



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:50 PM UTC

PDB ID : 9J4S / pdb_00009j4s
Title : Structural basis for recognition of SARS-CoV-2 conserved nucleocapside epitopes by dominant T cell receptors
Authors : Yuan, P.; Wu, D.C.
Deposited on : 2024-08-10
Resolution : 2.95 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:

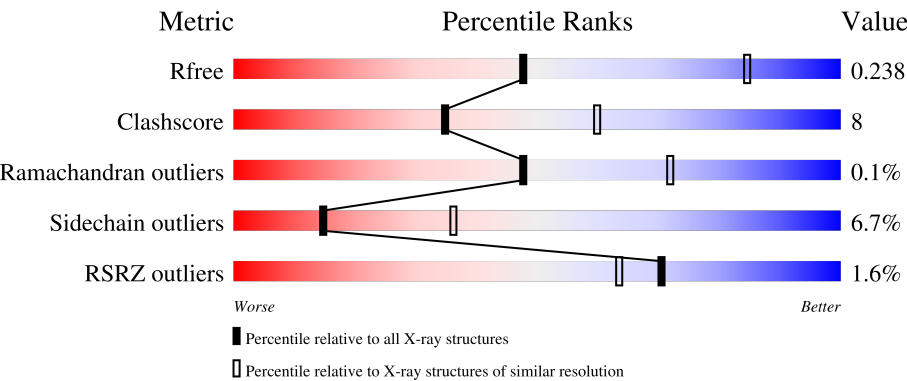
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	245	% 78%18%...
1	G	245	2% 79%18%..
2	B	208	% 76%15%.. 5%
2	I	208	% 75%20%..
3	C	276	% 73%18%7%..

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Mol	Chain	Length	Quality of chain
3	F	276	
4	D	100	
4	H	100	
5	E	9	
5	J	9	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	I	301	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13301 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 T cell receptor CLA1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	242	Total	C	N	O	S	0	0	0
			1912	1208	331	368	5			
1	A	241	Total	C	N	O	S	0	0	0
			1898	1197	331	365	5			

- Molecule 2 is a protein called T cell receptor CLA1 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	201	Total	C	N	O	S	2	0	0
			1562	989	253	312	8			
2	B	197	Total	C	N	O	S	0	0	0
			1551	984	253	306	8			

- Molecule 3 is a protein called HLA class I histocompatibility antigen, B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	274	Total	C	N	O	S	0	0	0
			2252	1397	412	437	6			
3	F	273	Total	C	N	O	S	0	0	0
			2225	1383	402	434	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P01889
F	0	MET	-	initiating methionine	UNP P01889

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	100	Total	C	N	O	S	0	0	0
			833	530	140	159	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	99	Total	C	N	O	S	0	0	0
			825	525	139	158	3			

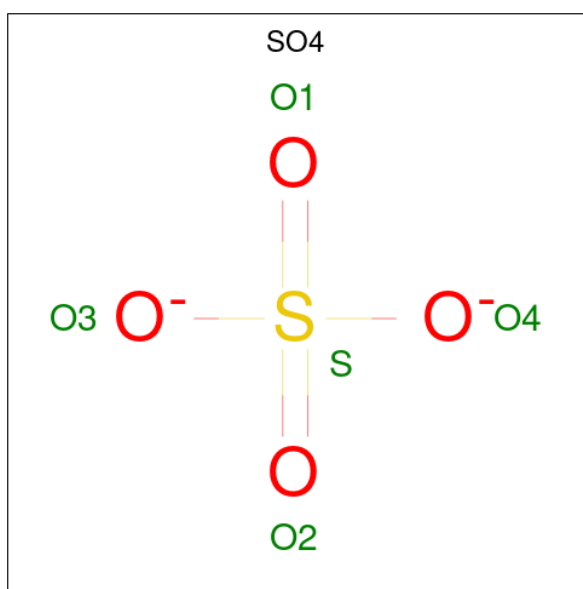
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP P61769
H	1	MET	-	initiating methionine	UNP P61769

- Molecule 5 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	9	Total	C	N	O	0	0	0
			94	67	13	14			
5	J	9	Total	C	N	O	0	0	0
			94	67	13	14			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



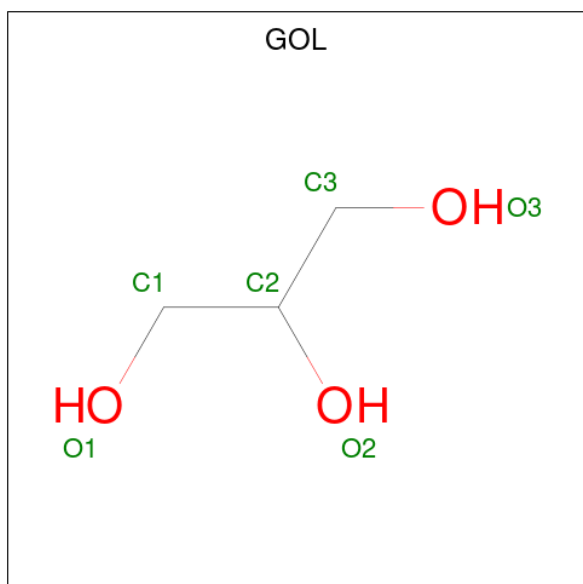
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	1	Total	O	0	0
			1	1		
8	A	2	Total	O	0	0
			2	2		

