



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:18 PM EDT

PDB ID : 6CIK / pdb_00006cik
Title : Pre-Reaction Complex, RAG1(E962Q)/2-intact/nicked 12/23RSS complex in Mn²⁺
Authors : Chuenchor, W.; Chen, X.; Kim, M.S.; Gellert, M.; Yang, W.
Deposited on : 2018-02-24
Resolution : 3.15 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
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

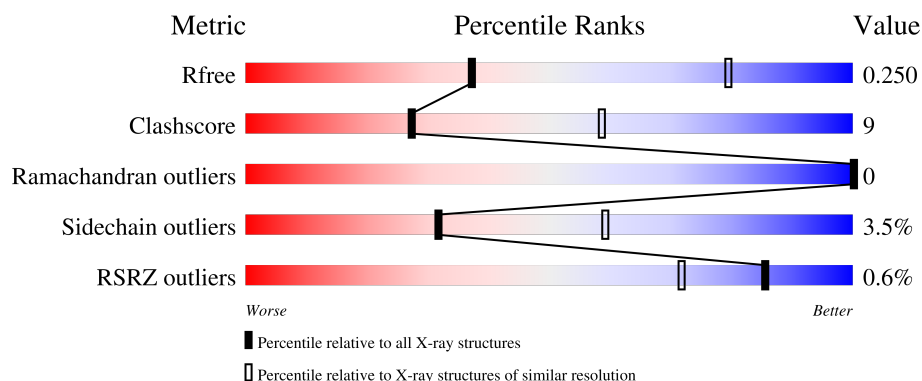
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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.



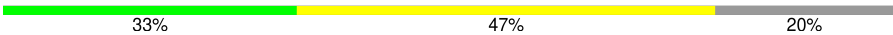
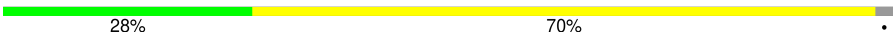
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	625	77% 19% ..
1	C	625	72% 23% ..
2	B	359	78% 16% 5%
2	D	359	82% 10% 7%
3	N	163	45% 8% 45%

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Mol	Chain	Length	Quality of chain
4	F	39	 36% 54% 10%
5	I	40	 40% 48% 12%
6	G	55	 51% 42% 7%
7	J	15	 33% 47% 20%
8	M	40	 28% 70% .

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18735 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 V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	1	0
			4716	2971	826	885	34			
1	C	602	Total	C	N	O	S	0	1	0
			4711	2970	826	881	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	962	GLN	GLU	engineered mutation	UNP P15919
C	962	GLN	GLU	engineered mutation	UNP P15919

- Molecule 2 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	341	Total	C	N	O	S	0	1	0
			2652	1695	450	490	17			
2	D	335	Total	C	N	O	S	0	1	0
			2569	1646	436	469	18			

- Molecule 3 is a protein called High mobility group protein B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	90	Total	C	N	O	S	0	0	0
			552	350	98	102	2			

- Molecule 4 is a DNA chain called Intact 12RSS substrate reverse strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	35	Total	C	N	O	P	0	0	0
			723	345	129	214	35			

- Molecule 5 is a DNA chain called Intact 12RSS substrate forward strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	35	Total	C	N	O	P	0	0	0
			709	340	131	204	34			

- Molecule 6 is a DNA chain called Nicked 23RSS intermediate reverse strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	51	Total	C	N	O	P	0	0	0
			1043	499	179	314	51			

- Molecule 7 is a DNA chain called DNA (5'-D(*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	12	Total	C	N	O	P	0	0	0
			244	117	39	76	12			

- Molecule 8 is a DNA chain called Nicked 23RSS intermediate forward strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	39	Total	C	N	O	P	0	0	0
			805	381	162	223	39			

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		
9	C	1	Total	Zn	0	0
			1	1		

- Molecule 10 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Mn	0	0
			1	1		
10	C	1	Total	Mn	0	0
			1	1		

- Molecule 11 is water.

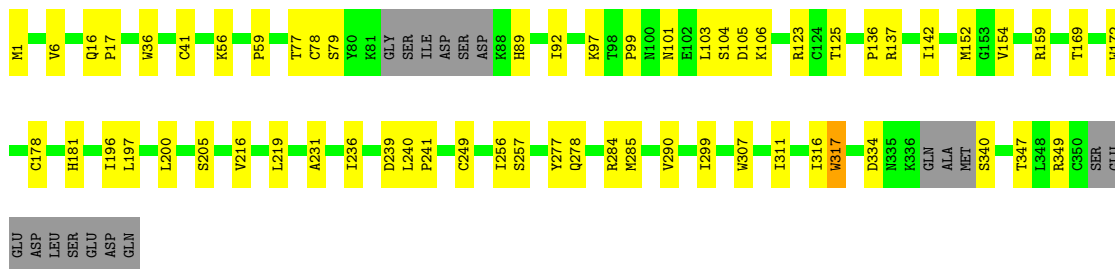
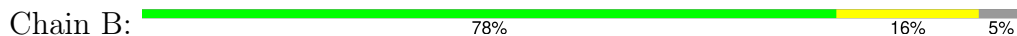
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	O	0	0
			2	2		

