



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:27 PM UTC

PDB ID : 5EUO / pdb_00005euo
Title : PF6-M1-HLA-A2
Authors : Yang, X.
Deposited on : 2015-11-18
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

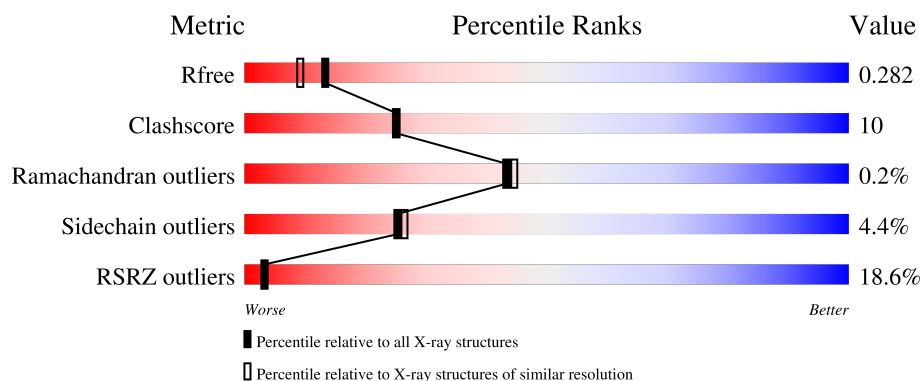
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



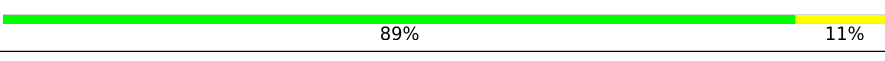
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	31% 75% 21% ...
1	C	276	5% 85% 12% .
2	B	100	48% 70% 26% .
2	D	100	5% 78% 21% .
3	E	208	16% 74% 16% 9%

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Mol	Chain	Length	Quality of chain
3	G	208	
4	F	240	
4	H	240	
5	I	9	
5	J	9	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13444 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 I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2237	1398	408	422	9			
1	C	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892
C	0	MET	-	initiating methionine	UNP P01892

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called PF6 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	190	Total	C	N	O	S	0	0	0
			1454	910	245	292	7			
3	G	191	Total	C	N	O	S	0	0	0
			1460	913	246	294	7			

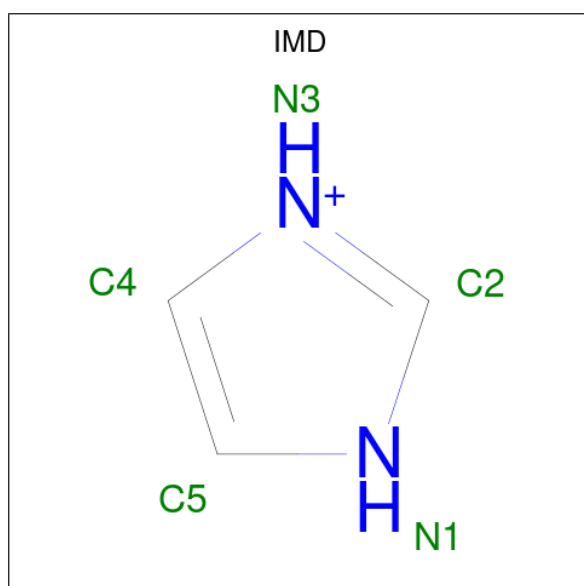
- Molecule 4 is a protein called PF6 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	239	Total	C	N	O	S	0	0	0
			1922	1214	332	370	6			
4	H	237	Total	C	N	O	S	0	0	0
			1906	1205	327	368	6			

- Molecule 5 is a protein called Matrix protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	9	Total	C	N	O	0	0	0
			69	49	9	11			
5	J	9	Total	C	N	O	0	0	0
			69	49	9	11			

- Molecule 6 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			5	3	2		
6	G	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	28	Total	O	0	0
			28	28		

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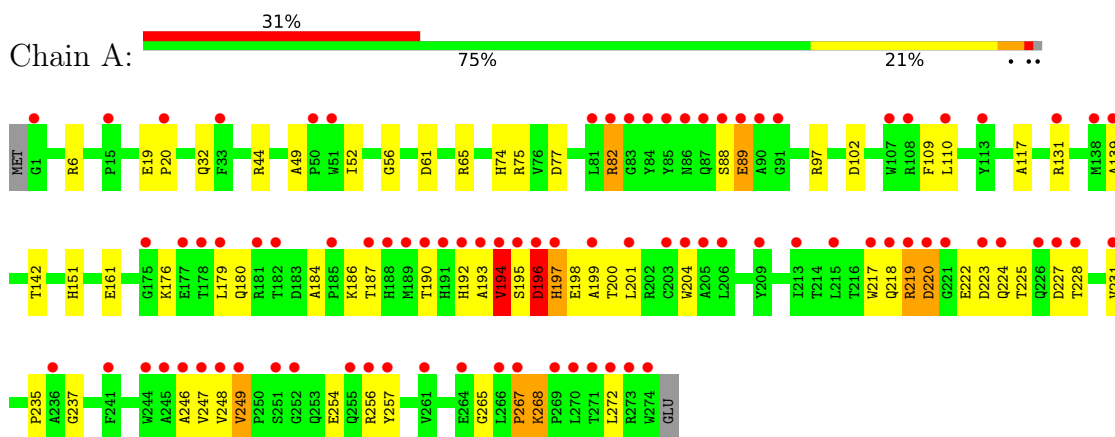
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total 11	O 11	0	0
7	C	96	Total 96	O 96	0	0
7	D	23	Total 23	O 23	0	0
7	E	29	Total 29	O 29	0	0
7	F	80	Total 80	O 80	0	0
7	G	38	Total 38	O 38	0	0
7	H	83	Total 83	O 83	0	0
7	I	6	Total 6	O 6	0	0
7	J	3	Total 3	O 3	0	0

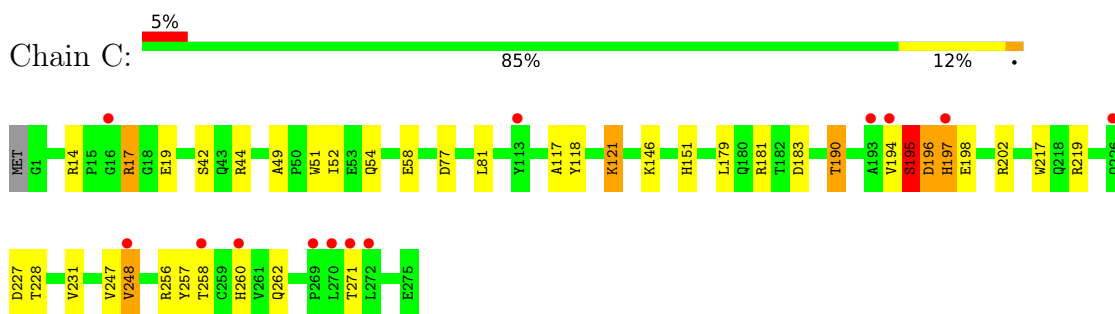
3 Residue-property plots [i](#)

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.