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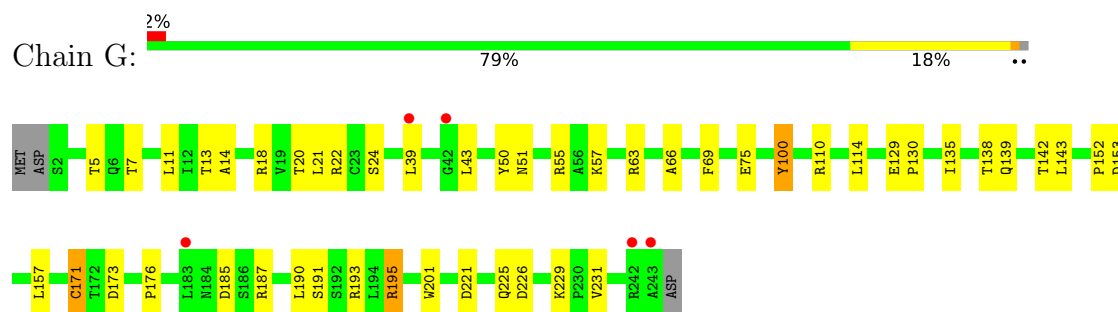
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	O	0	0
			1	1		

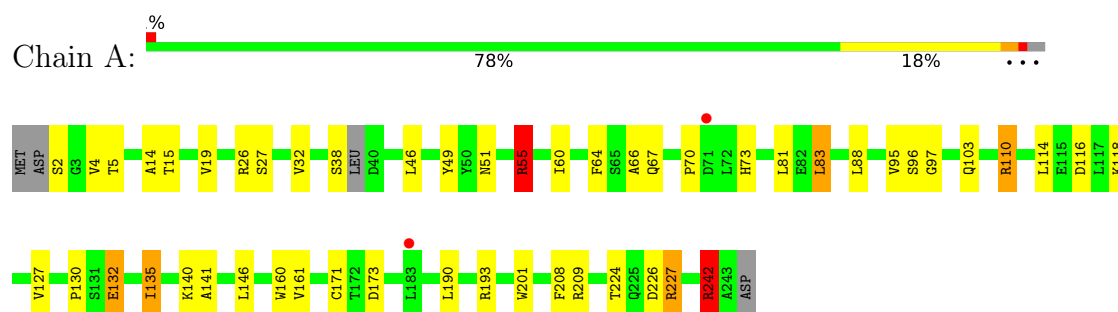
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

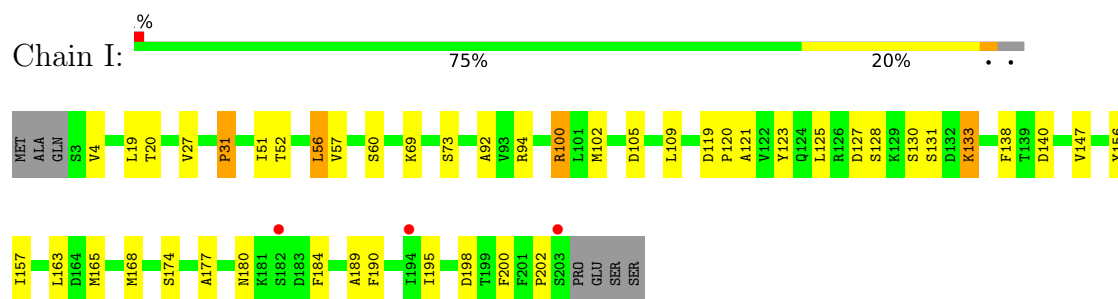
- Molecule 1: T cell receptor CLA1 beta



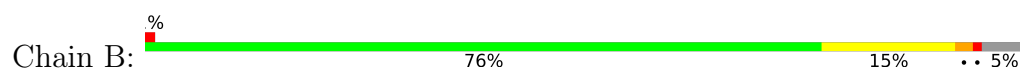
- Molecule 1: T cell receptor CLA1 beta

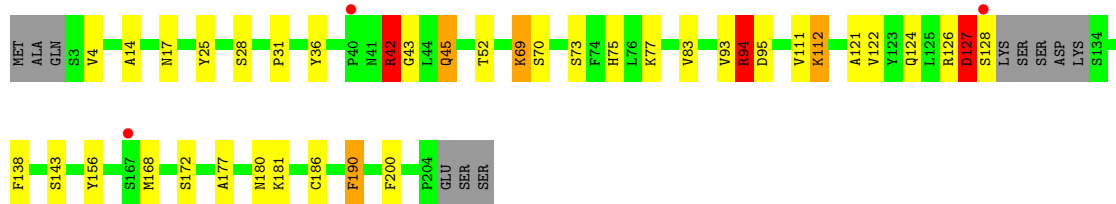


- Molecule 2: T cell receptor CLA1 alpha

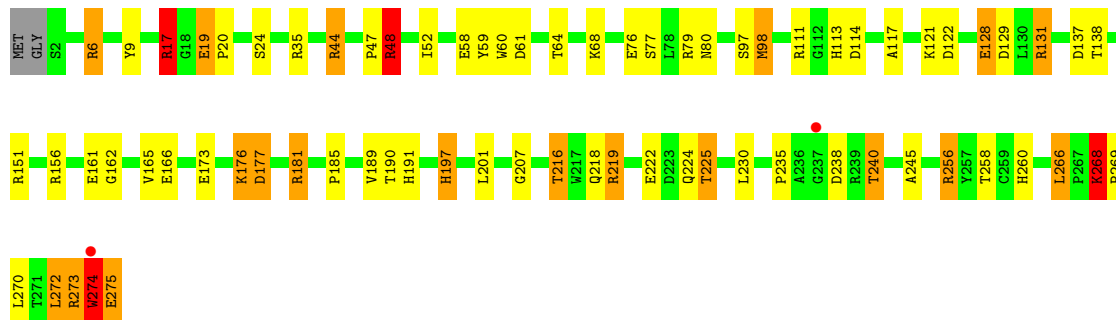
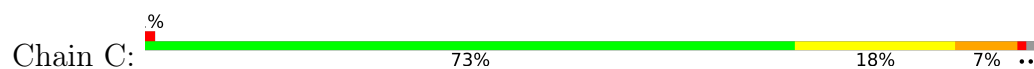


