



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:22 PM UTC

PDB ID : 1FYT / pdb_00001fyt
Title : CRYSTAL STRUCTURE OF A COMPLEX OF A HUMAN ALPHA/BETA-T CELL RECEPTOR, INFLUENZA HA ANTIGEN PEPTIDE, AND MHC CLASS II MOLECULE, HLA-DR1
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Deposited on : 2000-10-03
Resolution : 2.60 Å(reported)

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

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

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

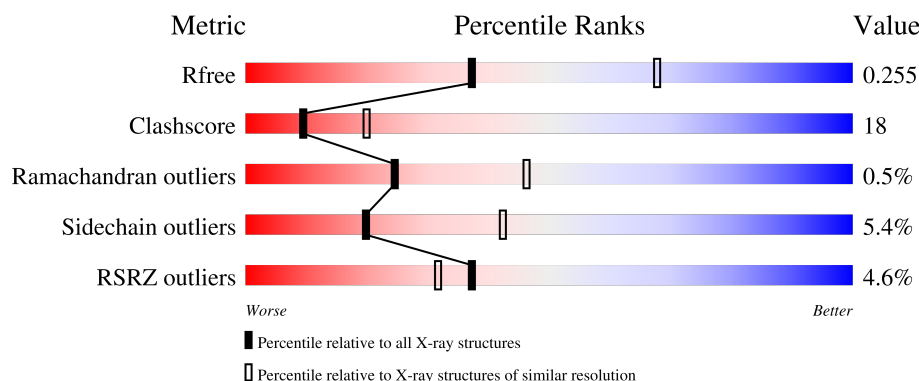
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	181	3% 64% 29% 6% ..
2	B	192	3% 63% 29% 7% .
3	C	13	46% 46% 8%
4	D	212	10% 52% 32% 9% 7%
5	E	245	2% 62% 31% . .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6644 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 HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1483	960	241	277	5			

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR-1 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total	C	N	O	S	0	0	0
			1467	926	260	275	6			

- Molecule 3 is a protein called HEMAGGLUTININ HA1 PEPTIDE CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			106	69	18	19			

- Molecule 4 is a protein called T-CELL RECEPTOR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1529	969	248	305	7			

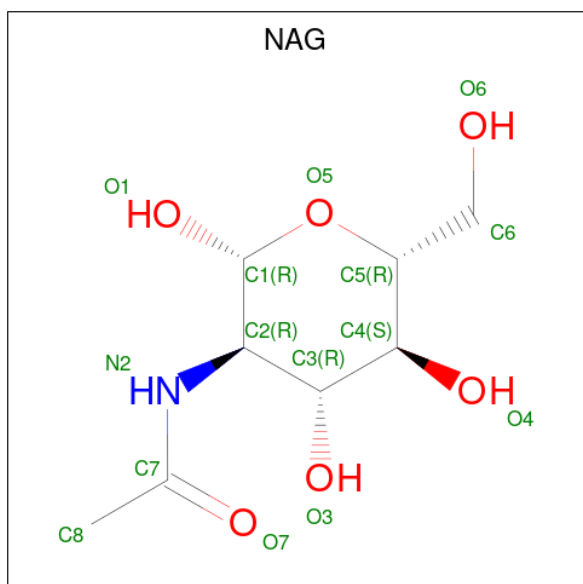
- Molecule 5 is a protein called T-CELL RECEPTOR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1931	1222	331	370	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	192	SER	CYS	engineered mutation	UNP P01850

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

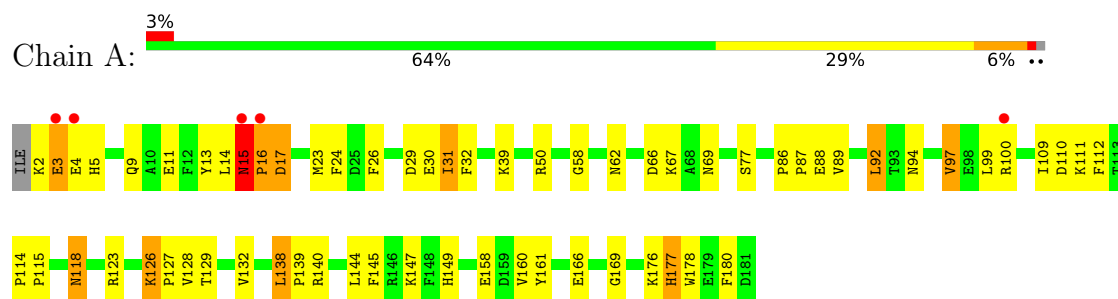
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	16	Total	O	0	0
			16	16		
7	B	17	Total	O	0	0
			17	17		
7	C	1	Total	O	0	0
			1	1		
7	D	29	Total	O	0	0
			29	29		
7	E	37	Total	O	0	0
			37	37		