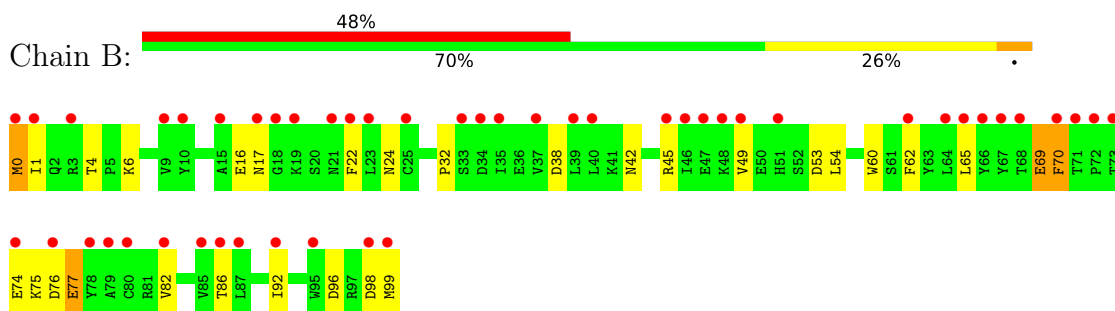
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



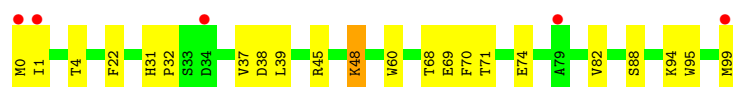
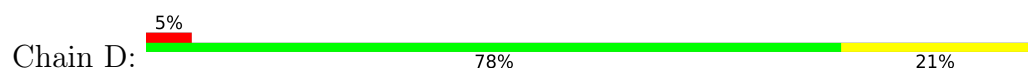
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



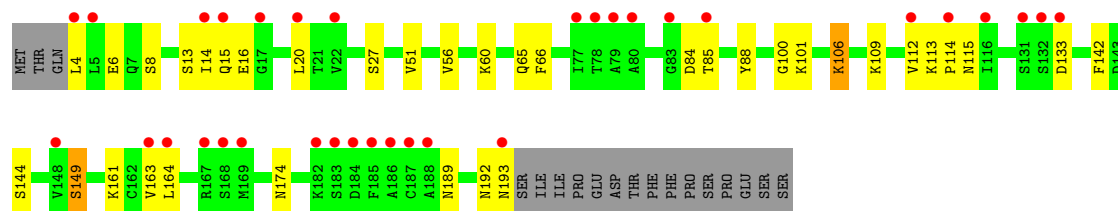
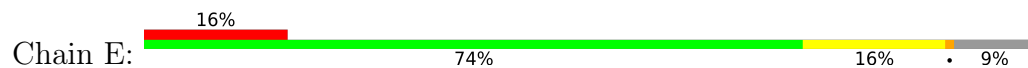
- Molecule 2: Beta-2-microglobulin



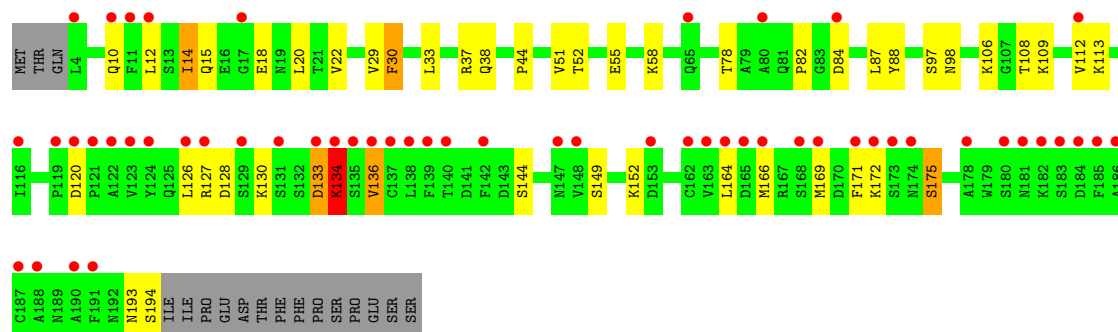
- Molecule 2: Beta-2-microglobulin



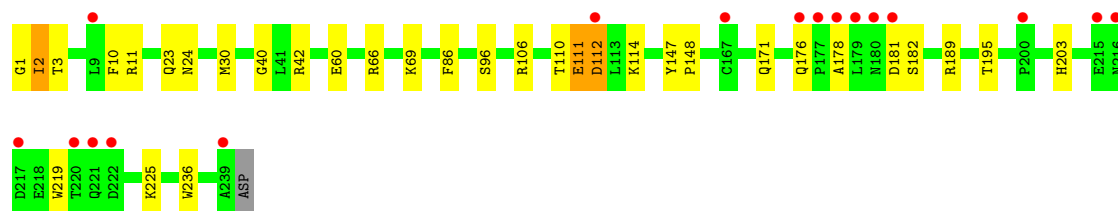
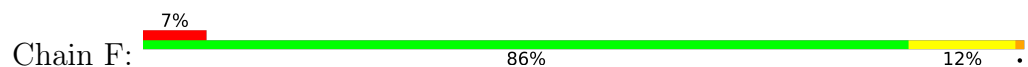
• Molecule 3: PF6 TCR alpha chain



• Molecule 3: PF6 TCR alpha chain

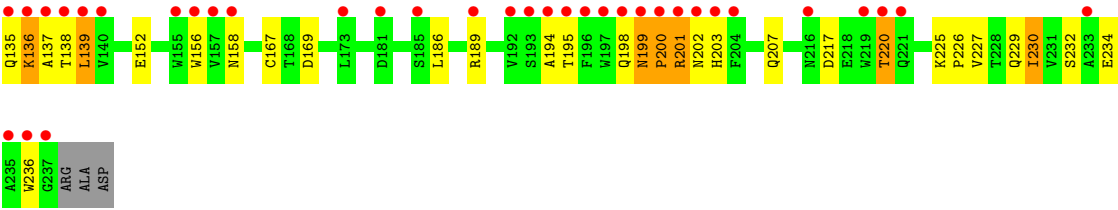


• Molecule 4: PF6 TCR beta chain



• Molecule 4: PF6 TCR beta chain

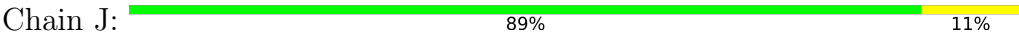




● Molecule 5: Matrix protein 1



● Molecule 5: Matrix protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.74Å 54.08Å 149.30Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	120.47 – 2.10 120.47 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (120.47-2.10) 99.9 (120.47-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.229 , 0.281 0.234 , 0.282	Depositor DCC
R_{free} test set	1984 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13444	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6143e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IMD