- Molecule 2: T cell receptor CLA1 alpha

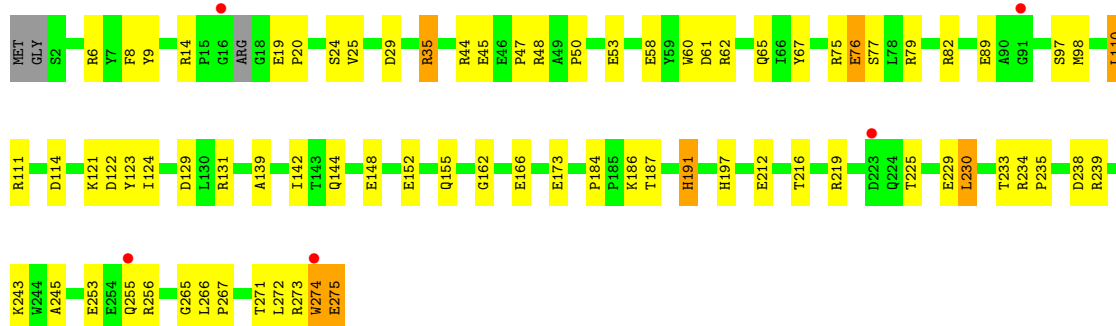




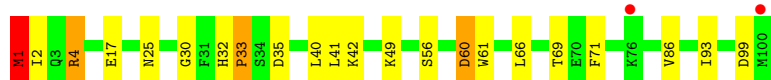
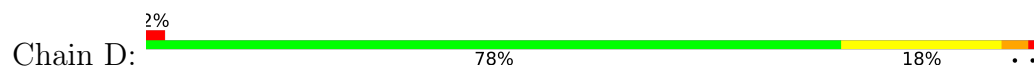
- Molecule 3: HLA class I histocompatibility antigen, B alpha chain



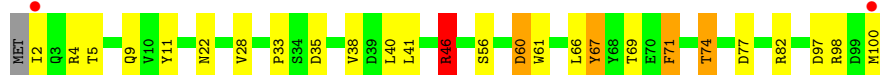
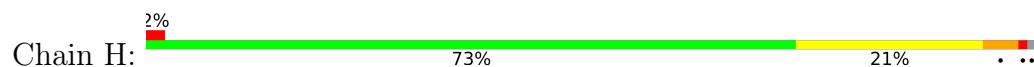
- Molecule 3: HLA class I histocompatibility antigen, B alpha chain



- Molecule 4: Beta-2-microglobulin



- Molecule 4: Beta-2-microglobulin



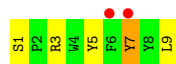
● Molecule 5: Nucleoprotein

Chain E:  89% 11%



● Molecule 5: Nucleoprotein

Chain J:  22% 44% 44% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.98Å 93.30Å 261.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.10 – 2.95 76.10 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.10-2.95) 100.0 (76.10-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.194 , 0.238 0.194 , 0.238	Depositor DCC
R_{free} test set	2450 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13301	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: GOL, SO4

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	0.68	0/1948	1.28	10/2654 (0.4%)
1	G	0.68	1/1963 (0.1%)	1.28	5/2674 (0.2%)
2	B	0.63	0/1589	1.27	4/2160 (0.2%)
2	I	0.67	1/1600 (0.1%)	1.28	8/2177 (0.4%)
3	C	0.66	0/2314	1.35	19/3142 (0.6%)
3	F	0.63	0/2286	1.34	11/3106 (0.4%)
4	D	0.63	0/856	1.27	3/1158 (0.3%)
4	H	0.60	0/848	1.26	7/1148 (0.6%)
5	E	0.68	0/100	1.15	0/135
5	J	0.56	0/100	1.39	0/135
All	All	0.65	2/13604 (0.0%)	1.30	67/18489 (0.4%)

