



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:57 PM UTC

PDB ID : 5C0A / pdb_00005c0a
Title : 1E6 TCR in complex with HLA-A02 carrying MVW peptide
Authors : Rizkallah, P.J.; Bulek, A.M.; Cole, D.K.; Sewell, A.K.
Deposited on : 2015-06-12
Resolution : 2.46 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

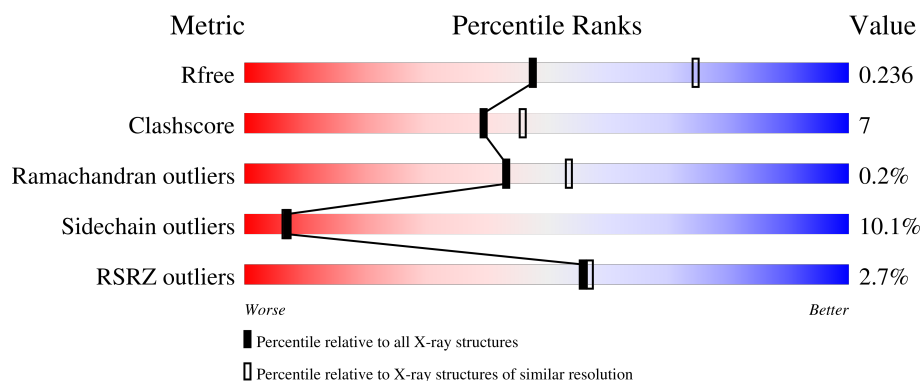
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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.



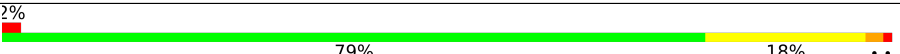
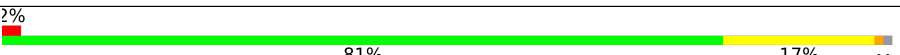
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	79% 17% .
1	F	276	84% 14% .
2	B	100	84% 13% .
2	G	100	88% 11% .
3	C	10	60% 40%

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Mol	Chain	Length	Quality of chain
3	H	10	 70% 30%
4	D	197	 6% 81% 15% •
4	I	197	 8% 75% 19% 6% •
5	E	246	 2% 79% 18% ••
5	J	246	 2% 81% 17% ••

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	EDO	A	302	-	-	X	-
6	EDO	J	303	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13708 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	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	F	276	Total	C	N	O	S	0	2	0
			2273	1419	415	430	9			

- 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
			837	533	141	159	4			
2	G	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
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Marker peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			83	57	11	14	1			
3	H	10	Total	C	N	O	S	0	0	0
			83	57	11	14	1			

- Molecule 4 is a protein called 1E6 TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1557	975	256	316	10			

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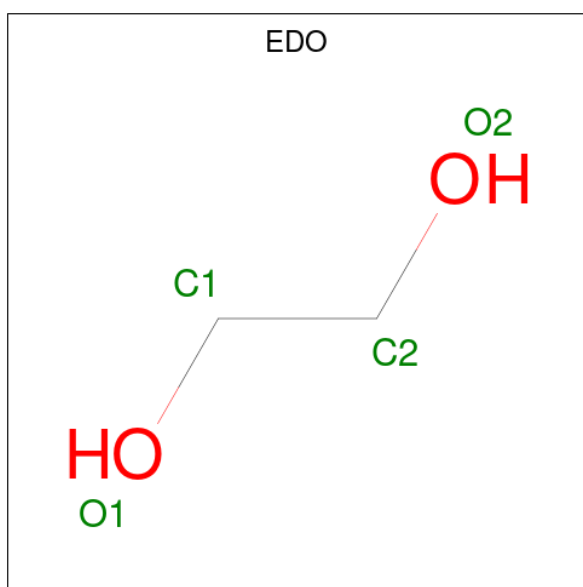
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	197	Total	C	N	O	S	0	0	0
			1557	975	256	316	10			

- Molecule 5 is a protein called 1E6 TCR Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1974	1249	341	374	10			
5	J	244	Total	C	N	O	S	0	0	0
			1961	1242	339	370	10			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