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	0.62	1/2302 (0.0%)	1.00	11/3125 (0.4%)
1	C	0.64	0/2312	0.87	3/3137 (0.1%)
2	B	0.49	0/859	0.87	2/1162 (0.2%)
2	D	0.64	0/860	0.84	2/1162 (0.2%)
3	E	0.60	0/1481	0.91	0/2004
3	G	0.72	2/1487 (0.1%)	1.03	12/2012 (0.6%)
4	F	0.64	1/1975 (0.1%)	0.84	3/2688 (0.1%)
4	H	0.61	0/1959	0.87	3/2667 (0.1%)
5	I	0.54	0/70	0.82	0/92
5	J	0.64	0/70	0.74	0/92
All	All	0.63	4/13375 (0.0%)	0.91	36/18141 (0.2%)

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	1
3	G	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	111	GLU	C-N	9.22	1.45	1.33
1	A	193	ALA	C-N	-6.42	1.25	1.33
3	G	133	ASP	C-N	-5.17	1.26	1.33
3	G	29	VAL	C-O	-5.07	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	HIS	O-C-N	14.38	141.08	122.39
1	A	194	VAL	O-C-N	-11.11	108.68	122.57
1	A	196	ASP	O-C-N	-11.00	107.96	122.59
1	A	196	ASP	CA-C-N	-8.72	106.65	120.60
1	A	196	ASP	C-N-CA	-8.72	106.65	120.60
3	G	97	SER	CA-C-N	-7.83	112.40	123.20
3	G	97	SER	C-N-CA	-7.83	112.40	123.20
3	G	133	ASP	CA-C-N	7.39	135.65	121.54
3	G	133	ASP	C-N-CA	7.39	135.65	121.54
3	G	97	SER	N-CA-C	-7.06	101.21	110.53
3	G	133	ASP	O-C-N	-6.83	114.17	122.71
3	G	30	PHE	N-CA-C	6.22	118.86	108.96
1	A	193	ALA	CA-C-N	6.22	133.16	121.97
1	A	193	ALA	C-N-CA	6.22	133.16	121.97
2	B	70	PHE	N-CA-C	6.13	117.89	109.18
1	C	231	VAL	CB-CA-C	-6.09	104.89	111.59
1	C	197	HIS	N-CA-CB	-5.97	102.96	110.90
1	A	220	ASP	N-CA-C	-5.72	105.14	111.71
1	A	197	HIS	N-CA-C	5.70	119.33	112.38
2	D	71	THR	CA-C-N	-5.66	114.13	119.85
2	D	71	THR	C-N-CA	-5.66	114.13	119.85
4	H	200	PRO	CA-C-O	-5.60	114.25	122.31
3	G	38	GLN	N-CA-C	5.42	117.22	108.34
3	G	127	ARG	CA-C-N	5.41	129.03	121.24
3	G	127	ARG	C-N-CA	5.41	129.03	121.24
2	B	82	VAL	N-CA-C	5.35	115.82	108.12
3	G	30	PHE	CB-CA-C	-5.34	101.31	110.22
1	C	17	ARG	N-CA-C	-5.16	104.79	111.71
3	G	175	SER	N-CA-C	5.16	116.25	108.46
4	F	111	GLU	CA-C-N	-5.07	113.02	121.64
4	F	111	GLU	C-N-CA	-5.07	113.02	121.64
4	F	112	ASP	N-CA-C	5.03	116.57	108.32
1	A	56	GLY	CA-C-N	5.02	124.63	119.56
1	A	56	GLY	C-N-CA	5.02	124.63	119.56
4	H	199	ASN	CA-C-N	-5.02	114.49	120.11
4	H	199	ASN	C-N-CA	-5.02	114.49	120.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ASP	Mainchain
3	G	134	LYS	Mainchain

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	2237	0	2090	61	3
1	C	2247	0	2096	33	0
2	B	836	0	803	21	0
2	D	837	0	803	11	0
3	E	1454	0	1418	25	0
3	G	1460	0	1422	39	0
4	F	1922	0	1825	22	0
4	H	1906	0	1807	53	2
5	I	69	0	75	2	0
5	J	69	0	75	2	0
6	C	5	0	5	0	0
6	G	5	0	5	0	0
7	A	28	0	0	0	0
7	B	11	0	0	1	0
7	C	96	0	0	2	0
7	D	23	0	0	0	0
7	E	29	0	0	0	0
7	F	80	0	0	3	0
7	G	38	0	0	3	0
7	H	83	0	0	4	0
7	I	6	0	0	1	0
7	J	3	0	0	0	0
All	All	13444	0	12424	246	3

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 10.