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
1	G	0	1
2	B	0	2
2	I	0	1
3	C	0	7
3	F	0	1
4	H	0	3
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	69	LYS	CD-CE	-5.77	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	24	SER	CA-CB	-5.08	1.47	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	275	GLU	CB-CA-C	9.21	127.60	110.10
1	G	7	THR	CA-CB-OG1	-8.98	96.13	109.60
3	C	201	LEU	N-CA-CB	-7.99	98.18	110.65
2	I	31	PRO	N-CA-CB	-7.83	95.03	103.25
3	C	128	GLU	N-CA-CB	7.21	122.53	110.41
3	C	17	ARG	CG-CD-NE	-7.09	96.40	112.00
3	F	225	THR	CA-CB-OG1	-7.06	99.01	109.60
2	I	105	ASP	CA-CB-CG	6.87	119.47	112.60
4	H	100	MET	CG-SD-CE	6.63	115.49	100.90
3	C	19	GLU	CB-CG-CD	6.60	123.83	112.60
3	C	216	THR	CA-CB-OG1	-6.44	99.94	109.60
3	F	45	GLU	CB-CG-CD	6.37	123.43	112.60
1	A	242	ARG	CD-NE-CZ	-6.27	115.62	124.40
3	F	62	ARG	CD-NE-CZ	6.19	133.06	124.40
3	C	176	LYS	CB-CA-C	-6.18	109.46	116.63
1	G	5	THR	CA-CB-OG1	-6.16	100.36	109.60
3	C	197	HIS	CB-CA-C	6.12	119.35	109.07
4	H	9	GLN	CB-CA-C	-6.08	101.74	110.62
3	C	48	ARG	CB-CA-C	-6.07	100.03	109.80
4	D	33	PRO	N-CD-CG	-6.07	96.52	103.80
2	I	168	MET	CG-SD-CE	6.07	114.25	100.90
2	I	105	ASP	CB-CA-C	-6.06	97.88	109.95
3	F	155	GLN	CB-CA-C	-5.97	100.70	110.85
1	G	157	LEU	N-CA-CB	-5.97	100.44	110.83
1	A	70	PRO	CA-C-N	5.97	130.15	120.60
1	A	70	PRO	C-N-CA	5.97	130.15	120.60
3	C	225	THR	CA-CB-OG1	-5.89	100.77	109.60
1	A	4	VAL	N-CA-CB	5.86	117.68	111.00
3	C	138	THR	CA-CB-OG1	-5.71	101.03	109.60
1	A	5	THR	CA-CB-OG1	-5.71	101.03	109.60
4	H	74	THR	CA-CB-OG1	-5.68	101.08	109.60
3	C	190	THR	CA-CB-OG1	-5.67	101.10	109.60
2	B	190	PHE	CA-CB-CG	-5.66	108.14	113.80
4	H	35	ASP	CB-CA-C	5.63	119.52	110.29
4	D	1	MET	CG-SD-CE	5.58	113.17	100.90
3	F	14	ARG	CB-CA-C	5.56	117.19	108.63
2	B	127	ASP	CB-CA-C	-5.55	99.37	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	129	ASP	CA-CB-CG	5.55	118.15	112.60
2	I	20	THR	CA-CB-OG1	-5.53	101.31	109.60
3	C	52	ILE	N-CA-C	-5.52	107.36	112.83
4	H	28	VAL	N-CA-CB	-5.51	103.80	111.41
4	D	35	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	224	THR	CA-CB-OG1	-5.48	101.38	109.60
1	G	152	PRO	N-CD-CG	-5.46	97.24	103.80
3	C	19	GLU	CB-CA-C	5.41	118.34	109.46
4	H	5	THR	CA-CB-OG1	-5.40	101.50	109.60
3	C	17	ARG	NE-CZ-NH1	-5.40	116.10	121.50
2	I	140	ASP	CA-CB-CG	5.39	117.99	112.60
3	F	76	GLU	CB-CG-CD	5.33	121.66	112.60
3	C	165	VAL	N-CA-CB	-5.32	103.31	110.54
3	C	35	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	51	ASN	CB-CA-C	-5.27	103.78	112.06
2	B	42	ARG	CG-CD-NE	5.23	123.51	112.00
3	F	29	ASP	CB-CA-C	5.23	120.83	110.42
2	I	133	LYS	CB-CA-C	5.22	119.42	110.81
1	A	46	LEU	CA-C-N	-5.18	116.30	122.11
1	A	46	LEU	C-N-CA	-5.18	116.30	122.11
1	A	103	GLN	CB-CA-C	5.18	118.29	109.84
4	H	67	TYR	CB-CA-C	-5.17	102.42	110.74
3	C	273	ARG	CD-NE-CZ	5.16	131.63	124.40
2	B	94	ARG	CD-NE-CZ	5.13	131.58	124.40
2	I	180	ASN	CB-CA-C	-5.11	102.86	110.88
3	F	216	THR	CA-CB-OG1	-5.08	101.98	109.60
3	C	268	LYS	CG-CD-CE	5.06	122.93	111.30
3	F	67	TYR	N-CA-CB	5.04	117.31	110.01
1	G	63	ARG	CB-CA-C	5.03	119.66	110.36
3	F	129	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	ARG	Sidechain
1	A	242	ARG	Sidechain
1	A	55	ARG	Sidechain
2	B	42	ARG	Sidechain
2	B	94	ARG	Sidechain
3	C	131	ARG	Sidechain
3	C	17	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	181	ARG	Sidechain
3	C	219	ARG	Sidechain
3	C	274	TRP	Peptide
3	C	48	ARG	Sidechain
3	C	6	ARG	Sidechain
3	F	234	ARG	Sidechain
1	G	195	ARG	Sidechain
4	H	4	ARG	Sidechain
4	H	46	ARG	Sidechain
4	H	82	ARG	Sidechain
2	I	94	ARG	Sidechain