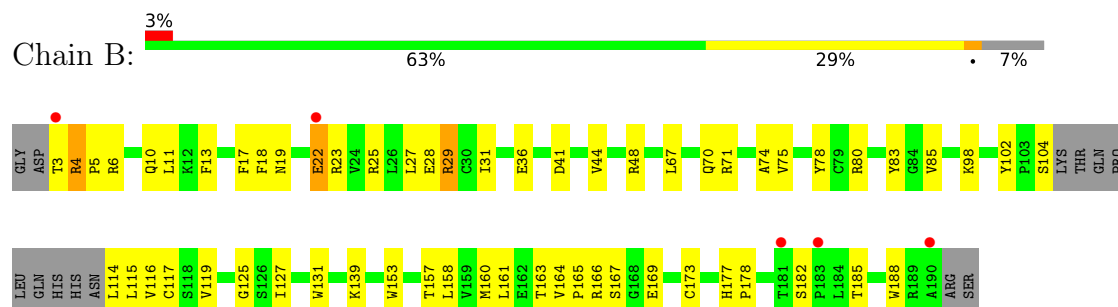
3 Residue-property plots

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.

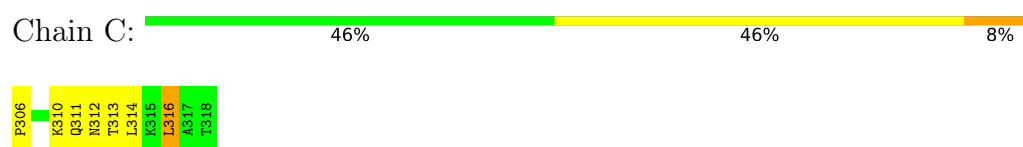
• Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN



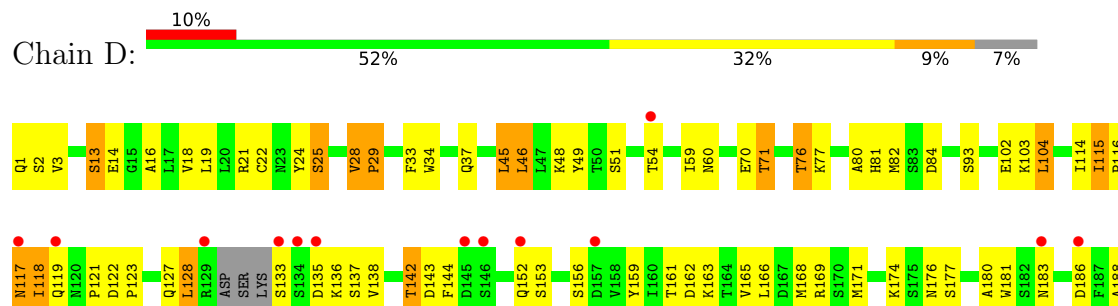
• Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR-1 BETA CHAIN

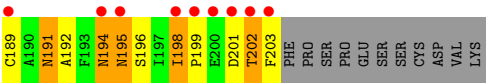


• Molecule 3: HEMAGGLUTININ HA1 PEPTIDE CHAIN

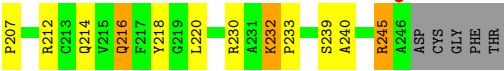
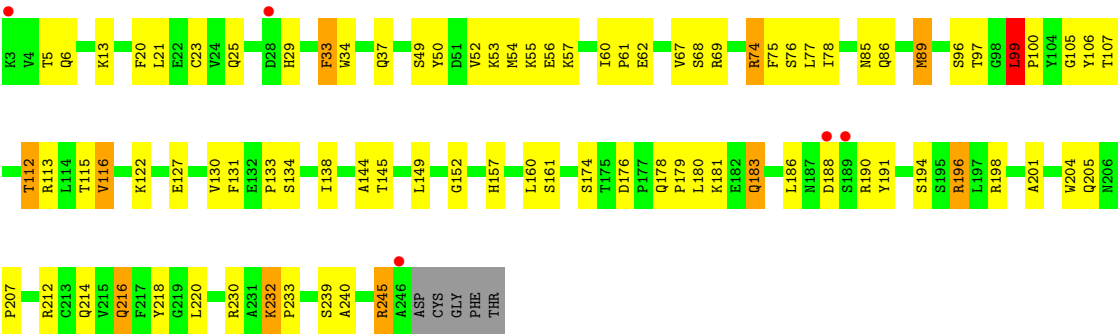


• Molecule 4: T-CELL RECEPTOR ALPHA CHAIN





● Molecule 5: T-CELL RECEPTOR BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.90Å 73.44Å 122.43Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-2.60) 99.5 (19.97-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.47 (at 2.60Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.221 , 0.255 0.221 , 0.255	Depositor DCC
R_{free} test set	1871 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6644	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 4.34% 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	0.57	1/1528 (0.1%)	1.12	19/2081 (0.9%)
2	B	0.48	0/1503	0.98	7/2040 (0.3%)
3	C	0.51	0/107	0.91	0/141
4	D	0.51	0/1564	1.12	19/2126 (0.9%)
5	E	0.51	0/1981	1.03	13/2686 (0.5%)
All	All	0.52	1/6683 (0.0%)	1.06	58/9074 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	PRO	C-O	6.39	1.32	1.24