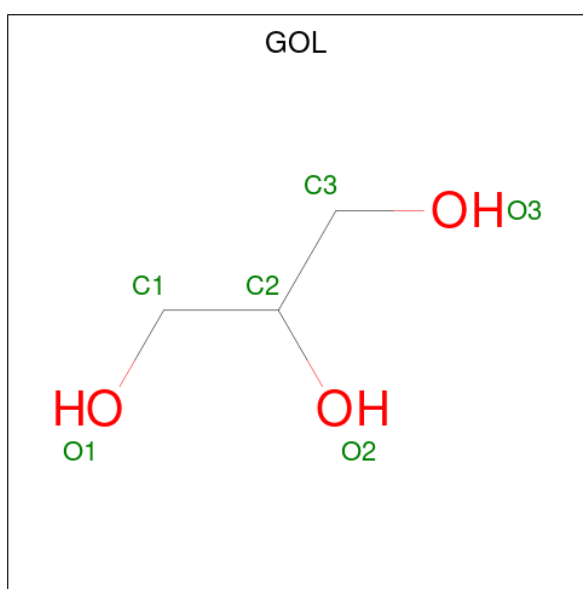
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	G	1	Total	C	O	0	0
			6	3	3		
8	J	1	Total	C	O	0	0
			6	3	3		

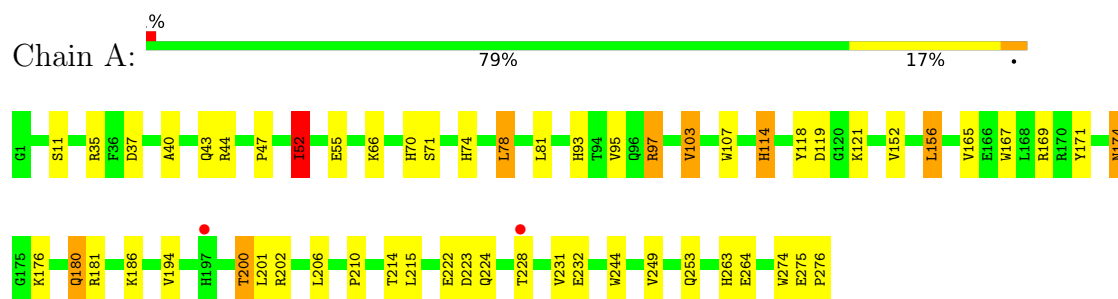
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	18	Total 18	O 18	0	0
9	B	6	Total 6	O 6	0	0
9	C	4	Total 4	O 4	0	0
9	D	8	Total 8	O 8	0	0
9	E	32	Total 32	O 32	0	0
9	F	48	Total 48	O 48	0	0
9	G	12	Total 12	O 12	0	0
9	H	8	Total 8	O 8	0	0
9	I	16	Total 16	O 16	0	0
9	J	18	Total 18	O 18	0	0

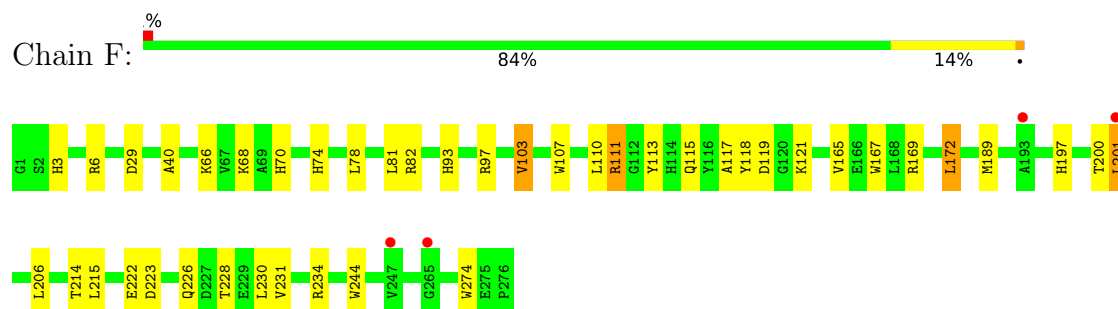
3 Residue-property plots

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

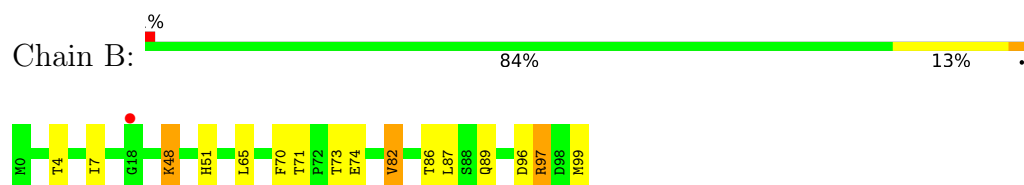
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



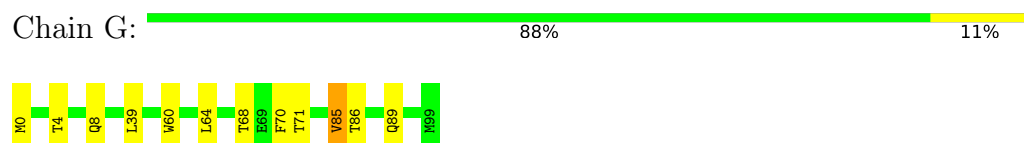
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin