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	1898	0	1783	26	1
1	G	1912	0	1810	24	0
2	B	1551	0	1467	25	0
2	I	1562	0	1458	19	0
3	C	2252	0	2092	38	0
3	F	2225	0	2052	51	1
4	D	833	0	792	12	0
4	H	825	0	780	12	0
5	E	94	0	84	1	0
5	J	94	0	84	5	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	D	10	0	0	1	0
6	F	10	0	0	1	0
6	G	5	0	0	0	0
6	I	10	0	0	2	0
7	F	6	0	8	1	0
8	A	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	13301	0	12410	193	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:273:ARG:O	3:F:274:TRP:HB2	1.51	1.04
3:F:191:HIS:HB3	3:F:275:GLU:HB3	1.50	0.93
3:C:191:HIS:HB3	3:C:275:GLU:HB3	1.54	0.89
1:A:83:LEU:HD12	1:A:83:LEU:N	1.89	0.87
3:F:79:ARG:NH1	6:F:302:SO4:O3	2.08	0.87
3:C:268:LYS:HG3	3:C:269:PRO:HD2	1.57	0.85
3:F:20:PRO:HD2	3:F:75:ARG:HD2	1.59	0.84
3:C:185:PRO:HD2	3:C:266:LEU:HD23	1.63	0.81
2:B:42:ARG:HD2	2:B:43:GLY:H	1.48	0.77
3:F:219:ARG:NH1	3:F:256:ARG:HH21	1.84	0.75
3:C:191:HIS:CB	3:C:275:GLU:HB3	2.17	0.74
3:F:219:ARG:HH11	3:F:256:ARG:HH21	1.35	0.74
3:F:25:VAL:HG21	4:H:56:SER:HB3	1.70	0.72
1:A:83:LEU:HD12	1:A:83:LEU:H	1.56	0.70
2:B:42:ARG:HD2	2:B:43:GLY:N	2.07	0.69
3:C:6:ARG:HH12	3:C:113:HIS:CE1	2.11	0.68
3:F:44:ARG:NH2	3:F:61:ASP:OD1	2.27	0.68
3:C:238:ASP:OD1	3:C:240:THR:OG1	2.12	0.66
3:C:230:LEU:HD13	3:C:245:ALA:HB2	1.77	0.66
3:C:44:ARG:NH2	3:C:61:ASP:OD1	2.28	0.65
1:G:130:PRO:HA	2:I:125:LEU:HD23	1.79	0.63
3:F:20:PRO:HD2	3:F:75:ARG:CD	2.28	0.63
1:A:83:LEU:N	1:A:83:LEU:CD1	2.60	0.63
1:A:83:LEU:H	1:A:83:LEU:CD1	2.12	0.62
3:F:230:LEU:HD13	3:F:245:ALA:HB2	1.81	0.62
3:F:110:LEU:HD23	3:F:111:ARG:NH2	2.15	0.62
1:G:221:ASP:O	1:G:229:LYS:NZ	2.33	0.61
1:A:2:SER:O	1:A:26:ARG:HA	2.01	0.61
3:F:8:PHE:HB2	3:F:25:VAL:HG23	1.82	0.60
1:A:130:PRO:HD2	1:A:201:TRP:CZ2	2.36	0.60
3:C:64:THR:HG22	3:C:68:LYS:HE2	1.83	0.60
5:J:5:TYR:HB2	5:J:7:TYR:OH	2.02	0.60
2:B:14:ALA:HB3	2:B:17:ASN:HD22	1.67	0.60
3:C:173:GLU:O	3:C:176:LYS:HG3	2.02	0.59
1:A:32:VAL:HG12	1:A:49:TYR:HB2	1.85	0.59
1:A:140:LYS:HE2	2:B:168:MET:HE3	1.84	0.58
1:A:116:ASP:OD2	1:A:118:LYS:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:144:GLN:O	3:F:148:GLU:HG3	2.03	0.58
2:I:127:ASP:HB3	2:I:130:SER:O	2.04	0.58
1:A:88:LEU:HD13	1:A:110:ARG:HG2	1.85	0.58
3:F:77:SER:HB3	5:J:9:LEU:HB2	1.86	0.57
3:F:235:PRO:HG2	4:H:66:LEU:HD13	1.86	0.57
1:A:15:THR:HG21	1:A:83:LEU:HD11	1.84	0.57
2:B:112:LYS:HB3	2:B:143:SER:HB3	1.87	0.57
2:I:121:ALA:HB1	2:I:123:TYR:CE1	2.40	0.57
3:C:122:ASP:OD1	4:D:61:TRP:NE1	2.37	0.57
2:I:138:PHE:HB2	2:I:190:PHE:CE2	2.40	0.56
4:H:22:ASN:HB3	4:H:71:PHE:HE1	1.70	0.56
1:G:18:ARG:HD2	1:G:18:ARG:C	2.31	0.56
1:G:229:LYS:HG2	1:G:231:VAL:HG13	1.87	0.56
2:I:131:SER:C	2:I:133:LYS:H	2.14	0.55
3:C:79:ARG:NH2	3:C:80:ASN:OD1	2.40	0.55
4:D:42:LYS:NZ	6:D:202:SO4:O4	2.39	0.55
3:F:82:ARG:HD2	3:F:89:GLU:HA	1.87	0.55
1:G:153:ASP:HB2	1:G:176:PRO:HG2	1.88	0.55
3:F:273:ARG:O	3:F:274:TRP:CB	2.41	0.55
1:G:130:PRO:HD2	1:G:201:TRP:CZ2	2.41	0.55
3:C:47:PRO:O	3:C:48:ARG:HD2	2.07	0.55
2:I:100:ARG:NE	6:I:301:SO4:O3	2.39	0.55
2:B:127:ASP:CG	2:B:128:SER:N	2.65	0.55
3:C:121:LYS:HB3	4:D:2:ILE:HD12	1.89	0.54
2:B:156:TYR:O	2:B:177:ALA:HA	2.08	0.54
3:C:117:ALA:HB2	4:D:61:TRP:CE2	2.43	0.54
1:A:135:ILE:HD11	1:A:141:ALA:HB2	1.91	0.53
3:F:131:ARG:HH11	3:F:131:ARG:HG3	1.72	0.53
3:C:19:GLU:HG3	3:C:20:PRO:HD2	1.91	0.53
2:I:156:TYR:O	2:I:177:ALA:HA	2.08	0.53
1:A:132:GLU:H	1:A:132:GLU:CD	2.16	0.53
3:F:114:ASP:OD2	5:J:3:ARG:NH1	2.29	0.53
4:H:22:ASN:HB3	4:H:71:PHE:CE1	2.43	0.53
2:B:77:LYS:HE3	3:F:122:ASP:OD2	2.09	0.52
4:D:25:ASN:HB3	4:D:66:LEU:HD11	1.92	0.52
2:I:200:PHE:CE2	2:I:202:PRO:HG3	2.45	0.52
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.75	0.52
2:B:126:ARG:HG2	2:B:126:ARG:NH1	2.25	0.51
1:G:138:THR:O	1:G:139:GLN:HB2	2.09	0.51
2:B:126:ARG:HG2	2:B:126:ARG:HH11	1.74	0.51
4:H:74:THR:OG1	4:H:77:ASP:OD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ARG:HG2	3:C:44:ARG:HH11	1.76	0.51
4:D:1:MET:HG2	4:D:2:ILE:N	2.26	0.51
4:D:60:ASP:O	4:D:61:TRP:HB2	2.11	0.51
3:F:187:THR:HB	3:F:272:LEU:HD11	1.93	0.50
1:A:60:ILE:HG13	1:A:64:PHE:HB2	1.93	0.50
1:G:39:LEU:HD11	1:G:110:ARG:HH12	1.76	0.50
3:C:111:ARG:NE	3:C:128:GLU:OE1	2.44	0.50
3:C:219:ARG:HD2	3:C:256:ARG:HE	1.77	0.50
3:F:271:THR:O	3:F:272:LEU:HD23	2.11	0.49
3:C:189:VAL:HG23	3:C:272:LEU:HD12	1.95	0.49
1:G:129:GLU:OE1	2:I:128:SER:HA	2.11	0.49
4:H:38:VAL:HB	4:H:67:TYR:CZ	2.47	0.49