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	TYR	CA-C-N	9.55	129.48	120.03
2	B	102	TYR	C-N-CA	9.55	129.48	120.03
1	A	15	ASN	N-CA-C	9.39	130.56	109.81
4	D	196	SER	N-CA-C	9.20	123.81	111.30
4	D	137	SER	N-CA-C	-8.26	95.93	109.40
4	D	194	ASN	N-CA-C	-8.09	97.07	109.85
5	E	127	GLU	N-CA-C	-8.00	96.36	109.40
1	A	88	GLU	N-CA-C	-7.95	95.46	108.41
1	A	15	ASN	CA-C-N	-7.89	109.98	119.84
1	A	15	ASN	C-N-CA	-7.89	109.98	119.84
1	A	138	LEU	CA-C-N	7.50	127.42	119.85
1	A	138	LEU	C-N-CA	7.50	127.42	119.85
5	E	99	LEU	CA-C-N	7.48	129.19	119.84
5	E	99	LEU	C-N-CA	7.48	129.19	119.84
4	D	119	GLN	N-CA-C	7.14	118.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	60	ILE	CA-C-N	7.00	126.48	118.85
5	E	60	ILE	C-N-CA	7.00	126.48	118.85
5	E	106	TYR	N-CA-C	6.98	120.09	110.24
4	D	103	LYS	N-CA-C	6.92	120.00	110.24
4	D	183	ASN	N-CA-C	-6.62	104.42	113.30
4	D	153	SER	N-CA-C	6.31	119.92	110.14
4	D	29	PRO	CA-C-N	6.21	125.97	119.76
4	D	29	PRO	C-N-CA	6.21	125.97	119.76
1	A	17	ASP	N-CA-C	6.13	119.59	111.75
4	D	156	SER	N-CA-C	-6.08	105.72	113.01
4	D	21	ARG	N-CA-C	5.91	119.53	110.20
5	E	107	THR	N-CA-C	-5.84	98.76	108.34
2	B	98	LYS	N-CA-C	-5.79	99.80	109.24
1	A	3	GLU	N-CA-C	5.78	118.65	110.50
5	E	105	GLY	N-CA-C	5.75	119.83	112.13
5	E	74	ARG	N-CA-C	5.66	118.13	108.90
4	D	122	ASP	CA-C-N	5.65	126.90	119.84
4	D	122	ASP	C-N-CA	5.65	126.90	119.84
1	A	158	GLU	N-CA-C	5.54	120.03	113.16
4	D	135	ASP	N-CA-C	-5.49	106.43	114.39
1	A	50	ARG	N-CA-C	-5.49	106.75	113.50
2	B	4	ARG	CA-C-N	5.47	126.67	119.84
2	B	4	ARG	C-N-CA	5.47	126.67	119.84
1	A	114	PRO	CA-C-N	5.47	126.67	119.84
1	A	114	PRO	C-N-CA	5.47	126.67	119.84
4	D	115	ILE	CA-C-N	5.39	125.15	119.76
4	D	115	ILE	C-N-CA	5.39	125.15	119.76
4	D	169	ARG	N-CA-C	5.39	117.60	111.02
1	A	144	LEU	N-CA-C	-5.34	102.09	110.36
4	D	142	THR	N-CA-C	5.33	117.09	109.14
5	E	183	GLN	CA-C-N	5.32	126.50	119.84
5	E	183	GLN	C-N-CA	5.32	126.50	119.84
4	D	102	GLU	N-CA-C	-5.32	102.14	110.17
2	B	44	VAL	N-CA-C	-5.30	107.25	111.81
2	B	125	GLY	N-CA-C	5.29	121.22	114.66
1	A	126	LYS	CA-C-N	5.17	125.09	119.76
1	A	126	LYS	C-N-CA	5.17	125.09	119.76
1	A	118	ASN	OD1-CG-ND2	5.11	127.71	122.60
1	A	97	VAL	N-CA-C	5.10	115.62	108.89
1	A	177	HIS	N-CA-C	5.09	118.36	110.17
5	E	232	LYS	CA-C-N	5.06	126.16	119.84
5	E	232	LYS	C-N-CA	5.06	126.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ILE	N-CA-C	-5.02	105.95	110.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1483	0	1418	52	0
2	B	1467	0	1403	49	0
3	C	106	0	119	13	0
4	D	1529	0	1459	77	0
5	E	1931	0	1857	63	0
6	A	28	0	26	2	0
7	A	16	0	0	1	0
7	B	17	0	0	1	0
7	C	1	0	0	0	0
7	D	29	0	0	0	0
7	E	37	0	0	1	0
All	All	6644	0	6282	229	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 18.