All (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:O	1:A:197:HIS:N	1.79	1.14
1:A:219:ARG:HD3	1:A:256:ARG:HH12	1.03	1.10
1:A:194:VAL:HG12	1:A:195:SER:H	1.28	0.99
1:A:196:ASP:O	1:A:198:GLU:N	1.95	0.98
1:A:219:ARG:CD	1:A:256:ARG:HH12	1.76	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:30:MET:SD	7:H:379:HOH:O	2.22	0.96
1:A:219:ARG:HD3	1:A:256:ARG:NH1	1.80	0.95
3:E:85:THR:HG22	3:E:112:VAL:H	1.34	0.93
4:H:134:THR:HG23	4:H:136:LYS:H	1.31	0.92
1:A:222:GLU:CG	1:A:223:ASP:H	1.83	0.90
1:C:190:THR:HG22	1:C:202:ARG:HB3	1.55	0.89
3:G:128:ASP:OD2	7:G:401:HOH:O	1.91	0.89
4:F:110:THR:OG1	4:F:181:ASP:OD2	1.90	0.88
1:A:194:VAL:HG21	1:A:200:THR:OG1	1.77	0.85
3:G:164:LEU:HB3	4:H:167:CYS:HB2	1.60	0.83
4:H:23:GLN:HE21	4:H:25:LEU:H	1.25	0.82
1:A:220:ASP:OD1	1:A:256:ARG:HG2	1.80	0.81
1:C:195:SER:OG	1:C:196:ASP:N	2.13	0.81
1:C:228:THR:HG22	1:C:247:VAL:HG12	1.61	0.79
1:A:187:THR:HB	1:A:272:LEU:HD11	1.65	0.79
1:A:225:THR:O	1:A:228:THR:HG22	1.84	0.77
1:A:220:ASP:OD1	1:A:256:ARG:HD2	1.85	0.77
4:H:207:GLN:HE21	4:H:230:ILE:HD12	1.51	0.75
4:H:34:ARG:HB2	4:H:44:ILE:HD11	1.67	0.75
3:G:37:ARG:NH2	3:G:88:TYR:OH	2.20	0.74
2:D:39:LEU:HD12	2:D:68:THR:HG22	1.68	0.73
4:H:23:GLN:HE21	4:H:25:LEU:N	1.86	0.73
3:E:142:PHE:HE2	3:E:161:LYS:HE3	1.55	0.72
3:G:10:GLN:H	3:G:10:GLN:CD	1.97	0.71
1:A:194:VAL:CG2	1:A:200:THR:OG1	2.38	0.71
1:A:223:ASP:OD1	1:A:224:GLN:N	2.24	0.70
3:E:13:SER:OG	3:E:113:LYS:HE2	1.92	0.70
1:A:190:THR:HG22	1:A:192:HIS:CE1	2.26	0.69
1:A:222:GLU:HG2	1:A:223:ASP:H	1.56	0.69
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.73	0.69
2:B:42:ASN:ND2	2:B:76:ASP:OD1	2.21	0.69
4:H:34:ARG:NH2	4:H:82:ASN:O	2.26	0.68
1:A:220:ASP:OD1	1:A:256:ARG:CG	2.43	0.66
1:A:222:GLU:HG3	1:A:223:ASP:H	1.57	0.66
1:A:222:GLU:CG	1:A:223:ASP:N	2.56	0.66
1:C:77:ASP:HB3	5:I:9:LEU:HD12	1.77	0.65
1:C:260:HIS:CD2	1:C:271:THR:HG22	2.32	0.64
2:B:42:ASN:HA	2:B:77:GLU:HG2	1.80	0.64
3:G:51:VAL:HG23	3:G:52:THR:HG23	1.80	0.64
1:A:220:ASP:OD1	1:A:256:ARG:CD	2.45	0.63
7:C:405:HOH:O	3:G:52:THR:HG22	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:189:ASN:O	3:E:192:ASN:ND2	2.31	0.63
1:A:195:SER:O	1:A:196:ASP:C	2.41	0.63
4:H:123:VAL:HG13	4:H:139:LEU:HD21	1.79	0.62
2:B:17:ASN:HD21	2:B:74:GLU:N	1.97	0.62
4:H:50:VAL:HG23	7:H:341:HOH:O	1.99	0.62
1:A:190:THR:CG2	1:A:192:HIS:HE1	2.12	0.62
1:A:194:VAL:HG12	1:A:195:SER:N	1.97	0.62
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.33	0.62
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.83	0.61
1:C:194:VAL:HG12	1:C:194:VAL:O	2.00	0.61
4:H:23:GLN:NE2	4:H:27:HIS:H	1.98	0.61
2:B:17:ASN:HD21	2:B:74:GLU:H	1.48	0.60
1:A:219:ARG:CG	1:A:256:ARG:HH12	2.13	0.60
1:A:190:THR:HG22	1:A:192:HIS:HE1	1.65	0.60
4:H:12:LYS:HB3	4:H:15:GLN:HE21	1.66	0.60
4:F:203:HIS:HB2	4:F:236:TRP:CZ3	2.38	0.59
3:G:37:ARG:HH12	3:G:84:ASP:HA	1.67	0.59
3:G:166:MET:SD	3:G:171:PHE:HD2	2.26	0.58
1:C:14:ARG:NE	1:C:19:GLU:O	2.26	0.58
2:B:4:THR:HA	2:B:86:THR:HG21	1.85	0.58
1:A:77:ASP:HB3	5:J:9:LEU:HD12	1.86	0.58
2:B:22:PHE:CZ	2:B:69:GLU:HG3	2.39	0.57
3:G:87:LEU:HD12	3:G:109:LYS:HG3	1.87	0.57
4:F:176:GLN:HE21	4:F:178:ALA:H	1.53	0.57
1:C:258:THR:HG22	7:C:423:HOH:O	2.04	0.57
1:C:181:ARG:NH1	1:C:183:ASP:OD2	2.38	0.56
3:G:37:ARG:NH2	3:G:88:TYR:CZ	2.73	0.56
2:D:22:PHE:CE1	2:D:69:GLU:HB3	2.39	0.56
3:E:13:SER:OG	3:E:113:LYS:CE	2.53	0.56
4:H:23:GLN:NE2	4:H:25:LEU:H	1.99	0.56
4:F:10:PHE:O	4:F:11:ARG:NH1	2.37	0.56
3:G:120:ASP:OD2	4:H:133:HIS:HE1	1.88	0.56
1:C:195:SER:OG	1:C:197:HIS:N	2.38	0.56
3:G:37:ARG:NH1	3:G:84:ASP:HA	2.20	0.56
2:B:22:PHE:CE2	2:B:69:GLU:HG3	2.41	0.56
4:F:176:GLN:NE2	4:F:178:ALA:HB3	2.20	0.56
4:F:30:MET:HE2	4:F:69:LYS:O	2.05	0.56
1:A:82:ARG:HH12	1:A:89:GLU:HB3	1.70	0.56
1:C:258:THR:HG23	1:C:260:HIS:HE1	1.71	0.55
4:H:130:GLU:O	4:H:134:THR:HG22	2.06	0.55
4:H:194:ALA:O	4:H:198:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:15:GLN:NE2	3:E:113:LYS:HB2	2.22	0.55
1:A:227:ASP:HB3	1:A:248:VAL:HG22	1.88	0.54
2:B:38:ASP:OD1	2:B:45:ARG:NH1	2.36	0.54
1:C:58:GLU:H	1:C:58:GLU:CD	2.14	0.54
4:F:176:GLN:O	4:F:176:GLN:HG3	2.06	0.54
4:H:195:THR:O	4:H:199:ASN:ND2	2.40	0.54
1:C:227:ASP:HB3	1:C:248:VAL:HG22	1.90	0.54
3:E:56:VAL:HG22	3:E:65:GLN:HG3	1.89	0.54
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.89	0.54
4:H:7:LYS:NZ	4:H:152:GLU:OE2	2.33	0.54
4:H:207:GLN:NE2	4:H:230:ILE:HD12	2.22	0.53
1:C:258:THR:HG23	1:C:260:HIS:CE1	2.44	0.53
3:G:98:ASN:O	5:I:4:GLY:HA3	2.09	0.53
4:H:128:GLU:O	4:H:132:SER:HB3	2.09	0.52
4:F:112:ASP:CG	4:F:114:LYS:HG2	2.35	0.52
3:E:14:ILE:O	3:E:112:VAL:HA	2.10	0.52
1:A:19:GLU:HG2	1:A:75:ARG:HH21	1.75	0.51
4:H:60:GLU:CD	4:H:60:GLU:H	2.17	0.51
4:H:135:GLN:H	4:H:135:GLN:CD	2.18	0.51
1:C:14:ARG:HH11	1:C:17:ARG:HH12	1.57	0.51
3:G:52:THR:OG1	3:G:55:GLU:HB2	2.10	0.51
4:H:13:GLU:HG2	4:H:111:GLU:HA	1.92	0.51
3:E:16:GLU:OE2	3:E:115:ASN:HB2	2.11	0.51
1:A:32:GLN:NE2	2:B:53:ASP:OD2	2.39	0.51
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.45	0.51
2:B:96:ASP:OD2	2:B:99:MET:HE2	2.11	0.51
4:H:195:THR:HG22	7:H:370:HOH:O	2.11	0.51
3:G:106:LYS:NZ	7:G:402:HOH:O	2.43	0.50
4:H:158:ASN:HD21	4:H:202:ASN:HA	1.75	0.50
4:H:200:PRO:HA	4:H:202:ASN:N	2.26	0.50
2:D:38:ASP:OD1	2:D:45:ARG:NH1	2.44	0.50
4:H:26:ASN:OD1	4:H:69:LYS:NZ	2.37	0.50
4:H:227:VAL:O	4:H:229:GLN:HG2	2.11	0.50
1:C:190:THR:HG21	2:D:99:MET:OXT	2.11	0.50