3:F:47:PRO:O	3:F:48:ARG:HD2	2.12	0.48
3:F:253:GLU:HB3	3:F:256:ARG:HD3	1.93	0.48
2:I:92:ALA:HA	2:I:102:MET:O	2.13	0.48
3:C:114:ASP:OD2	3:C:156:ARG:NH1	2.40	0.48
4:D:49:LYS:HE3	4:D:69:THR:OG1	2.13	0.48
3:C:77:SER:HB3	5:E:9:LEU:HB2	1.96	0.48
3:C:177:ASP:O	3:C:181:ARG:HB2	2.14	0.48
3:F:6:ARG:HH11	3:F:6:ARG:HG2	1.79	0.48
3:F:191:HIS:HB3	3:F:275:GLU:CB	2.32	0.48
2:B:124:GLN:NE2	2:B:126:ARG:HH22	2.12	0.47
1:A:2:SER:N	1:A:27:SER:HG	2.12	0.47
1:G:11:LEU:HD12	1:G:11:LEU:HA	1.63	0.47
3:C:162:GLY:O	3:C:166:GLU:HG2	2.15	0.47
1:A:96:SER:OG	1:A:97:GLY:N	2.47	0.47
2:B:122:VAL:HG12	2:B:186:CYS:HB3	1.97	0.46
3:C:6:ARG:HB2	3:C:98:MET:HE3	1.98	0.46
3:F:274:TRP:CD1	3:F:275:GLU:H	2.32	0.46
2:B:69:LYS:HB3	2:B:69:LYS:HE3	1.58	0.46
2:I:100:ARG:HB3	6:I:301:SO4:O3	2.15	0.46
3:F:139:ALA:HA	3:F:142:ILE:HD12	1.97	0.46
2:B:4:VAL:HG13	2:B:93:VAL:HG12	1.96	0.46
3:C:9:TYR:CD1	3:C:24:SER:HB2	2.51	0.46
3:F:233:THR:OG1	3:F:243:LYS:HD2	2.16	0.46
4:H:41:LEU:HD23	4:H:46:ARG:HA	1.98	0.46
2:B:138:PHE:HB2	2:B:190:PHE:CE2	2.51	0.45
3:C:47:PRO:HB3	3:C:60:TRP:CH2	2.51	0.45
2:I:19:LEU:HD22	2:I:109:LEU:HD21	1.98	0.45
3:F:50:PRO:O	3:F:53:GLU:HB2	2.17	0.45
1:G:173:ASP:OD1	1:G:193:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:119:ASP:N	2:I:120:PRO:HD3	2.31	0.45
3:F:186:LYS:HE3	3:F:186:LYS:HB2	1.79	0.45
2:B:83:VAL:HA	2:B:111:VAL:HB	1.98	0.45
2:B:121:ALA:HA	2:B:200:PHE:O	2.17	0.45
3:F:184:PRO:HB3	3:F:265:GLY:C	2.41	0.45
1:A:14:ALA:HA	1:A:114:LEU:O	2.17	0.44
1:G:69:PHE:HE2	1:G:75:GLU:HG3	1.82	0.44
1:A:160:TRP:HB2	1:A:209:ARG:HB3	1.98	0.44
3:F:152:GLU:OE2	5:J:7:TYR:HD2	2.01	0.44
2:B:181:LYS:HE3	2:B:181:LYS:HB2	1.85	0.43
3:F:6:ARG:NE	3:F:98:MET:SD	2.92	0.43
1:A:242:ARG:HH11	1:A:242:ARG:HD2	1.61	0.43
5:J:5:TYR:HB2	5:J:7:TYR:CZ	2.53	0.43
1:A:19:VAL:HG22	1:A:81:LEU:HD11	2.01	0.43
3:F:76:GLU:O	3:F:77:SER:C	2.60	0.43
1:A:127:VAL:O	2:B:127:ASP:CB	2.67	0.42
1:G:171:CYS:HB3	2:I:163:LEU:HB3	2.01	0.42
3:C:6:ARG:CB	3:C:98:MET:HE3	2.49	0.42
3:F:58:GLU:H	3:F:58:GLU:CD	2.27	0.42
2:I:184:PHE:CZ	2:I:189:ALA:HB2	2.55	0.42
1:A:161:VAL:HG12	1:A:208:PHE:CD1	2.55	0.42
3:F:131:ARG:HH11	3:F:131:ARG:CG	2.32	0.42
3:F:162:GLY:O	3:F:166:GLU:HG3	2.19	0.42
4:D:4:ARG:HB3	4:D:30:GLY:O	2.19	0.42
1:A:173:ASP:OD1	1:A:193:ARG:NH2	2.52	0.42
3:C:207:GLY:HA2	3:C:240:THR:HB	2.00	0.42
1:G:153:ASP:OD1	1:G:153:ASP:N	2.51	0.42
2:B:126:ARG:NH1	2:B:126:ARG:CG	2.83	0.42
3:F:266:LEU:HA	3:F:267:PRO:HD2	1.87	0.42
3:C:272:LEU:HD23	3:C:272:LEU:N	2.35	0.42
1:A:66:ALA:O	1:A:67:GLN:HB2	2.20	0.42
3:C:224:GLN:O	3:C:225:THR:C	2.63	0.41
1:G:20:THR:C	1:G:21:LEU:HD23	2.46	0.41
2:B:94:ARG:NH1	2:B:95:ASP:O	2.53	0.41
1:G:195:ARG:HD3	2:I:165:MET:SD	2.59	0.41
3:C:44:ARG:HG2	3:C:44:ARG:NH1	2.36	0.41
3:F:35:ARG:HG2	3:F:48:ARG:HD3	2.02	0.41
1:G:39:LEU:HD12	1:G:39:LEU:H	1.85	0.41
3:C:137:ASP:OD1	3:C:137:ASP:N	2.53	0.41
3:F:9:TYR:CD1	3:F:24:SER:HB2	2.55	0.41
4:H:60:ASP:O	4:H:61:TRP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:197:HIS:HD2	7:F:301:GOL:O2	2.03	0.41
3:F:256:ARG:H	3:F:256:ARG:HG2	1.70	0.41
2:B:73:SER:HB2	2:B:75:HIS:CE1	2.55	0.41
3:C:270:LEU:HD23	3:C:270:LEU:HA	1.88	0.41
3:F:47:PRO:HB3	3:F:60:TRP:CH2	2.55	0.41
1:G:55:ARG:NE	1:G:55:ARG:HA	2.36	0.41
3:F:121:LYS:HB2	4:H:2:ILE:CD1	2.51	0.41
3:F:235:PRO:O	4:H:11:TYR:OH	2.22	0.41
1:G:21:LEU:HD23	1:G:21:LEU:N	2.36	0.41
2:B:36:TYR:HA	2:B:45:GLN:O	2.20	0.41
3:F:123:TYR:HD2	3:F:124:ILE:HG22	1.86	0.41
3:F:238:ASP:O	3:F:239:ARG:HB2	2.21	0.41
4:H:40:LEU:HD12	4:H:69:THR:HB	2.01	0.41
4:H:97:ASP:O	4:H:98:ARG:HB2	2.21	0.41
2:I:56:LEU:HD22	2:I:56:LEU:HA	1.92	0.41
1:A:110:ARG:HH11	1:A:110:ARG:HG3	1.85	0.41
2:B:4:VAL:HG13	2:B:93:VAL:CG1	2.52	0.41
3:C:218:GLN:HG3	3:C:260:HIS:CD2	2.56	0.41
1:G:13:THR:OG1	1:G:14:ALA:N	2.53	0.40
2:B:25:TYR:CE1	2:B:31:PRO:HG3	2.55	0.40
3:C:9:TYR:HD1	3:C:24:SER:HB2	1.86	0.40
3:C:235:PRO:HG2	4:D:66:LEU:HD22	2.03	0.40
3:F:82:ARG:CD	3:F:89:GLU:HA	2.51	0.40
2:I:138:PHE:HB2	2:I:190:PHE:CZ	2.57	0.40
1:G:50:TYR:O	1:G:51:ASN:C	2.65	0.40
1:G:100:TYR:HB2	2:I:51:ILE:HD12	2.02	0.40
1:G:66:ALA:HA	1:G:75:GLU:O	2.21	0.40
3:C:58:GLU:O	3:C:59:TYR:C	2.65	0.40
4:D:32:HIS:HA	4:D:33:PRO:C	2.46	0.40
4:D:40:LEU:O	4:D:41:LEU:HD23	2.21	0.40
3:F:184:PRO:HB3	3:F:265:GLY:O	2.22	0.40
1:G:14:ALA:HA	1:G:114:LEU:O	2.21	0.40
3:F:230:LEU:HD11	3:F:243:LYS:HE3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:NH1	3:F:65:GLN:OE1[3_659]	2.12	0.08