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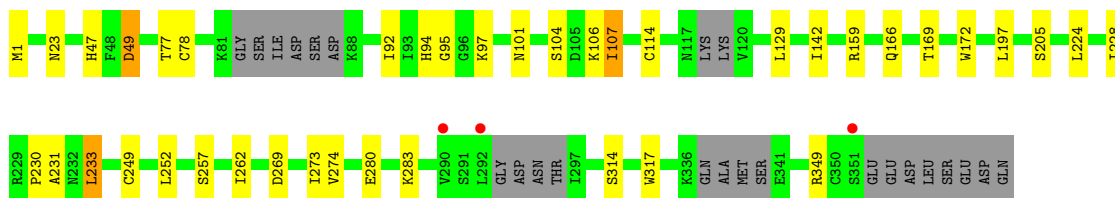
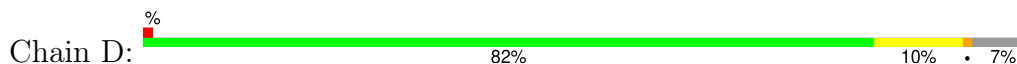
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total 1	O 1	0	0
11	C	2	Total 2	O 2	0	0
11	D	1	Total 1	O 1	0	0
11	G	1	Total 1	O 1	0	0

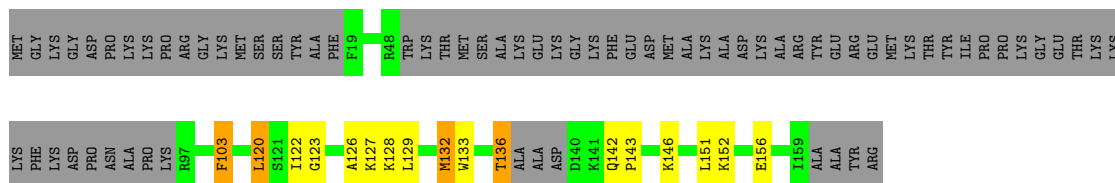
- Molecule 2: V(D)J recombination-activating protein 2



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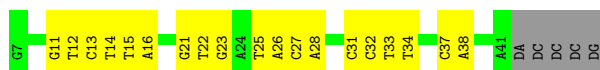
- Molecule 3: High mobility group protein B1



- Molecule 4: Intact 12RSS substrate reverse strand



- Molecule 5: Intact 12RSS substrate forward strand

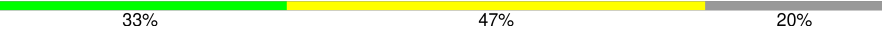


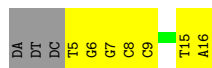
- Molecule 6: Nicked 23RSS intermediate reverse strand

Chain G: 



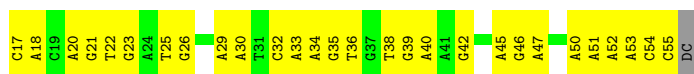
- Molecule 7: DNA (5'-D(*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3')

Chain J: 



- Molecule 8: Nicked 23RSS intermediate forward strand

Chain M: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.42Å 123.15Å 186.33Å 90.00° 105.03° 90.00°	Depositor
Resolution (Å)	37.84 – 3.15 37.84 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.84-3.15) 99.5 (37.84-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.209 , 0.249 0.208 , 0.250	Depositor DCC
R_{free} test set	3050 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	104.9	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18735	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: ZN, MN

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	0.44	0/4815	0.66	0/6511
1	C	0.44	0/4809	0.66	0/6499
2	B	0.40	0/2723	0.62	0/3697
2	D	0.36	0/2634	0.58	0/3573
3	N	0.41	0/562	0.58	0/770
4	F	0.42	0/810	0.61	0/1250
5	I	0.43	0/795	0.63	0/1223
6	G	0.41	0/1166	0.62	0/1798
7	J	0.43	0/271	0.52	0/416
8	M	0.46	0/907	0.67	0/1395
All	All	0.42	0/19492	0.64	0/27132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4716	0	4529	78	0
1	C	4711	0	4544	93	0
2	B	2652	0	2573	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2569	0	2454	23	0
3	N	552	0	380	11	0
4	F	723	0	398	26	0
5	I	709	0	395	21	0
6	G	1043	0	580	22	0
7	J	244	0	138	10	0
8	M	805	0	435	25	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	2	0	0	0	0
11	D	1	0	0	0	0
11	G	1	0	0	1	0
All	All	18735	0	16426	317	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 9.