3:E:149:SER:OG	3:E:193:ASN:O	2.19	0.50
4:H:217:ASP:O	4:H:225:LYS:NZ	2.36	0.50
3:E:100:GLY:HA2	4:F:96:SER:HB2	1.93	0.50
4:H:23:GLN:HE22	4:H:27:HIS:H	1.59	0.50
4:H:131:ILE:HG23	4:H:194:ALA:HB1	1.94	0.49
3:G:152:LYS:H	3:G:193:ASN:HD22	1.61	0.49
3:E:101:LYS:HE3	7:F:305:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ARG:HD2	2:D:99:MET:OXT	2.12	0.49
4:H:130:GLU:CD	4:H:138:THR:H	2.19	0.49
1:A:219:ARG:HG3	1:A:257:TYR:HE1	1.78	0.49
1:C:151:HIS:CE1	3:G:51:VAL:HG21	2.48	0.49
1:C:217:TRP:CD1	1:C:247:VAL:HG13	2.48	0.49
3:G:152:LYS:H	3:G:193:ASN:ND2	2.10	0.49
1:A:151:HIS:ND1	3:E:51:VAL:HG11	2.28	0.49
3:G:82:PRO:HA	3:G:112:VAL:HB	1.95	0.49
1:A:190:THR:CG2	1:A:192:HIS:CE1	2.91	0.48
1:C:219:ARG:HG3	1:C:257:TYR:CZ	2.49	0.48
4:H:156:TRP:NE1	4:H:207:GLN:OE1	2.46	0.48
1:C:121:LYS:HG3	2:D:1:ILE:HG12	1.96	0.48
1:A:77:ASP:CG	5:J:9:LEU:HG	2.39	0.48
4:F:111:GLU:O	4:F:112:ASP:HB2	2.12	0.48
2:D:48:LYS:HB3	2:D:48:LYS:HE3	1.72	0.47
4:F:112:ASP:OD2	4:F:114:LYS:HG2	2.14	0.47
4:F:147:TYR:CZ	4:F:181:ASP:HB3	2.50	0.47
3:G:15:GLN:O	3:G:18:GLU:HG2	2.14	0.47
2:D:37:VAL:HG22	2:D:82:VAL:HG22	1.96	0.47
1:A:267:PRO:HB2	1:A:268:LYS:HG3	1.96	0.47
3:E:106:LYS:NZ	4:F:40:GLY:HA3	2.29	0.47
4:H:112:ASP:OD2	4:H:114:LYS:HB3	2.15	0.47
3:E:16:GLU:OE2	3:E:115:ASN:N	2.35	0.47
4:F:147:TYR:CD1	4:F:148:PRO:HA	2.50	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.46
1:C:219:ARG:HH11	1:C:256:ARG:NH2	2.13	0.46
3:E:163:VAL:HG22	3:E:174:ASN:OD1	2.15	0.46
3:E:15:GLN:HG2	3:E:113:LYS:HB2	1.98	0.46
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.50	0.46
4:F:195:THR:HG23	7:F:358:HOH:O	2.15	0.46
1:A:237:GLY:HA3	7:B:101:HOH:O	2.14	0.46
2:B:75:LYS:O	2:B:75:LYS:HG3	2.16	0.46
3:E:85:THR:HG22	3:E:112:VAL:N	2.16	0.46
1:A:74:HIS:NE2	1:A:97:ARG:HD2	2.31	0.45
1:C:51:TRP:O	1:C:54:GLN:HG2	2.15	0.45
4:H:50:VAL:HG22	4:H:69:LYS:HA	1.99	0.45
1:C:17:ARG:O	1:C:17:ARG:HG2	2.16	0.45
3:G:58:LYS:HB3	3:G:58:LYS:HE3	1.78	0.45
4:H:200:PRO:CB	4:H:201:ARG:HA	2.47	0.45
4:H:169:ASP:HB2	4:H:186:LEU:HD12	1.98	0.45
1:A:194:VAL:O	1:A:196:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:GLU:O	2:B:70:PHE:HD1	2.00	0.45
1:C:14:ARG:HD2	1:C:17:ARG:NH1	2.32	0.45
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.82	0.44
4:F:182:SER:N	7:F:303:HOH:O	2.46	0.44
1:A:204:TRP:HH2	2:B:99:MET:O	2.00	0.44
1:C:49:ALA:O	1:C:52:ILE:HG22	2.17	0.44
4:F:112:ASP:OD2	4:F:114:LYS:HD2	2.18	0.44
3:G:126:LEU:HG	4:H:126:PRO:HA	2.00	0.44
2:D:94:LYS:HG3	2:D:95:TRP:N	2.31	0.44
4:H:30:MET:HE2	4:H:69:LYS:O	2.17	0.44
4:H:126:PRO:HG3	4:H:137:ALA:HB1	1.99	0.44
1:A:201:LEU:O	1:A:246:ALA:HA	2.18	0.44
2:B:69:GLU:C	2:B:70:PHE:HD1	2.25	0.44
1:A:139:ALA:O	1:A:142:THR:HB	2.18	0.43
2:B:6:LYS:HB2	2:B:6:LYS:HE3	1.83	0.43
4:H:23:GLN:NE2	7:H:311:HOH:O	2.50	0.43
3:G:106:LYS:HA	3:G:106:LYS:HD3	1.69	0.43
3:G:175:SER:OG	4:H:189:ARG:HD3	2.17	0.43
1:A:61:ASP:HB3	1:A:65:ARG:NH1	2.34	0.43
1:A:199:ALA:HB3	1:A:249:VAL:HG22	2.00	0.43
3:E:114:PRO:O	3:E:144:SER:OG	2.37	0.43
3:G:128:ASP:C	3:G:130:LYS:N	2.76	0.43
1:A:19:GLU:CG	1:A:20:PRO:HD2	2.46	0.43
1:A:200:THR:HA	1:A:247:VAL:O	2.19	0.43
3:E:113:LYS:HB3	3:E:144:SER:HB3	2.01	0.43
3:G:128:ASP:O	3:G:130:LYS:N	2.51	0.43
1:A:109:PHE:CZ	1:A:161:GLU:HG2	2.54	0.42
1:A:176:LYS:HG3	1:A:180:GLN:OE1	2.19	0.42
2:B:96:ASP:C	2:B:98:ASP:H	2.27	0.42
3:G:30:PHE:CE2	3:G:33:LEU:HD12	2.54	0.42
1:A:6:ARG:HH22	1:A:102:ASP:CG	2.27	0.42
1:A:49:ALA:O	1:A:52:ILE:HG22	2.18	0.42
2:B:0:MET:HE1	2:B:32:PRO:HD3	2.01	0.42
2:B:54:LEU:HD11	2:B:62:PHE:CD1	2.54	0.42
3:G:169:MET:HB2	3:G:169:MET:HE3	1.71	0.42
4:H:220:THR:O	4:H:220:THR:OG1	2.35	0.42
1:C:42:SER:O	1:C:44:ARG:HG2	2.18	0.42
4:F:1:GLY:N	4:F:24:ASN:OD1	2.48	0.42
3:G:10:GLN:O	3:G:109:LYS:HD2	2.20	0.42
1:A:184:ALA:HB2	1:A:265:GLY:O	2.19	0.42
1:A:217:TRP:O	1:A:218:GLN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:TRP:CZ2	1:C:179:LEU:HD11	2.55	0.42
2:D:31:HIS:ND1	2:D:32:PRO:HA	2.35	0.42
3:G:14:ILE:HD11	3:G:112:VAL:HG22	2.02	0.42
4:H:118:PRO:HD3	4:H:226:PRO:HB3	2.02	0.42
1:C:258:THR:CG2	1:C:260:HIS:HE1	2.33	0.42
3:G:22:VAL:HG11	3:G:108:THR:HG21	2.01	0.42
4:H:85:ALA:HB3	4:H:87:TYR:CE1	2.55	0.42
3:G:120:ASP:OD2	4:H:133:HIS:CE1	2.71	0.42
1:A:219:ARG:HG2	1:A:256:ARG:NH1	2.35	0.41
1:C:190:THR:CG2	1:C:202:ARG:HB3	2.37	0.41
3:E:4:LEU:HD22	3:E:27:SER:HB3	2.02	0.41
3:G:44:PRO:HD2	4:H:101:PHE:CG	2.55	0.41
3:E:133:ASP:OD1	3:E:133:ASP:N	2.47	0.41
3:G:128:ASP:C	3:G:130:LYS:H	2.28	0.41
3:G:136:VAL:HG13	4:H:124:PHE:CE2	2.56	0.41
3:G:149:SER:HB3	3:G:194:SER:HB2	2.01	0.41
4:H:203:HIS:NE2	4:H:234:GLU:OE1	2.50	0.41
1:A:219:ARG:HG2	1:A:256:ARG:HH12	1.82	0.41
3:G:15:GLN:N	7:G:405:HOH:O	2.51	0.41
1:A:19:GLU:HG2	1:A:75:ARG:NH2	2.35	0.41
4:H:30:MET:HE2	4:H:66:ARG:NH2	2.35	0.41
1:C:146:LYS:HE2	7:I:106:HOH:O	2.20	0.41
3:E:15:GLN:CD	3:E:113:LYS:HB2	2.46	0.41
1:A:254:GLU:C	1:A:256:ARG:H	2.29	0.41
3:E:66:PHE:HD1	3:E:66:PHE:HA	1.75	0.40
3:E:84:ASP:O	3:E:88:TYR:OH	2.31	0.40
4:H:30:MET:CE	4:H:66:ARG:NE	2.84	0.40
1:A:222:GLU:HG3	1:A:223:ASP:N	2.27	0.40
4:F:86:PHE:HD1	4:F:106:ARG:HG2	1.86	0.40
3:G:113:LYS:HB3	3:G:144:SER:HB3	2.02	0.40
4:H:199:ASN:O	4:H:202:ASN:HB2	2.21	0.40
4:H:236:TRP:CD1	4:H:236:TRP:N	2.90	0.40
4:F:2:ILE:HG23	4:F:23:GLN:HB3	2.03	0.40
3:G:133:ASP:O	3:G:134:LYS:HB2	2.21	0.40
4:F:30:MET:HE3	4:F:66:ARG:NE	2.37	0.40
4:F:219:TRP:CB	4:F:225:LYS:HE2	2.52	0.40