All (229) 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)
4:D:202:THR:HG21	7:E:288:HOH:O	1.51	1.09
4:D:198:ILE:HD12	4:D:198:ILE:H	1.06	1.07
4:D:198:ILE:HD12	4:D:198:ILE:N	1.79	0.97
4:D:37:GLN:HE22	5:E:37:GLN:HE22	1.04	0.97
4:D:123:PRO:HB2	4:D:201:ASP:HB3	1.52	0.91
4:D:28:VAL:HG22	4:D:29:PRO:HD2	1.50	0.91
4:D:198:ILE:H	4:D:198:ILE:CD1	1.73	0.87
4:D:191:ASN:HD22	4:D:192:ALA:N	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASN:O	1:A:16:PRO:C	2.18	0.84
5:E:54:MET:HE3	5:E:56:GLU:HG2	1.60	0.82
5:E:183:GLN:OE1	5:E:186:LEU:HD22	1.82	0.79
4:D:28:VAL:HG22	4:D:29:PRO:CD	2.13	0.78
2:B:116:VAL:HG22	2:B:160:MET:HG2	1.64	0.78
1:A:123:ARG:HG3	1:A:161:TYR:CE1	2.19	0.77
2:B:182:SER:HB2	7:B:195:HOH:O	1.85	0.75
5:E:230:ARG:HH12	5:E:233:PRO:HG3	1.50	0.74
4:D:123:PRO:CB	4:D:201:ASP:HB3	2.19	0.71
4:D:71:THR:HG23	4:D:71:THR:O	1.89	0.71
4:D:37:GLN:NE2	5:E:37:GLN:HE22	1.85	0.71
1:A:62:ASN:CG	3:C:313:THR:HG23	2.16	0.70
5:E:245:ARG:HB2	5:E:245:ARG:HH11	1.55	0.69
1:A:9:GLN:HG3	1:A:24:PHE:CE1	2.27	0.69
5:E:216:GLN:HG2	5:E:218:TYR:CZ	2.30	0.66
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.76	0.66
5:E:115:THR:OG1	5:E:157:HIS:HE1	1.77	0.66
2:B:13:PHE:CE1	2:B:28:GLU:HG3	2.31	0.66
4:D:128:LEU:N	4:D:128:LEU:HD12	2.11	0.66
1:A:23:MET:HE2	1:A:30:GLU:HG3	1.78	0.65
4:D:70:GLU:O	4:D:71:THR:HG22	1.96	0.65
1:A:115:PRO:HG3	1:A:145:PHE:CE1	2.32	0.65
4:D:37:GLN:HE22	5:E:37:GLN:NE2	1.86	0.65
1:A:129:THR:O	1:A:132:VAL:HG22	1.97	0.64
5:E:89:MET:HE2	5:E:112:THR:N	2.12	0.64
5:E:230:ARG:NH1	5:E:233:PRO:HG3	2.12	0.64
4:D:1:GLN:HA	4:D:25:SER:O	1.98	0.64
1:A:77:SER:HA	6:A:501:NAG:H82	1.80	0.63
4:D:168:MET:HE2	4:D:171:MET:HE3	1.81	0.63
5:E:245:ARG:HH11	5:E:245:ARG:CB	2.12	0.63
2:B:85:VAL:HG13	3:C:306:PRO:HB2	1.80	0.62
2:B:161:LEU:HG	2:B:163:THR:HG23	1.81	0.62
2:B:67:LEU:HD11	3:C:314:LEU:HD11	1.81	0.62
4:D:166:LEU:HB3	5:E:174:SER:HB3	1.79	0.62
4:D:2:SER:OG	4:D:25:SER:HB2	1.98	0.62
4:D:82:MET:HE2	4:D:114:ILE:CG2	2.30	0.61
4:D:49:TYR:CZ	4:D:51:SER:HA	2.35	0.61
4:D:123:PRO:HB2	4:D:201:ASP:CB	2.29	0.61
5:E:52:VAL:HG12	5:E:53:LYS:HD2	1.81	0.61
4:D:46:LEU:HD23	4:D:59:ILE:HG12	1.83	0.61
4:D:116:PRO:HG2	4:D:165:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:GLY:O	5:E:190:ARG:HD3	2.01	0.61
4:D:45:LEU:HD11	4:D:48:LYS:HD3	1.83	0.60
4:D:81:HIS:HD2	4:D:82:MET:N	2.00	0.60
1:A:58:GLY:O	3:C:310:LYS:HE3	2.02	0.60
5:E:122:LYS:HD2	5:E:188:ASP:OD2	2.01	0.60
2:B:165:PRO:HB3	2:B:188:TRP:HZ3	1.67	0.60
2:B:29:ARG:HG2	2:B:36:GLU:OE2	2.03	0.59
2:B:165:PRO:HB3	2:B:188:TRP:CZ3	2.37	0.59
4:D:136:LYS:HG2	4:D:181:TRP:HD1	1.66	0.59
4:D:194:ASN:O	4:D:195:ASN:HB2	2.03	0.59
1:A:160:VAL:HG13	1:A:177:HIS:CE1	2.38	0.59
3:C:311:GLN:HE21	3:C:311:GLN:HA	1.67	0.59
4:D:202:THR:HG22	4:D:203:PHE:H	1.67	0.59
5:E:115:THR:OG1	5:E:157:HIS:CE1	2.55	0.58
5:E:85:ASN:OD1	5:E:86:GLN:HG3	2.02	0.58
1:A:2:LYS:O	2:B:18:PHE:HD2	1.87	0.58
2:B:70:GLN:OE1	2:B:71:ARG:HD3	2.04	0.58
3:C:312:ASN:HB2	5:E:97:THR:HG22	1.86	0.58
1:A:3:GLU:HA	2:B:18:PHE:CE2	2.39	0.58
5:E:145:THR:OG1	5:E:198:ARG:HG3	2.04	0.58
5:E:212:ARG:HD3	5:E:239:SER:HB2	1.84	0.57
4:D:127:GLN:HG3	4:D:189:CYS:SG	2.45	0.57
5:E:96:SER:HB3	5:E:99:LEU:HD22	1.87	0.57
4:D:191:ASN:HD22	4:D:192:ALA:H	1.49	0.56
1:A:39:LYS:HD3	5:E:56:GLU:OE2	2.05	0.56
1:A:86:PRO:HG3	1:A:169:GLY:O	2.05	0.56
2:B:3:THR:HG21	2:B:4:ARG:NH1	2.20	0.56
4:D:194:ASN:O	4:D:195:ASN:CB	2.53	0.56
1:A:123:ARG:HB2	1:A:128:VAL:HG21	1.85	0.56
4:D:82:MET:HE2	4:D:114:ILE:HG22	1.87	0.56
1:A:14:LEU:HD11	2:B:6:ARG:HB3	1.87	0.56
5:E:160:LEU:HD23	5:E:161:SER:N	2.21	0.55