All (317) 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:F:12:DT:H2'	4:F:13:DA:C8	2.09	0.88
8:M:50:DA:H2'	8:M:51:DA:C8	2.20	0.75
8:M:38:DT:H2'	8:M:39:DG:C8	2.22	0.74
4:F:9:DT:H3	5:I:38:DA:H2	1.37	0.72
8:M:51:DA:H1'	8:M:52:DA:H5''	1.70	0.71
4:F:13:DA:H2''	4:F:14:DA:C8	2.25	0.71
5:I:31:DC:H2''	5:I:32:DC:H5''	1.73	0.69
6:G:19:DC:H2''	6:G:20:DA:C8	2.28	0.69
1:C:848[B]:ARG:NH1	7:J:15:DT:O2	2.26	0.69
5:I:32:DC:H2'	5:I:33:DT:H72	1.76	0.68
4:F:11:DT:H2'	4:F:12:DT:C6	2.28	0.68
1:A:977:ARG:HG3	1:A:986:ASP:OD1	1.95	0.66
1:C:962:GLN:NE2	11:G:101:HOH:O	2.30	0.65
5:I:14:DT:H2''	5:I:15:DT:C6	2.31	0.65
4:F:16:DG:H2''	4:F:17:DG:C8	2.32	0.64
8:M:52:DA:H2''	8:M:53:DA:C8	2.32	0.64
1:C:996:SER:O	1:C:1000:GLN:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:11:DT:H2'	4:F:12:DT:C5	2.33	0.64
1:A:729:LEU:C	1:A:748:ARG:HG3	2.23	0.64
1:A:811:GLU:OE2	1:A:875:ARG:NE	2.31	0.63
5:I:21:DG:H2''	5:I:22:DT:H72	1.80	0.62
8:M:45:DA:H2''	8:M:46:DG:H5'	1.80	0.62
7:J:16:DA:O3'	8:M:17:DC:H5''	1.99	0.62
2:B:41:CYS:HB2	2:B:59:PRO:HB3	1.81	0.62
1:C:489:LYS:NZ	4:F:20:DG:OP1	2.33	0.62
8:M:29:DA:H2''	8:M:30:DA:H8	1.64	0.62
2:D:228:ILE:O	2:D:230:PRO:HD3	1.99	0.61
1:A:898:PRO:HG3	1:A:947:ILE:HD13	1.82	0.61
1:A:620:VAL:HB	1:A:658:MET:HG2	1.81	0.61
4:F:36:DC:H2''	4:F:37:DA:C8	2.35	0.61
2:D:95:GLY:HA2	2:D:104:SER:O	2.00	0.61
6:G:35:DC:H2'	6:G:36:DA:C8	2.37	0.60
1:C:716:GLU:O	1:C:783:PRO:HG3	2.02	0.60
1:C:857:LEU:HD12	1:C:862:THR:HG21	1.84	0.60
5:I:15:DT:H2''	5:I:16:DA:N7	2.16	0.60
1:A:624:PHE:HD2	1:A:655:LEU:HD22	1.65	0.60
1:C:469:ALA:O	1:C:473:ASN:HB2	2.01	0.60
6:G:14:DG:H2'	6:G:15:DG:C8	2.37	0.59
1:A:703:ARG:NH2	1:A:950:ASP:OD1	2.23	0.58
8:M:29:DA:H2''	8:M:30:DA:C8	2.39	0.58
4:F:26:DC:H2''	4:F:27:DT:C6	2.39	0.58
5:I:32:DC:H2'	5:I:33:DT:C7	2.33	0.57
5:I:11:DG:H2''	5:I:12:DT:C6	2.40	0.57
6:G:30:DT:H1'	6:G:31:DG:H5'	1.87	0.57
1:A:624:PHE:CD2	1:A:655:LEU:HD22	2.39	0.57
1:C:744:HIS:HB2	1:C:941:ALA:HB1	1.86	0.57
4:F:11:DT:C6	4:F:12:DT:H72	2.39	0.57
1:C:586:TYR:HA	1:C:694:ILE:HD13	1.86	0.57
2:B:1:MET:HA	2:B:349:ARG:O	2.03	0.56
1:A:687:LEU:O	1:A:697:THR:HA	2.04	0.56
1:A:745:SER:HA	1:A:945:GLU:OE2	2.05	0.56
1:C:703:ARG:NH2	1:C:950:ASP:OD1	2.36	0.56
6:G:7:DT:H2'	6:G:8:DT:C6	2.40	0.56
4:F:27:DT:H2''	4:F:28:DG:C8	2.41	0.56
3:N:103:PHE:CE1	8:M:33:DA:H1'	2.41	0.55
1:A:678:GLU:HG3	2:B:169:THR:HG21	1.87	0.55
1:A:634:GLY:HA3	1:A:636:GLN:OE1	2.06	0.55
1:A:545:VAL:HG23	2:B:316:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:283:LYS:HE2	2:D:314:SER:O	2.07	0.54
1:A:666:GLU:N	1:A:666:GLU:OE2	2.40	0.54
2:B:290:VAL:HG22	2:B:299:ILE:HG13	1.90	0.54
4:F:12:DT:H2''	4:F:13:DA:H5'	1.88	0.54
6:G:5:DT:H2''	6:G:6:DT:H5''	1.89	0.54
5:I:37:DC:H1'	5:I:38:DA:H5'	1.89	0.54
6:G:22:DA:H2''	6:G:23:DC:H5'	1.89	0.54
2:D:47[A]:HIS:NE2	2:D:49:ASP:OD2	2.39	0.53
8:M:22:DT:H2'	8:M:23:DG:C8	2.43	0.53
1:C:715:VAL:HB	1:C:785:ILE:HB	1.90	0.53
1:C:813:GLY:HA3	1:C:829:TRP:CD2	2.44	0.53
2:D:94:HIS:HD2	2:D:107:ILE:HG13	1.72	0.53
1:C:836:HIS:CB	1:C:869:LEU:HD11	2.39	0.53
1:A:475:PHE:HB3	1:A:974:MET:HE3	1.90	0.53
1:A:552:THR:HB	1:A:659:LEU:O	2.09	0.53
2:D:166:GLN:N	2:D:166:GLN:OE1	2.42	0.53
4:F:8:DT:H2''	4:F:9:DT:H5''	1.91	0.53
8:M:54:DC:H2'	8:M:55:DC:C6	2.44	0.52
5:I:22:DT:H2'	5:I:23:DG:C8	2.44	0.52
1:A:552:THR:HG21	1:A:667:THR:HG21	1.90	0.52
3:N:133:TRP:O	3:N:136:THR:HG22	2.10	0.52
1:A:719:GLU:OE2	1:A:723:SER:OG	2.26	0.51
1:C:949:ARG:HG2	1:C:950:ASP:OD1	2.11	0.51
1:A:713:ARG:NH2	1:A:725:TYR:O	2.44	0.51
1:C:754:LEU:HD23	1:C:783:PRO:HD2	1.93	0.51