All (3) 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:131:ARG:NH2	1:A:198:GLU:OE2[2_15511]	1.62	0.58
1:A:220:ASP:OD2	4:H:201:ARG:CB[2_16412]	1.62	0.58
1:A:220:ASP:OD2	4:H:201:ARG:CA[2_16412]	1.89	0.31

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	272/276 (99%)	251 (92%)	18 (7%)	3 (1%)	11	8
1	C	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	30	28
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	D	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	E	188/208 (90%)	179 (95%)	9 (5%)	0	100	100
3	G	189/208 (91%)	174 (92%)	15 (8%)	0	100	100
4	F	237/240 (99%)	230 (97%)	7 (3%)	0	100	100
4	H	235/240 (98%)	229 (97%)	6 (3%)	0	100	100
5	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1604/1666 (96%)	1530 (95%)	70 (4%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	C	195	SER
1	A	194	VAL
1	A	267	PRO

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	230/232 (99%)	219 (95%)	11 (5%)	23	23
1	C	231/232 (100%)	224 (97%)	7 (3%)	36	41
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	10
2	D	95/95 (100%)	89 (94%)	6 (6%)	16	14
3	E	166/184 (90%)	158 (95%)	8 (5%)	23	23
3	G	167/184 (91%)	160 (96%)	7 (4%)	26	28
4	F	210/211 (100%)	204 (97%)	6 (3%)	37	42
4	H	209/211 (99%)	199 (95%)	10 (5%)	23	23
5	I	7/7 (100%)	7 (100%)	0	100	100
5	J	7/7 (100%)	7 (100%)	0	100	100
All	All	1417/1458 (97%)	1355 (96%)	62 (4%)	25	26

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	82	ARG
1	A	88	SER
1	A	89	GLU
1	A	110	LEU
1	A	179	LEU
1	A	186	LYS
1	A	219	ARG
1	A	231	VAL
1	A	249	VAL
1	A	268	LYS
2	B	0	MET
2	B	1	ILE
2	B	16	GLU
2	B	49	VAL
2	B	69	GLU