2:B:27:LEU:HG	2:B:29:ARG:HD2	1.87	0.55
2:B:119:VAL:HG11	2:B:127:ILE:CD1	2.36	0.55
4:D:198:ILE:HG22	4:D:199:PRO:HD2	1.88	0.55
5:E:54:MET:HE3	5:E:56:GLU:CG	2.33	0.55
5:E:130:VAL:HG23	5:E:240:ALA:HB3	1.89	0.55
5:E:180:LEU:HD12	5:E:180:LEU:O	2.07	0.55
2:B:19:ASN:HD22	2:B:22:GLU:HG2	1.72	0.54
4:D:191:ASN:HD22	4:D:191:ASN:C	2.13	0.54
4:D:136:LYS:HG2	4:D:181:TRP:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:LYS:HG3	5:E:67:VAL:CG1	2.37	0.54
2:B:173:CYS:O	2:B:185:THR:HA	2.08	0.54
3:C:311:GLN:HA	3:C:311:GLN:NE2	2.23	0.54
2:B:3:THR:HB	2:B:6:ARG:HH21	1.73	0.53
2:B:11:LEU:HD12	2:B:29:ARG:O	2.08	0.53
4:D:123:PRO:HG2	4:D:198:ILE:HG12	1.91	0.53
1:A:123:ARG:HG3	1:A:161:TYR:CZ	2.43	0.53
5:E:20:PHE:CE2	5:E:78:ILE:HG12	2.44	0.53
5:E:25:GLN:HE22	5:E:29:HIS:N	2.07	0.53
2:B:163:THR:O	2:B:165:PRO:HD3	2.09	0.52
4:D:71:THR:O	4:D:71:THR:CG2	2.56	0.52
2:B:75:VAL:HG12	2:B:80:ARG:NH1	2.24	0.52
2:B:3:THR:HG21	2:B:4:ARG:HH11	1.74	0.52
2:B:164:VAL:O	2:B:166:ARG:HG3	2.10	0.52
5:E:216:GLN:HG2	5:E:218:TYR:CE1	2.45	0.52
2:B:119:VAL:HG11	2:B:127:ILE:HD11	1.92	0.52
1:A:16:PRO:HD2	2:B:6:ARG:HD3	1.92	0.51
2:B:4:ARG:HH11	2:B:4:ARG:HG2	1.75	0.51
4:D:18:VAL:O	4:D:76:THR:HA	2.10	0.51
1:A:89:VAL:O	1:A:176:LYS:HE2	2.11	0.51
4:D:13:SER:O	4:D:16:ALA:HB3	2.10	0.51
5:E:62:GLU:H	5:E:62:GLU:CD	2.19	0.51
2:B:17:PHE:CE2	2:B:83:TYR:HB2	2.47	0.50
4:D:81:HIS:CD2	4:D:82:MET:N	2.78	0.50
4:D:81:HIS:HD2	4:D:82:MET:H	1.59	0.50
1:A:69:ASN:HB3	3:C:316:LEU:HD22	1.94	0.50
1:A:109:ILE:HG22	1:A:112:PHE:CE1	2.47	0.50
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.94	0.49
2:B:22:GLU:HG3	2:B:23:ARG:N	2.28	0.49
2:B:157:THR:O	2:B:158:LEU:HD12	2.12	0.49
5:E:160:LEU:HD23	5:E:160:LEU:C	2.37	0.49
4:D:93:SER:HB2	4:D:104:LEU:HD22	1.94	0.49
1:A:62:ASN:OD1	3:C:313:THR:HG23	2.13	0.49
1:A:147:LYS:NZ	1:A:149:HIS:CE1	2.81	0.49
4:D:118:ILE:HG22	4:D:121:PRO:HG3	1.93	0.49
5:E:49:SER:OG	5:E:69:ARG:HD3	2.12	0.49
2:B:74:ALA:O	2:B:78:TYR:HB3	2.13	0.49
4:D:22:CYS:HB2	4:D:34:TRP:CZ2	2.49	0.48
4:D:127:GLN:C	4:D:128:LEU:HD12	2.38	0.48
5:E:201:ALA:O	5:E:205:GLN:HG3	2.13	0.48
5:E:52:VAL:HG12	5:E:53:LYS:CD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:134:SER:O	5:E:138:ILE:HG13	2.13	0.48
4:D:116:PRO:HB3	4:D:174:LYS:HD2	1.96	0.48
1:A:3:GLU:HA	2:B:18:PHE:CD2	2.49	0.47
5:E:6:GLN:OE1	5:E:112:THR:HG23	2.14	0.47
5:E:50:TYR:HB2	5:E:54:MET:SD	2.54	0.47
1:A:99:LEU:O	1:A:100:ARG:HB2	2.15	0.47
1:A:77:SER:HA	6:A:501:NAG:C8	2.45	0.47
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.96	0.47
5:E:99:LEU:HA	5:E:100:PRO:HD3	1.68	0.47
2:B:3:THR:CG2	2:B:4:ARG:HH11	2.27	0.47
4:D:198:ILE:O	4:D:201:ASP:OD2	2.33	0.47
4:D:33:PHE:N	4:D:33:PHE:CD1	2.84	0.46
4:D:202:THR:HG22	4:D:203:PHE:N	2.29	0.46
4:D:166:LEU:C	4:D:166:LEU:HD12	2.40	0.46
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.51	0.46
1:A:32:PHE:CD1	1:A:32:PHE:C	2.93	0.46
1:A:87:PRO:HB3	1:A:109:ILE:HG23	1.98	0.46
1:A:15:ASN:O	1:A:17:ASP:N	2.48	0.46
5:E:33:PHE:N	5:E:33:PHE:CD1	2.83	0.46
2:B:31:ILE:N	2:B:31:ILE:HD12	2.31	0.46
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.51	0.45
1:A:97:VAL:HG21	1:A:178:TRP:CZ2	2.52	0.45
4:D:19:LEU:HD12	4:D:76:THR:HG23	1.98	0.45
4:D:19:LEU:CD1	4:D:76:THR:HG23	2.46	0.45
4:D:163:LYS:HA	4:D:177:SER:O	2.17	0.45
4:D:168:MET:HE3	5:E:198:ARG:O	2.16	0.45
2:B:29:ARG:CG	2:B:36:GLU:OE2	2.65	0.45
5:E:188:ASP:O	5:E:188:ASP:CG	2.60	0.45
5:E:220:LEU:HD12	5:E:233:PRO:HD2	1.99	0.45
4:D:60:ASN:O	4:D:77:LYS:NZ	2.48	0.45
5:E:25:GLN:HE22	5:E:29:HIS:H	1.63	0.45
4:D:191:ASN:O	4:D:192:ALA:C	2.60	0.45
4:D:14:GLU:HG3	4:D:117:ASN:HD21	1.82	0.44