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	237/245 (97%)	222 (94%)	15 (6%)	0	100	100
1	G	240/245 (98%)	228 (95%)	12 (5%)	0	100	100
2	B	193/208 (93%)	185 (96%)	8 (4%)	0	100	100
2	I	199/208 (96%)	192 (96%)	7 (4%)	0	100	100
3	C	272/276 (99%)	257 (94%)	14 (5%)	1 (0%)	30	53
3	F	269/276 (98%)	253 (94%)	15 (6%)	1 (0%)	30	53
4	D	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
4	H	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
5	E	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1619/1676 (97%)	1534 (95%)	83 (5%)	2 (0%)	48	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	274	TRP
3	C	274	TRP

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	204/212 (96%)	192 (94%)	12 (6%)	18	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	207/212 (98%)	193 (93%)	14 (7%)	14	35
2	B	176/186 (95%)	166 (94%)	10 (6%)	18	42
2	I	175/186 (94%)	161 (92%)	14 (8%)	11	28
3	C	233/234 (100%)	212 (91%)	21 (9%)	9	24
3	F	229/234 (98%)	219 (96%)	10 (4%)	25	51
4	D	94/95 (99%)	85 (90%)	9 (10%)	8	22
4	H	93/95 (98%)	89 (96%)	4 (4%)	26	52
5	E	9/9 (100%)	9 (100%)	0	100	100
5	J	9/9 (100%)	7 (78%)	2 (22%)	1	2
All	All	1429/1472 (97%)	1333 (93%)	96 (7%)	15	36

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	22	ARG
1	G	43	LEU
1	G	57	LYS
1	G	100	TYR
1	G	135	ILE
1	G	142	THR
1	G	143	LEU
1	G	171	CYS
1	G	185	ASP
1	G	187	ARG
1	G	190	LEU
1	G	191	SER
1	G	225	GLN
1	G	226	ASP
2	I	4	VAL
2	I	27	VAL
2	I	31	PRO
2	I	52	THR
2	I	56	LEU
2	I	57	VAL
2	I	60	SER
2	I	73	SER
2	I	100	ARG
2	I	147	VAL
2	I	157	ILE

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Mol	Chain	Res	Type
2	I	174	SER
2	I	195	ILE
2	I	198	ASP
1	A	38	SER
1	A	55	ARG
1	A	73	HIS
1	A	83	LEU
1	A	95	VAL
1	A	110	ARG
1	A	132	GLU
1	A	135	ILE
1	A	146	LEU
1	A	171	CYS
1	A	190	LEU
1	A	226	ASP
2	B	28	SER
2	B	42	ARG
2	B	45	GLN
2	B	52	THR
2	B	69	LYS
2	B	70	SER
2	B	112	LYS
2	B	127	ASP
2	B	172	SER
2	B	180	ASN
3	C	17	ARG
3	C	44	ARG
3	C	76	GLU
3	C	97	SER
3	C	98	MET
3	C	131	ARG
3	C	151	ARG
3	C	161	GLU
3	C	177	ASP
3	C	197	HIS
3	C	216	THR
3	C	222	GLU
3	C	240	THR
3	C	256	ARG
3	C	258	THR
3	C	266	LEU
3	C	268	LYS