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Mol	Chain	Res	Type
2	B	77	GLU
2	B	92	ILE
1	C	121	LYS
1	C	190	THR
1	C	195	SER
1	C	196	ASP
1	C	198	GLU
1	C	248	VAL
1	C	262	GLN
2	D	0	MET
2	D	4	THR
2	D	48	LYS
2	D	70	PHE
2	D	74	GLU
2	D	88	SER
3	E	6	GLU
3	E	8	SER
3	E	20	LEU
3	E	60	LYS
3	E	106	LYS
3	E	109	LYS
3	E	149	SER
3	E	164	LEU
4	F	2	ILE
4	F	3	THR
4	F	42	ARG
4	F	60	GLU
4	F	171	GLN
4	F	189	ARG
3	G	12	LEU
3	G	14	ILE
3	G	20	LEU
3	G	78	THR
3	G	134	LYS
3	G	136	VAL
3	G	172	LYS
4	H	54	GLN
4	H	96	SER
4	H	132	SER
4	H	134	THR
4	H	136	LYS
4	H	139	LEU

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Mol	Chain	Res	Type
4	H	201	ARG
4	H	220	THR
4	H	230	ILE
4	H	232	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	115	GLN
1	A	188	HIS
1	A	260	HIS
2	B	13	HIS
2	B	17	ASN
1	C	260	HIS
3	E	181	ASN
4	F	115	ASN
4	F	163	HIS
4	F	176	GLN
3	G	34	GLN
3	G	118	ASN
3	G	145	GLN
3	G	189	ASN
3	G	193	ASN
4	H	15	GLN
4	H	23	GLN
4	H	133	HIS
4	H	158	ASN
4	H	163	HIS
4	H	198	GLN
4	H	199	ASN
4	H	207	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	IMD	G	301	-	5,5,5	0.70	0	5,5,5	0.34	0
6	IMD	C	301	-	5,5,5	0.74	0	5,5,5	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IMD	G	301	-	-	-	0/1/1/1
6	IMD	C	301	-	-	-	0/1/1/1

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

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	274/276 (99%)	1.51	85 (31%) 1 1	31, 50, 76, 86	0
1	C	275/276 (99%)	0.48	13 (4%) 36 38	22, 36, 58, 76	0
2	B	100/100 (100%)	2.10	48 (48%) 0 0	40, 63, 76, 82	0
2	D	100/100 (100%)	0.85	5 (5%) 34 36	24, 45, 66, 74	0
3	E	190/208 (91%)	1.20	33 (17%) 4 4	30, 51, 72, 81	0
3	G	191/208 (91%)	1.44	55 (28%) 1 1	26, 51, 78, 88	0
4	F	239/240 (99%)	0.67	17 (7%) 22 23	26, 38, 61, 70	0
4	H	237/240 (98%)	1.01	46 (19%) 3 3	21, 39, 68, 83	0
5	I	9/9 (100%)	-0.07	0 100 100	24, 26, 28, 32	0
5	J	9/9 (100%)	0.40	0 100 100	31, 33, 36, 42	0
All	All	1624/1666 (97%)	1.08	302 (18%) 3 3	21, 44, 72, 88	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	200	PRO	6.4
2	B	79	ALA	6.3
2	B	70	PHE	6.0
4	H	201	ARG	5.8
1	A	197	HIS	5.6
2	D	1	ILE	5.5
4	H	204	PHE	5.2
4	H	237	GLY	5.2
1	A	220	ASP	5.1
1	A	256	ARG	5.1
2	B	49	VAL	5.0
4	H	236	TRP	4.8
2	D	0	MET	4.7

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Mol	Chain	Res	Type	RSRZ
4	H	197	TRP	4.7
3	G	184	ASP	4.7
1	A	249	VAL	4.6
2	B	0	MET	4.6
4	F	179	LEU	4.6
2	B	1	ILE	4.5
1	C	197	HIS	4.4
1	A	221	GLY	4.4
3	E	4	LEU	4.2
4	H	173	LEU	4.2
3	G	4	LEU	4.1
4	H	137	ALA	4.1
3	G	187	CYS	4.1
3	G	134	LYS	4.0
4	H	235	ALA	3.9
2	B	95	TRP	3.9
1	A	195	SER	3.8
1	A	247	VAL	3.8
1	A	248	VAL	3.8
3	G	171	PHE	3.8
3	G	188	ALA	3.8
2	B	37	VAL	3.8
1	A	274	TRP	3.8
1	A	257	TYR	3.8
1	A	193	ALA	3.8
1	A	190	THR	3.8
2	B	46	ILE	3.7
3	G	17	GLY	3.7
2	B	78	TYR	3.7
4	H	131	ILE	3.7
1	A	139	ALA	3.7
4	H	195	THR	3.7
1	A	204	TRP	3.7
4	H	129	ALA	3.7
1	A	270	LEU	3.6
3	G	137	CYS	3.6
2	B	23	LEU	3.6
4	H	203	HIS	3.6
4	H	124	PHE	3.5
1	A	84	TYR	3.5
2	B	73	THR	3.5
3	G	178	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	G	173	SER	3.5
1	A	138	MET	3.5
4	H	194	ALA	3.5
1	A	83	GLY	3.4
1	A	272	LEU	3.4
3	E	164	LEU	3.4
2	B	17	ASN	3.4
3	G	116	ILE	3.4
1	A	217	TRP	3.4
2	B	15	ALA	3.4
3	G	122	ALA	3.4
4	H	198	GLN	3.4
4	H	199	ASN	3.4
1	A	182	THR	3.4
3	G	124	TYR	3.4
1	A	227	ASP	3.4
1	A	194	VAL	3.3
4	H	192	VAL	3.3
4	F	176	GLN	3.3
3	G	172	LYS	3.3
3	G	186	ALA	3.3
1	A	215	LEU	3.3
1	A	255	GLN	3.3
3	G	153	ASP	3.3
3	E	78	THR	3.2
4	H	123	VAL	3.2
4	H	132	SER	3.2
4	H	34	ARG	3.2
1	A	206	LEU	3.2
1	A	213	ILE	3.2
2	B	40	LEU	3.2
3	E	17	GLY	3.2
3	G	112	VAL	3.1
3	G	123	VAL	3.1
2	B	39	LEU	3.1
3	E	132	SER	3.1
1	A	178	THR	3.1
1	A	224	GLN	3.1
2	B	35	ILE	3.1
3	E	183	SER	3.1
3	E	187	CYS	3.1
3	E	79	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	99	MET	3.1
4	H	135	GLN	3.1
2	B	67	TYR	3.0
1	A	228	THR	3.0
3	G	164	LEU	3.0
3	E	193	ASN	3.0
1	A	201	LEU	3.0
3	E	148	VAL	3.0
3	G	148	VAL	3.0
4	H	185	SER	3.0
3	G	181	ASN	3.0
3	G	166	MET	3.0
3	G	190	ALA	3.0
3	E	15	GLN	2.9
1	A	246	ALA	2.9
4	H	193	SER	2.9
3	G	138	LEU	2.9
4	H	157	VAL	2.9
1	C	260	HIS	2.9
1	A	108	ARG	2.9
1	C	113	TYR	2.9
4	F	178	ALA	2.9
4	H	202	ASN	2.9
3	G	163	VAL	2.9
4	H	220	THR	2.9
4	F	239	ALA	2.9
4	F	112	ASP	2.9
3	E	168	SER	2.9
2	D	79	ALA	2.9
2	B	18	GLY	2.9
4	H	196	PHE	2.8
3	E	80	ALA	2.8
3	G	84	ASP	2.8
1	A	266	LEU	2.8
4	H	139	LEU	2.8
1	A	177	GLU	2.8
1	C	194	VAL	2.8
1	A	86	ASN	2.8
1	A	88	SER	2.8
3	G	136	VAL	2.8
2	B	33	SER	2.8
3	G	169	MET	2.8