1:A:13:TYR:CZ	1:A:67:LYS:HG2	2.52	0.44
1:A:126:LYS:HA	1:A:127:PRO:HD3	1.87	0.44
4:D:188:ALA:O	4:D:191:ASN:ND2	2.50	0.44
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.53	0.44
5:E:13:LYS:O	5:E:116:VAL:HA	2.17	0.44
4:D:14:GLU:HA	4:D:80:ALA:HB3	2.00	0.44
1:A:86:PRO:HG3	1:A:169:GLY:C	2.43	0.44
2:B:29:ARG:HG2	2:B:29:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ARG:HB2	2:B:5:PRO:HD2	2.00	0.43
5:E:67:VAL:HG21	5:E:75:PHE:CZ	2.53	0.43
5:E:205:GLN:O	5:E:207:PRO:HD3	2.18	0.43
4:D:166:LEU:HD12	4:D:166:LEU:O	2.18	0.43
4:D:191:ASN:C	4:D:191:ASN:ND2	2.76	0.43
4:D:159:TYR:O	4:D:180:ALA:HA	2.18	0.43
5:E:131:PHE:CE1	5:E:149:LEU:HD12	2.53	0.43
1:A:111:LYS:HG2	1:A:140:ARG:CZ	2.49	0.43
1:A:110:ASP:OD1	1:A:140:ARG:HD2	2.19	0.43
5:E:21:LEU:HD12	5:E:77:LEU:HD23	2.00	0.43
1:A:11:GLU:OE1	1:A:62:ASN:HB3	2.18	0.43
1:A:69:ASN:CB	3:C:316:LEU:HD22	2.49	0.43
1:A:160:VAL:CG1	1:A:177:HIS:CE1	3.01	0.43
2:B:167:SER:C	2:B:169:GLU:H	2.24	0.43
4:D:142:THR:OG1	4:D:143:ASP:N	2.52	0.43
4:D:186:ASP:O	4:D:186:ASP:CG	2.62	0.43
5:E:23:CYS:HB2	5:E:34:TRP:CZ2	2.53	0.43
5:E:133:PRO:CG	5:E:144:ALA:HB1	2.49	0.43
1:A:4:GLU:HG2	1:A:5:HIS:CD2	2.54	0.42
3:C:311:GLN:HE21	3:C:311:GLN:CA	2.27	0.42
4:D:123:PRO:HG3	4:D:144:PHE:HA	1.99	0.42
5:E:133:PRO:HD2	5:E:204:TRP:CZ2	2.54	0.42
5:E:212:ARG:NH1	5:E:214:GLN:OE1	2.52	0.42
4:D:161:THR:HG21	5:E:194:SER:OG	2.20	0.42
5:E:232:LYS:HA	5:E:233:PRO:HD3	1.80	0.42
4:D:49:TYR:CE1	4:D:51:SER:HA	2.54	0.42
5:E:89:MET:HE3	5:E:113:ARG:N	2.35	0.42
1:A:16:PRO:HG2	2:B:5:PRO:O	2.20	0.42
5:E:176:ASP:OD1	5:E:196:ARG:NH2	2.50	0.42
5:E:179:PRO:HB3	5:E:191:TYR:HB3	2.01	0.42
1:A:92:LEU:HD23	1:A:92:LEU:N	2.34	0.42
4:D:14:GLU:HG3	4:D:117:ASN:ND2	2.34	0.42
1:A:138:LEU:HA	1:A:139:PRO:HD3	1.82	0.42
4:D:24:TYR:CD1	4:D:24:TYR:C	2.98	0.42
4:D:168:MET:CE	4:D:171:MET:HE3	2.49	0.42
1:A:99:LEU:HD21	1:A:180:PHE:CD2	2.54	0.42
1:A:160:VAL:CG1	1:A:177:HIS:HE1	2.33	0.41
2:B:11:LEU:HD23	3:C:313:THR:HG22	2.02	0.41
5:E:89:MET:CE	5:E:112:THR:C	2.93	0.41
4:D:123:PRO:HB3	4:D:198:ILE:HD13	2.02	0.41
5:E:57:LYS:HB3	5:E:61:PRO:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:81:HIS:CD2	4:D:82:MET:H	2.37	0.41
5:E:133:PRO:HG2	5:E:144:ALA:HB1	2.01	0.41
1:A:62:ASN:ND2	3:C:310:LYS:HE2	2.35	0.41
1:A:11:GLU:OE1	1:A:66:ASP:OD2	2.39	0.41
1:A:17:ASP:OD1	2:B:6:ARG:NH1	2.46	0.41
1:A:86:PRO:HA	1:A:87:PRO:HD3	1.78	0.41
4:D:115:ILE:HA	4:D:116:PRO:HD3	1.75	0.41
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.54	0.40
4:D:165:VAL:HG22	4:D:176:ASN:OD1	2.22	0.40
1:A:94:ASN:HB3	7:A:519:HOH:O	2.21	0.40
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.70	0.40
4:D:128:LEU:HD13	4:D:138:VAL:HG23	2.03	0.40
5:E:212:ARG:HD3	5:E:239:SER:CB	2.49	0.40
2:B:29:ARG:HB3	2:B:31:ILE:HD11	2.03	0.40
2:B:18:PHE:O	2:B:19:ASN:HB3	2.21	0.40
4:D:77:LYS:HE2	4:D:84:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	178/181 (98%)	168 (94%)	9 (5%)	1 (1%)	21	42
2	B	175/192 (91%)	171 (98%)	4 (2%)	0	100	100
3	C	11/13 (85%)	11 (100%)	0	0	100	100
4	D	194/212 (92%)	178 (92%)	13 (7%)	3 (2%)	8	18
5	E	238/245 (97%)	229 (96%)	9 (4%)	0	100	100
All	All	796/843 (94%)	757 (95%)	35 (4%)	4 (0%)	24	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	195	ASN
1	A	15	ASN
4	D	152	GLN
4	D	118	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	165/166 (99%)	164 (99%)	1 (1%)	78	91
2	B	161/173 (93%)	155 (96%)	6 (4%)	30	57
3	C	12/12 (100%)	11 (92%)	1 (8%)	10	23
4	D	173/190 (91%)	156 (90%)	17 (10%)	7	17
5	E	214/218 (98%)	200 (94%)	14 (6%)	15	35
All	All	725/759 (96%)	686 (95%)	39 (5%)	20	42