1:C:825:GLU:HG2	1:C:828:ARG:HH22	1.75	0.51
1:C:593:VAL:HG13	1:C:629:ILE:HG12	1.93	0.51
2:B:123:ARG:HG2	2:B:125:THR:HG23	1.93	0.51
1:C:482:HIS:HB2	1:C:500:LEU:HD11	1.92	0.51
1:A:730:CYS:O	1:A:748:ARG:NH1	2.43	0.51
6:G:16:DC:H2'	6:G:17:DT:C6	2.46	0.51
1:A:654:PRO:HG3	1:A:991:HIS:HB3	1.92	0.51
1:C:515:HIS:ND1	1:C:568:MET:HG3	2.25	0.51
1:C:602:MET:HE1	1:C:968:PHE:CD1	2.46	0.51
1:C:711:LEU:O	1:C:715:VAL:HG22	2.11	0.51
1:C:770:GLU:CD	1:C:770:GLU:H	2.19	0.51
1:C:826:ARG:HG2	1:C:829:TRP:CZ3	2.46	0.51
2:B:278:GLN:HG3	2:B:284:ARG:HB2	1.93	0.51
1:C:892:VAL:HG21	1:C:909:TYR:HD2	1.76	0.50
1:C:501:HIS:NE2	4:F:19:DT:OP2	2.45	0.50
8:M:34:DA:H2''	8:M:35:DG:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:886:TYR:OH	1:C:890:LYS:HD3	2.12	0.50
1:A:813:GLY:HA3	1:A:829:TRP:CE2	2.46	0.50
1:A:910:SER:O	1:A:914:GLN:HG3	2.11	0.50
2:B:36:TRP:NE1	2:B:99:PRO:HB2	2.27	0.50
1:C:673:SER:OG	1:C:674:PRO:HD3	2.11	0.50
1:A:515:HIS:ND1	1:A:568:MET:HG3	2.27	0.49
2:B:137:ARG:HG2	2:B:178:CYS:SG	2.53	0.49
1:C:534:ILE:HG21	1:C:985:GLU:HG3	1.93	0.49
5:I:25:DT:H2''	5:I:26:DA:C8	2.47	0.49
1:A:849:MET:HB2	4:F:34:DG:OP1	2.13	0.49
1:C:566:ALA:O	1:C:570:MET:HG2	2.11	0.49
1:C:850:ASN:HD21	1:C:852:ASN:HB2	1.78	0.49
8:M:17:DC:H2'	8:M:18:DA:C8	2.48	0.49
6:G:16:DC:H3'	6:G:17:DT:H72	1.95	0.49
1:C:605:VAL:HG11	1:C:968:PHE:CE2	2.48	0.49
1:C:624:PHE:HD1	1:C:655:LEU:HD22	1.77	0.49
1:A:575:LEU:HA	1:A:578:MET:HE2	1.94	0.49
1:C:997:LYS:O	1:C:1001:LYS:HG2	2.12	0.49
1:A:805:TYR:OH	1:A:830:GLN:NE2	2.46	0.49
2:D:78:CYS:HB3	2:D:142:ILE:O	2.13	0.49
1:A:547:GLU:OE1	2:B:159:ARG:NH1	2.42	0.49
1:A:898:PRO:HD2	1:A:951:GLY:O	2.13	0.49
2:D:1:MET:HA	2:D:349:ARG:O	2.12	0.49
6:G:42:DT:H2''	6:G:43:DA:C8	2.48	0.49
1:A:674:PRO:HG3	2:B:172:TRP:HB3	1.94	0.48
1:C:979:SER:HA	4:F:27:DT:H5'	1.95	0.48
5:I:27:DC:H2''	5:I:28:DA:C8	2.48	0.48
5:I:32:DC:H2''	5:I:33:DT:H5'	1.95	0.48
6:G:14:DG:H2''	6:G:15:DG:O5'	2.13	0.48
6:G:41:DG:H1'	6:G:42:DT:H5'	1.94	0.48
2:B:56:LYS:HD3	4:F:40:DC:OP2	2.14	0.48
1:C:850:ASN:ND2	1:C:852:ASN:H	2.11	0.48
6:G:22:DA:C2'	6:G:23:DC:H5'	2.44	0.48
7:J:7:DG:H1'	7:J:8:DC:H5'	1.96	0.48
1:A:741:LEU:HD12	1:A:741:LEU:HA	1.76	0.48
2:B:239:ASP:C	2:B:241:PRO:HD3	2.39	0.48
1:C:910:SER:O	1:C:914:GLN:HG3	2.14	0.48
8:M:20:DA:H2''	8:M:21:DG:O5'	2.13	0.48
1:A:570:MET:HE1	1:A:641:PHE:CD2	2.49	0.48
1:A:746:ILE:HG13	1:A:945:GLU:OE1	2.14	0.48
1:C:740:ASN:O	1:C:744:HIS:HE1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:CYS:HB3	2:B:142:ILE:O	2.14	0.48
7:J:5:DT:H2'	7:J:6:DG:C8	2.49	0.48
2:B:77:THR:HA	2:B:92:ILE:O	2.14	0.47
2:B:181:HIS:CD2	2:B:196:ILE:HG13	2.49	0.47
1:A:969:ARG:HH12	4:F:30:DG:P	2.37	0.47
7:J:8:DC:H2''	7:J:9:DC:C5	2.50	0.47
1:C:536:ASP:OD2	1:C:538:LEU:HB2	2.14	0.47
2:B:200:LEU:HD11	2:B:236:ILE:HD11	1.97	0.47
3:N:129:LEU:HA	3:N:132:MET:HE3	1.95	0.47
2:B:231:ALA:HB2	2:B:257:SER:HB2	1.97	0.47
1:C:679:ARG:HA	1:C:682:MET:CE	2.45	0.47
1:C:804:PHE:CB	1:C:858:MET:HE1	2.45	0.47
1:A:711:LEU:HD12	1:A:711:LEU:HA	1.77	0.46
1:C:967:LEU:HD11	1:C:994:TYR:CE2	2.50	0.46
2:B:219:LEU:HD22	2:B:256:ILE:HG12	1.97	0.46
1:C:730:CYS:O	1:C:748:ARG:HD2	2.14	0.46
8:M:17:DC:H5'	8:M:17:DC:H6	1.80	0.46
2:B:6:VAL:HG21	2:B:347:THR:HG23	1.98	0.46
2:D:197:LEU:HD13	2:D:249:CYS:HB2	1.97	0.46
4:F:12:DT:H2'	4:F:13:DA:H8	1.74	0.46
1:A:622:PHE:CD1	1:A:675:LEU:HD13	2.51	0.46
1:A:750:HIS:CE1	1:A:783:PRO:HB2	2.50	0.46
2:B:142:ILE:HA	2:B:154:VAL:O	2.15	0.46
1:C:767:GLU:HB3	1:C:771:GLU:HB2	1.98	0.46
2:B:334:ASP:O	2:B:340:SER:N	2.48	0.46
1:C:570:MET:HE2	1:C:570:MET:HB3	1.78	0.46
