res	Type
2	B	218	ASN
3	C	90	GLN
3	C	113	ASN
4	D	20	ASN
4	D	65	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	C	201	3	14,14,15	1.21	1 (7%)	17,19,21	1.61	3 (17%)

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
5	NAG	C	201	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	NAG	C1-C2	3.27	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	201	NAG	C2-N2-C7	3.66	127.81	122.90
5	C	201	NAG	O5-C5-C6	3.01	113.52	107.66
5	C	201	NAG	O7-C7-N2	2.17	125.81	121.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	201	NAG	O5-C5-C6-O6
5	C	201	NAG	C4-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	207/210 (98%)	0.24	8 (3%)	43 24	17, 46, 99, 128	0
2	B	241/242 (99%)	0.49	13 (5%)	31 17	20, 66, 119, 131	0
3	C	181/183 (98%)	0.70	14 (7%)	19 10	24, 72, 125, 145	0
4	D	150/215 (69%)	1.04	22 (14%)	6 3	22, 80, 141, 151	1 (0%)
All	All	779/850 (91%)	0.58	57 (7%)	21 11	17, 66, 127, 151	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	LYS	4.2
4	D	157	VAL	4.0
3	C	101	LEU	3.9
4	D	116	VAL	3.8
2	B	16	GLY	3.7
3	C	98	PRO	3.6
4	D	118	SER	3.6
4	D	50	ALA	3.6
3	C	53	LEU	3.6
4	D	147	LEU	3.5
2	B	161	GLY	3.5
4	D	-14	ALA	3.5
4	D	186	VAL	3.2
3	C	99	VAL	3.2
4	D	151	GLY	3.2
3	C	156	ILE	3.1
3	C	162	ILE	3.0
2	B	167	GLY	3.0
4	D	24	ARG	3.0
4	D	117	CYS	2.9
3	C	2	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	207	PRO	2.8
1	A	169	ARG	2.7
3	C	100	LEU	2.7
2	B	205	HIS	2.7
4	D	184	ILE	2.6
4	D	22	THR	2.6
3	C	182	PRO	2.6
1	A	170	SER	2.6
3	C	1	ASP	2.6
2	B	206	PHE	2.5
2	B	213	TYR	2.5
2	B	115	LEU	2.5
4	D	158	LEU	2.5
4	D	160	MET	2.5
3	C	74	ILE	2.5
1	A	136	LYS	2.4
2	B	241	ALA	2.4
4	D	159	VAL	2.4
4	D	173	CYS	2.4
4	D	49	ARG	2.3
3	C	85	THR	2.3
3	C	179	HIS	2.3
4	D	97	PRO	2.3
2	B	242	ASP	2.2
2	B	238	TRP	2.2
4	D	123	TYR	2.2
2	B	226	ALA	2.2
4	D	183	PRO	2.2
2	B	157	TRP	2.2
3	C	160	ASP	2.1
1	A	200	GLU	2.1
2	B	228	PRO	2.1
4	D	82	TYR	2.1
1	A	120	ASN	2.0
4	D	93	ARG	2.0
1	A	171	MET	2.0

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

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

6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
5	NAG	C	201	14/15	0.93	0.08	67,77,81,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.