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
2	B	22	GLU
2	B	29	ARG
2	B	48	ARG
2	B	104	SER
2	B	114	LEU
2	B	139	LYS
3	C	316	LEU
4	D	3	VAL
4	D	13	SER
4	D	25	SER
4	D	28	VAL
4	D	45	LEU
4	D	46	LEU
4	D	54	THR
4	D	71	THR

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Mol	Chain	Res	Type
4	D	76	THR
4	D	104	LEU
4	D	117	ASN
4	D	128	LEU
4	D	133	SER
4	D	162	ASP
4	D	191	ASN
4	D	198	ILE
4	D	202	THR
5	E	5	THR
5	E	33	PHE
5	E	68	SER
5	E	74	ARG
5	E	76	SER
5	E	89	MET
5	E	99	LEU
5	E	112	THR
5	E	116	VAL
5	E	178	GLN
5	E	181	LYS
5	E	196	ARG
5	E	216	GLN
5	E	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	149	HIS
1	A	177	HIS
2	B	10	GLN
2	B	19	ASN
2	B	150	ASN
2	B	156	GLN
3	C	311	GLN
4	D	1	GLN
4	D	23	ASN
4	D	37	GLN
4	D	81	HIS
4	D	117	ASN
4	D	191	ASN
5	E	157	HIS