1:C:545:VAL:HG13	2:D:280:GLU:OE2	2.16	0.46
1:C:674:PRO:HG3	2:D:172:TRP:HB3	1.97	0.46
1:C:678:GLU:HG3	2:D:169:THR:HG21	1.98	0.46
5:I:33:DT:C2'	5:I:34:DT:H71	2.46	0.46
1:A:492:THR:C	1:A:494:ARG:H	2.24	0.45
1:A:729:LEU:O	1:A:748:ARG:HG3	2.16	0.45
1:A:849:MET:SD	1:A:850:ASN:N	2.86	0.45
1:C:889:MET:HE3	1:C:913:SER:HB2	1.98	0.45
2:D:94:HIS:CD2	2:D:107:ILE:HG13	2.52	0.45
4:F:35:DA:H1'	4:F:36:DC:H5'	1.97	0.45
1:A:653:LYS:HB3	1:A:992:TRP:CZ3	2.52	0.45
8:M:25:DT:H2''	8:M:26:DG:C8	2.52	0.45
2:B:154:VAL:HG11	2:B:216:VAL:HG21	1.99	0.45
1:C:719:GLU:HG3	1:C:778:GLY:O	2.15	0.45
8:M:39:DG:H2''	8:M:40:DA:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:SER:O	1:A:747:THR:HG23	2.16	0.45
2:B:152:MET:HB2	2:B:240:LEU:HD11	1.99	0.45
1:C:847:MET:HB2	1:C:847:MET:HE3	1.62	0.45
3:N:123:GLY:O	3:N:127:LYS:HB2	2.17	0.45
4:F:12:DT:C2'	4:F:13:DA:H5'	2.46	0.45
1:A:792:ASP:HB3	1:A:957:ALA:HA	1.97	0.45
1:C:453:ALA:O	1:C:457:GLY:N	2.50	0.45
2:D:233:LEU:HG	2:D:252:LEU:HB2	1.99	0.45
1:C:668:LEU:HD12	1:C:668:LEU:HA	1.78	0.44
1:A:587:LEU:HD12	1:A:588:ASN:H	1.81	0.44
1:C:892:VAL:HG12	1:C:947:ILE:CD1	2.46	0.44
3:N:127:LYS:HG3	6:G:24:DT:H5''	1.99	0.44
1:C:725:TYR:OH	1:C:774:ASP:HA	2.18	0.44
4:F:13:DA:H8	4:F:13:DA:OP2	2.00	0.44
4:F:25:DA:C5	4:F:26:DC:C4	3.06	0.44
5:I:11:DG:H2'	5:I:12:DT:H72	2.00	0.44
7:J:6:DG:C2'	7:J:7:DG:C8	3.00	0.44
7:J:6:DG:H2'	7:J:7:DG:N7	2.32	0.44
1:C:443:ASN:ND2	6:G:17:DT:O4'	2.48	0.44
3:N:128:LYS:O	3:N:129:LEU:C	2.59	0.44
1:A:512:PRO:HG2	1:A:557:PHE:CE1	2.53	0.44
1:C:853:PHE:CE2	1:C:857:LEU:HD22	2.53	0.44
2:D:283:LYS:HG2	2:D:317:TRP:CZ2	2.53	0.44
5:I:15:DT:H2''	5:I:16:DA:C8	2.52	0.44
1:C:631:ILE:HG22	1:C:638:VAL:HG13	2.00	0.44
5:I:12:DT:H2''	5:I:13:DC:C6	2.53	0.44
1:A:605:VAL:HG12	1:A:605:VAL:O	2.18	0.44
1:C:701:ILE:HG21	1:C:701:ILE:HD13	1.74	0.44
5:I:33:DT:H2''	5:I:34:DT:H71	2.00	0.44
6:G:22:DA:H2''	6:G:23:DC:OP1	2.18	0.44
1:A:879:LEU:HD23	1:A:879:LEU:HA	1.76	0.44
1:A:659:LEU:HG	1:A:984:MET:HE2	1.99	0.44
2:B:105:ASP:HB3	2:B:136:PRO:HG3	1.99	0.44
3:N:142:GLN:N	3:N:143:PRO:HD2	2.33	0.44
1:C:605:VAL:HG12	1:C:972:ARG:NH2	2.32	0.43
1:C:886:TYR:CZ	1:C:890:LYS:HD3	2.53	0.43
5:I:12:DT:H2''	5:I:13:DC:H6	1.81	0.43
2:B:317:TRP:N	2:B:317:TRP:CD1	2.86	0.43
1:A:467:CYS:HB2	1:A:503:LEU:HD11	2.01	0.43
1:A:591:PHE:HB2	1:A:698:PHE:CD1	2.53	0.43
1:A:718:LEU:HD12	1:A:718:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:HIS:CD2	8:M:42:DG:H4'	2.53	0.43
1:C:730:CYS:O	1:C:748:ARG:NH1	2.39	0.43
2:D:224:LEU:HD12	2:D:224:LEU:HA	1.76	0.43
1:A:969:ARG:NH1	4:F:30:DG:OP1	2.44	0.43
2:D:159:ARG:HE	2:D:159:ARG:HB3	1.67	0.43
3:N:120:LEU:HD12	3:N:120:LEU:HA	1.63	0.43
3:N:152:LYS:O	3:N:156:GLU:HG2	2.19	0.43
1:A:735:LEU:O	1:A:738:SER:OG	2.37	0.43
1:A:794:LEU:O	1:A:798:ILE:HG13	2.19	0.43
1:A:846:ILE:HD12	1:A:848:ARG:O	2.19	0.43
1:C:713:ARG:NH1	1:C:725:TYR:O	2.52	0.43
1:C:873:GLU:HA	1:C:876:HIS:CG	2.53	0.43
5:I:11:DG:H2''	5:I:12:DT:H6	1.84	0.43
2:B:285:MET:HE3	2:B:307:TRP:CD1	2.54	0.43
1:C:492:THR:O	1:C:494:ARG:HG3	2.18	0.43
3:N:122:ILE:HD13	8:M:36:DT:O2	2.18	0.43
3:N:126:ALA:HB2	8:M:35:DG:H21	1.84	0.43
1:A:536:ASP:OD1	1:A:538:LEU:HB2	2.18	0.43
1:A:688:THR:HA	1:A:696:ARG:O	2.18	0.43
2:B:97:LYS:HG2	2:B:103:LEU:HD21	2.01	0.43
1:A:512:PRO:HG2	1:A:557:PHE:CD1	2.54	0.43
1:A:584:ASP:CG	1:A:586:TYR:CZ	2.97	0.43
8:M:32:DC:H6	8:M:32:DC:H2'	1.69	0.43
1:A:832:THR:HG22	1:A:869:LEU:HD13	2.01	0.42
1:C:761:ARG:HH21	2:D:106:LYS:HD3	1.84	0.42
6:G:7:DT:H2''	6:G:8:DT:O5'	2.18	0.42
1:A:823:LYS:HE3	1:A:827:LYS:HD2	2.01	0.42