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Mol	Chain	Res	Type
3	C	272	LEU
3	C	273	ARG
3	C	274	TRP
3	C	275	GLU
4	D	1	MET
4	D	4	ARG
4	D	17	GLU
4	D	56	SER
4	D	60	ASP
4	D	71	PHE
4	D	86	VAL
4	D	93	ILE
4	D	99	ASP
3	F	19	GLU
3	F	35	ARG
3	F	97	SER
3	F	110	LEU
3	F	173	GLU
3	F	191	HIS
3	F	212	GLU
3	F	229	GLU
3	F	230	LEU
3	F	255	GLN
4	H	33	PRO
4	H	46	ARG
4	H	60	ASP
4	H	71	PHE
5	J	1	SER
5	J	7	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	67	GLN
1	G	213	GLN
1	G	220	ASN
1	G	225	GLN
2	I	10	GLN
2	I	45	GLN
1	A	36	GLN
1	A	73	HIS
1	A	167	HIS

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Mol	Chain	Res	Type
1	A	220	ASN
2	B	17	ASN
2	B	38	GLN
2	B	144	GLN
3	C	32	GLN
3	C	113	HIS
3	C	115	GLN
3	C	174	ASN
3	C	192	HIS
3	C	255	GLN
3	C	260	HIS
4	D	14	HIS
3	F	32	GLN
3	F	197	HIS
3	F	224	GLN
3	F	260	HIS

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](#)

10 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	SO4	D	201	-	4,4,4	0.28	0	6,6,6	0.12	0
6	SO4	G	301	-	4,4,4	0.31	0	6,6,6	0.05	0
6	SO4	I	301	-	4,4,4	0.26	0	6,6,6	0.31	0
6	SO4	D	202	-	4,4,4	0.28	0	6,6,6	0.13	0
6	SO4	F	303	-	4,4,4	0.33	0	6,6,6	0.07	0
6	SO4	A	301	-	4,4,4	0.30	0	6,6,6	0.32	0
7	GOL	F	301	-	5,5,5	0.21	0	5,5,5	0.57	0
6	SO4	F	302	-	4,4,4	0.34	0	6,6,6	0.14	0
6	SO4	C	301	-	4,4,4	0.26	0	6,6,6	0.13	0
6	SO4	I	302	-	4,4,4	0.30	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	F	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	301	GOL	O1-C1-C2-C3
7	F	301	GOL	C1-C2-C3-O3
7	F	301	GOL	O1-C1-C2-O2
7	F	301	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	301	SO4	2	0
6	D	202	SO4	1	0
7	F	301	GOL	1	0
6	F	302	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	241/245 (98%)	-0.35	2 (0%) 82 78	16, 35, 71, 99	0
1	G	242/245 (98%)	-0.29	5 (2%) 63 55	13, 34, 73, 96	0
2	B	197/208 (94%)	-0.06	3 (1%) 72 65	21, 45, 81, 102	0
2	I	201/208 (96%)	-0.01	3 (1%) 72 65	14, 42, 83, 128	1 (0%)
3	C	274/276 (99%)	-0.26	2 (0%) 84 80	16, 37, 78, 121	0
3	F	273/276 (98%)	-0.11	5 (1%) 67 59	17, 44, 80, 109	0
4	D	100/100 (100%)	-0.19	2 (2%) 65 57	20, 44, 74, 109	0
4	H	99/100 (99%)	0.16	2 (2%) 65 57	21, 53, 83, 100	0
5	E	9/9 (100%)	-0.86	0 100 100	17, 21, 30, 33	0
5	J	9/9 (100%)	0.37	2 (22%) 2 2	25, 41, 76, 93	0
All	All	1645/1676 (98%)	-0.17	26 (1%) 70 63	13, 41, 80, 128	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	274	TRP	3.9
3	F	91	GLY	3.5
3	F	255	GLN	3.3
1	G	183	LEU	3.2
3	F	16	GLY	3.1
5	J	6	PHE	2.8
3	C	274	TRP	2.7
1	G	243	ALA	2.7
2	B	167	SER	2.7
1	G	242	ARG	2.5
2	B	128	SER	2.5
4	H	2	ILE	2.5
1	G	39	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	2.3
3	C	237	GLY	2.3
4	D	76	LYS	2.3
4	D	100	MET	2.2
1	A	71	ASP	2.2
4	H	100	MET	2.2
5	J	7	TYR	2.2
2	I	194	ILE	2.1
1	G	42	GLY	2.1
3	F	223	ASP	2.1
2	I	182	SER	2.0
2	B	40	PRO	2.0
2	I	203	SER	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(Å ²)	Q<0.9
6	SO4	F	302	5/5	0.81	0.14	95,112,116,119	0
6	SO4	I	302	5/5	0.82	0.14	83,100,106,121	0
6	SO4	C	301	5/5	0.83	0.14	77,78,88,90	0
6	SO4	F	303	5/5	0.83	0.12	77,83,92,92	0
6	SO4	A	301	5/5	0.84	0.14	55,86,93,95	0
6	SO4	D	202	5/5	0.84	0.15	77,88,115,124	0
7	GOL	F	301	6/6	0.84	0.20	30,49,57,58	0
6	SO4	D	201	5/5	0.89	0.16	94,102,111,111	0
6	SO4	G	301	5/5	0.91	0.09	77,82,84,87	0
6	SO4	I	301	5/5	0.97	0.11	36,42,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.