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Mol	Chain	Res	Type
5	E	216	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](#)

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	A	501	1	14,14,15	0.61	0	17,19,21	0.83	1 (5%)
6	NAG	A	511	1	14,14,15	0.64	0	17,19,21	1.05	2 (11%)

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	A	501	1	-	4/6/23/26	0/1/1/1
6	NAG	A	511	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	511	NAG	C2-N2-C7	-2.35	119.75	122.90
6	A	501	NAG	C2-N2-C7	-2.24	119.90	122.90
6	A	511	NAG	C8-C7-N2	2.18	119.73	116.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	NAG	O5-C5-C6-O6
6	A	501	NAG	C4-C5-C6-O6
6	A	501	NAG	C8-C7-N2-C2
6	A	511	NAG	C8-C7-N2-C2
6	A	501	NAG	O7-C7-N2-C2
6	A	511	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	180/181 (99%)	-0.10	5 (2%) 55 49	20, 35, 58, 77	0
2	B	179/192 (93%)	-0.05	5 (2%) 55 49	20, 34, 60, 68	0
3	C	13/13 (100%)	-0.23	0 100 100	27, 31, 49, 54	0
4	D	198/212 (93%)	0.52	22 (11%) 10 8	20, 42, 69, 79	0
5	E	240/245 (97%)	-0.14	5 (2%) 63 58	19, 33, 53, 69	0
All	All	810/843 (96%)	0.05	37 (4%) 37 32	19, 36, 62, 79	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	203	PHE	4.8
5	E	188	ASP	4.4
4	D	135	ASP	4.0
4	D	202	THR	3.7
4	D	189	CYS	3.6
4	D	194	ASN	3.4
2	B	3	THR	3.4
5	E	246	ALA	3.4
4	D	195	ASN	3.1
4	D	133	SER	3.0
4	D	183	ASN	2.9
2	B	190	ALA	2.9
2	B	183	PRO	2.8
4	D	129	ARG	2.8
4	D	200	GLU	2.8
4	D	157	ASP	2.8
4	D	199	PRO	2.6
4	D	198	ILE	2.6
4	D	152	GLN	2.6
1	A	3	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	22	GLU	2.5
5	E	3	LYS	2.4
1	A	100	ARG	2.4
4	D	119	GLN	2.4
4	D	54	THR	2.3
1	A	16	PRO	2.3
1	A	4	GLU	2.3
1	A	15	ASN	2.2
4	D	117	ASN	2.2
4	D	134	SER	2.2
5	E	28	ASP	2.2
4	D	146	SER	2.2
4	D	145	ASP	2.1
4	D	201	ASP	2.1
4	D	186	ASP	2.0
5	E	189	SER	2.0
2	B	181	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
6	NAG	A	501	14/15	0.67	0.18	83,88,91,92	0
6	NAG	A	511	14/15	0.75	0.16	63,68,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.