1:C:729:LEU:HD11	1:C:789:PRO:O	2.19	0.42
1:C:745:SER:HA	1:C:945:GLU:OE2	2.18	0.42
5:I:13:DC:H2'	5:I:14:DT:H71	2.00	0.42
1:A:761:ARG:HH21	2:B:106:LYS:HD2	1.84	0.42
1:C:519:TRP:CE2	1:C:687:LEU:HD13	2.54	0.42
1:C:662:GLU:HG3	1:C:710:LYS:HZ1	1.85	0.42
1:C:672:LEU:HA	1:C:672:LEU:HD23	1.61	0.42
2:B:79:SER:HG	2:B:89:HIS:HE2	1.64	0.42
1:C:898:PRO:HG3	1:C:947:ILE:HD13	2.02	0.42
1:C:993:LEU:HA	1:C:993:LEU:HD23	1.85	0.42
1:A:570:MET:HB3	1:A:570:MET:HE2	1.75	0.42
4:F:13:DA:OP2	4:F:13:DA:H2'	2.20	0.42
6:G:7:DT:H3'	6:G:8:DT:H71	2.01	0.42
8:M:50:DA:H2''	8:M:51:DA:C5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:25:DT:H6	6:G:25:DT:H2'	1.70	0.42
1:C:563:LEU:HD23	1:C:563:LEU:HA	1.83	0.42
1:C:795:HIS:CD2	1:C:935:TYR:CZ	3.08	0.42
1:A:466:VAL:HG22	1:A:1002:PHE:CD1	2.55	0.42
1:A:760:TRP:HA	1:A:772:LEU:HD11	2.01	0.42
1:C:598:SER:HA	1:C:706:GLY:O	2.20	0.41
1:A:605:VAL:HG11	1:A:968:PHE:CE2	2.55	0.41
2:B:36:TRP:CE2	2:B:99:PRO:HB2	2.55	0.41
1:C:520:GLN:HA	1:C:521:PRO:HA	1.85	0.41
6:G:36:DA:H1'	6:G:37:DC:H5'	2.02	0.41
1:C:883:MET:O	1:C:887:LEU:HG	2.20	0.41
4:F:28:DG:H1'	4:F:29:DT:H5'	2.01	0.41
1:C:729:LEU:HD12	1:C:789:PRO:HG2	2.02	0.41
1:C:826:ARG:HA	1:C:829:TRP:CE3	2.56	0.41
1:A:887:LEU:HD23	1:A:887:LEU:HA	1.92	0.41
6:G:23:DC:H6	6:G:23:DC:H2'	1.74	0.41
6:G:37:DC:H2''	6:G:38:DT:C6	2.55	0.41
1:A:598:SER:HA	1:A:706:GLY:HA3	2.02	0.41
1:A:620:VAL:HB	1:A:658:MET:CG	2.50	0.41
1:A:752:GLU:O	1:A:756:ARG:HG3	2.21	0.41
2:B:16:GLN:HG3	2:B:17:PRO:O	2.21	0.41
2:D:77:THR:HA	2:D:92:ILE:O	2.19	0.41
7:J:16:DA:H2''	8:M:17:DC:C6	2.56	0.41
1:A:534:ILE:HD13	1:A:985:GLU:HB2	2.03	0.41
1:A:560:ASP:O	1:A:564:VAL:HG23	2.21	0.41
2:B:97:LYS:HG2	2:B:103:LEU:CD2	2.50	0.41
1:C:532:VAL:HG11	1:C:558:ARG:NH1	2.36	0.41
1:C:621:ARG:HG3	1:C:657:LEU:HD21	2.03	0.41
2:D:23:ASN:HD22	2:D:23:ASN:HA	1.71	0.41
1:A:545:VAL:HG22	2:B:277:TYR:CZ	2.55	0.41
1:A:630:THR:HG22	1:A:639:LYS:HA	2.03	0.41
1:C:559:TYR:HA	1:C:655:LEU:HD11	2.03	0.41
1:C:603:GLY:O	1:C:618:LYS:HA	2.20	0.41
1:C:986:ASP:O	1:C:990:HIS:HB2	2.21	0.41
2:D:262:ILE:HB	2:D:274:VAL:HG22	2.02	0.41
8:M:46:DG:H1'	8:M:47:DA:C8	2.56	0.41
8:M:53:DA:H2''	8:M:54:DC:C6	2.55	0.41
1:C:624:PHE:O	1:C:653:LYS:N	2.49	0.40
1:C:659:LEU:HA	1:C:659:LEU:HD23	1.84	0.40
1:C:848[B]:ARG:HG3	7:J:16:DA:H4'	2.02	0.40
2:B:307:TRP:CE3	2:B:311:ILE:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ARG:O	1:C:472:VAL:C	2.63	0.40
1:C:511:LEU:HD23	1:C:511:LEU:HA	1.92	0.40
2:D:231:ALA:HB2	2:D:257:SER:HB2	2.03	0.40
1:A:556:ARG:HD2	1:A:675:LEU:HD21	2.04	0.40
1:C:644:PRO:O	1:C:646:PRO:HD3	2.21	0.40
2:D:107:ILE:HD12	2:D:129:LEU:HD11	2.03	0.40
7:J:9:DC:H6	7:J:9:DC:H2'	1.72	0.40
2:B:197:LEU:HD13	2:B:249:CYS:HB2	2.04	0.40
1:C:791:ILE:HD12	1:C:791:ILE:HA	1.93	0.40
1:C:816:TYR:CD1	1:C:817:LYS:HG3	2.56	0.40
1:A:554:ALA:HB2	1:A:658:MET:HB2	2.04	0.40
1:A:575:LEU:HA	1:A:578:MET:CE	2.52	0.40
1:A:655:LEU:O	1:A:655:LEU:HD12	2.22	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	604/625 (97%)	588 (97%)	16 (3%)	0	100	100
1	C	597/625 (96%)	572 (96%)	25 (4%)	0	100	100
2	B	336/359 (94%)	326 (97%)	10 (3%)	0	100	100
2	D	326/359 (91%)	315 (97%)	11 (3%)	0	100	100
3	N	84/163 (52%)	77 (92%)	7 (8%)	0	100	100
All	All	1947/2131 (91%)	1878 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	493/549 (90%)	476 (97%)	17 (3%)	32	60
1	C	495/549 (90%)	476 (96%)	19 (4%)	29	58
2	B	292/316 (92%)	288 (99%)	4 (1%)	59	73
2	D	274/316 (87%)	265 (97%)	9 (3%)	33	60
3	N	29/139 (21%)	23 (79%)	6 (21%)	1	6
All	All	1583/1869 (85%)	1528 (96%)	55 (4%)	32	59