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Mol	Chain	Res	Type	RSRZ
3	G	140	THR	2.8
2	B	92	ILE	2.8
2	B	98	ASP	2.7
2	B	66	TYR	2.7
3	G	126	LEU	2.7
1	C	258	THR	2.7
1	A	181	ARG	2.7
2	B	9	VAL	2.7
1	A	51	TRP	2.7
3	G	162	CYS	2.7
3	E	186	ALA	2.7
1	A	89	GLU	2.7
3	G	121	PRO	2.7
1	A	251	SER	2.7
4	F	181	ASP	2.7
4	F	222	ASP	2.7
3	G	127	ARG	2.7
1	A	264	GLU	2.6
3	G	185	PHE	2.6
4	H	138	THR	2.6
3	E	184	ASP	2.6
3	G	129	SER	2.6
1	A	203	CYS	2.6
4	F	167	CYS	2.6
4	H	134	THR	2.6
3	G	191	PHE	2.6
1	A	113	TYR	2.6
1	A	273	ARG	2.6
3	E	116	ILE	2.6
4	F	215	GLU	2.6
4	H	216	ASN	2.6
1	C	271	THR	2.6
3	G	180	SER	2.6
1	A	231	VAL	2.6
2	B	85	VAL	2.6
1	C	16	GLY	2.6
3	G	174	ASN	2.6
1	A	85	TYR	2.5
1	A	205	ALA	2.5
4	F	177	PRO	2.5
1	A	191	HIS	2.5
1	C	272	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	9	LEU	2.5
1	A	252	GLY	2.5
2	D	34	ASP	2.5
4	H	127	SER	2.5
3	G	11	PHE	2.5
1	A	91	GLY	2.5
2	B	10	TYR	2.4
4	H	126	PRO	2.4
2	B	19	LYS	2.4
3	G	182	LYS	2.4
2	B	21	ASN	2.4
4	F	216	ASN	2.4
1	A	267	PRO	2.4
1	A	90	ALA	2.4
3	E	167	ARG	2.4
2	B	22	PHE	2.4
2	B	74	GLU	2.4
3	G	120	ASP	2.4
4	H	181	ASP	2.4
3	G	183	SER	2.4
2	B	72	PRO	2.4
3	G	12	LEU	2.4
1	A	226	GLN	2.4
3	G	133	ASP	2.4
1	A	241	PHE	2.4
3	G	142	PHE	2.4
1	A	261	VAL	2.4
3	G	131	SER	2.4
1	C	269	PRO	2.4
4	F	200	PRO	2.4
1	C	193	ALA	2.3
3	G	80	ALA	2.3
4	H	111	GLU	2.3
1	A	175	GLY	2.3
3	E	133	ASP	2.3
2	B	62	PHE	2.3
3	E	169	MET	2.3
3	E	14	ILE	2.3
3	G	119	PRO	2.3
2	B	80	CYS	2.3
4	H	156	TRP	2.3
4	H	219	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	2.3
1	A	209	TYR	2.3
2	B	64	LEU	2.3
1	A	223	ASP	2.3
3	G	168	SER	2.3
2	B	47	GLU	2.3
4	H	140	VAL	2.3
1	C	226	GLN	2.3
3	E	85	THR	2.3
1	A	107	TRP	2.3
2	B	45	ARG	2.3
2	B	65	LEU	2.3
1	A	192	HIS	2.3
1	A	15	PRO	2.3
2	B	86	THR	2.3
2	B	34	ASP	2.3
1	A	1	GLY	2.3
3	E	5	LEU	2.3
1	A	244	TRP	2.3
3	E	131	SER	2.2
3	G	65	GLN	2.2
3	G	135	SER	2.2
3	G	139	PHE	2.2
4	F	220	THR	2.2
1	A	196	ASP	2.2
4	H	233	ALA	2.2
2	B	68	THR	2.2
4	F	180	ASN	2.2
1	C	248	VAL	2.2
3	E	163	VAL	2.2
4	H	114	LYS	2.2
4	H	136	LYS	2.2
1	A	82	ARG	2.2
1	A	219	ARG	2.2
4	H	189	ARG	2.2
3	E	77	ILE	2.2
3	E	185	PHE	2.2
1	A	218	GLN	2.2
1	C	270	LEU	2.2
2	B	87	LEU	2.2
3	E	20	LEU	2.2
2	B	82	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	22	VAL	2.1
4	F	221	GLN	2.1
4	H	158	ASN	2.1
1	A	50	PRO	2.1
1	A	185	PRO	2.1
1	A	187	THR	2.1
3	E	114	PRO	2.1
4	H	155	TRP	2.1
1	A	33	PHE	2.1
3	E	112	VAL	2.1
1	A	189	MET	2.1
3	G	165	ASP	2.1
1	A	271	THR	2.1
3	G	10	GLN	2.1
1	A	188	HIS	2.1
3	E	188	ALA	2.1
2	B	76	ASP	2.1
4	H	221	GLN	2.1
1	A	131	ARG	2.1
1	A	269	PRO	2.1
2	B	3	ARG	2.1
1	A	236	ALA	2.1
1	A	245	ALA	2.1
1	A	81	LEU	2.0
1	A	110	LEU	2.0
3	G	147	ASN	2.0
2	B	25	CYS	2.0
4	F	217	ASP	2.0
2	B	48	LYS	2.0
3	E	83	GLY	2.0
2	D	99	MET	2.0
1	A	87	GLN	2.0
1	A	179	LEU	2.0
2	B	51	HIS	2.0
3	E	182	LYS	2.0
1	A	20	PRO	2.0
2	B	71	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IMD	C	301	5/5	0.72	0.16	42,42,48,52	0
6	IMD	G	301	5/5	0.93	0.15	37,39,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.