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	437	LEU
1	A	473	ASN
1	A	486	ARG
1	A	552	THR
1	A	584	ASP
1	A	618	LYS
1	A	655	LEU
1	A	825	GLU
1	A	849	MET
1	A	850	ASN
1	A	895	SER
1	A	931	LYS
1	A	934	ASN
1	A	947	ILE
1	A	948	GLU
1	A	979	SER
1	A	984	MET
2	B	101	ASN
2	B	104	SER
2	B	205	SER
2	B	317	TRP
1	C	454	ILE
1	C	473	ASN

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Mol	Chain	Res	Type
1	C	561	SER
1	C	633	HIS
1	C	636	GLN
1	C	655	LEU
1	C	680	GLU
1	C	741	LEU
1	C	745	SER
1	C	755	GLN
1	C	809	GLN
1	C	835	LYS
1	C	847	MET
1	C	859	THR
1	C	904	GLU
1	C	934	ASN
1	C	969	ARG
1	C	990	HIS
1	C	996	SER
2	D	49	ASP
2	D	97	LYS
2	D	101	ASN
2	D	107	ILE
2	D	114	CYS
2	D	205	SER
2	D	233	LEU
2	D	269	ASP
2	D	273	ILE
3	N	103	PHE
3	N	120	LEU
3	N	132	MET
3	N	136	THR
3	N	146	LYS
3	N	151	LEU

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	447	GLN
1	A	766	HIS
1	A	830	GLN
1	A	965	ASN
2	B	278	GLN
2	B	295	ASN

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Mol	Chain	Res	Type
1	C	482	HIS
1	C	636	GLN
1	C	744	HIS
1	C	795	HIS
1	C	809	GLN
1	C	830	GLN
1	C	850	ASN
1	C	1006	HIS
2	D	23	ASN
2	D	101	ASN

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	607/625 (97%)	-0.38	6 (0%) 79 62	51, 99, 165, 187	1 (0%)
1	C	602/625 (96%)	-0.41	3 (0%) 87 75	66, 100, 171, 196	1 (0%)
2	B	341/359 (94%)	-0.44	0 100 100	65, 109, 147, 173	1 (0%)
2	D	335/359 (93%)	-0.22	3 (0%) 81 64	76, 126, 161, 183	1 (0%)
3	N	90/163 (55%)	0.19	0 100 100	129, 177, 229, 246	0
4	F	35/39 (89%)	-0.19	0 100 100	109, 149, 222, 227	0
5	I	35/40 (87%)	-0.32	0 100 100	100, 159, 216, 223	0
6	G	51/55 (92%)	-0.36	0 100 100	87, 146, 212, 220	0
7	J	12/15 (80%)	-0.11	0 100 100	141, 168, 212, 214	0
8	M	39/40 (97%)	-0.42	0 100 100	81, 134, 211, 215	0
All	All	2147/2320 (92%)	-0.34	12 (0%) 85 72	51, 113, 182, 246	4 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	404	GLN	3.4
1	A	978	GLN	3.2
1	A	607	GLU	2.8
1	C	848[A]	ARG	2.6
1	A	443	ASN	2.6
1	A	608	LYS	2.6
1	C	460	SER	2.3
2	D	292	LEU	2.3
2	D	290	VAL	2.3
1	A	698	PHE	2.2
1	A	721	SER	2.1
2	D	351	SER	2.1

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

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

6.3 Carbohydrates [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
10	MN	C	1102	1/1	0.96	0.12	90,90,90,90	0
10	MN	A	1102	1/1	0.98	0.12	90,90,90,90	0
9	ZN	C	1101	1/1	0.99	0.03	90,90,90,90	0
9	ZN	A	1101	1/1	1.00	0.07	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.