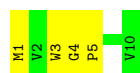


- Molecule 2: Beta-2-microglobulin



- Molecule 3: Marker peptide

Chain C:  60% 40%



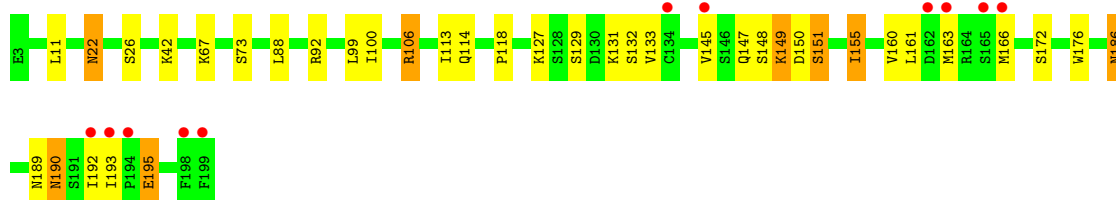
- Molecule 3: Marker peptide

Chain H:  70% 30%



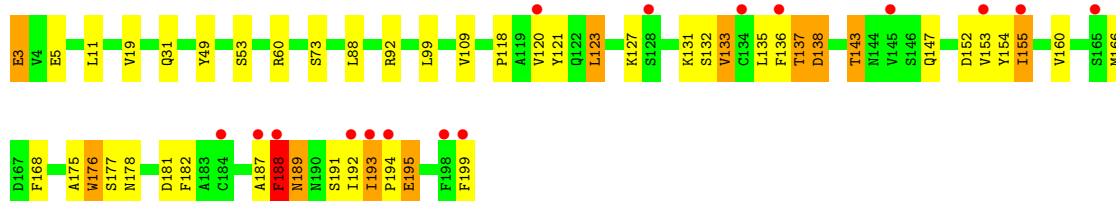
- Molecule 4: 1E6 TCR Alpha Chain

Chain D:  6% 81% 15%



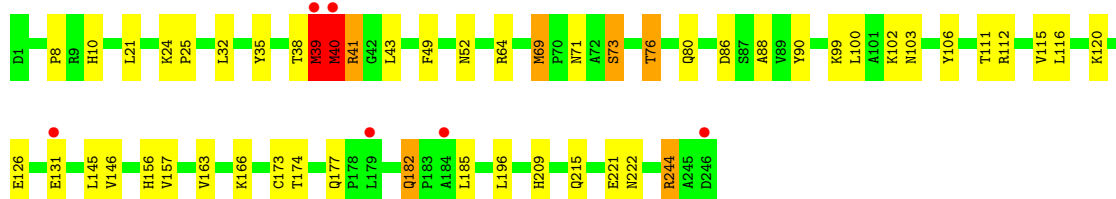
- Molecule 4: 1E6 TCR Alpha Chain

Chain I:  8% 75% 19% 6%



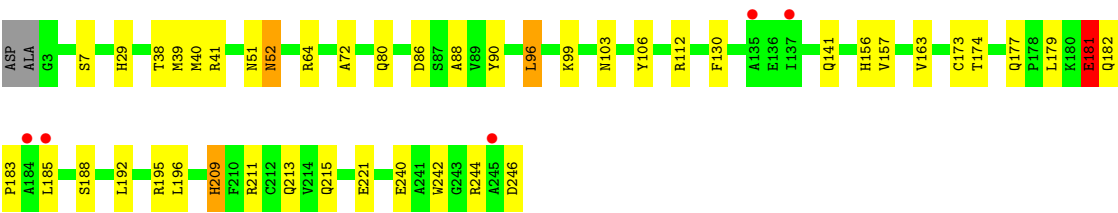
- Molecule 5: 1E6 TCR Beta Chain

Chain E:  2% 79% 18%



- Molecule 5: 1E6 TCR Beta Chain

Chain J:  2% 81% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.88Å 100.02Å 123.28Å 96.67° 98.58° 95.80°	Depositor
Resolution (Å)	31.24 – 2.46 31.24 – 2.46	Depositor EDS
% Data completeness (in resolution range)	97.7 (31.24-2.46) 97.7 (31.24-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.193 , 0.232 0.196 , 0.236	Depositor DCC
R_{free} test set	3655 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13708	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: EDO, 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	0.87	1/2320 (0.0%)	0.98	5/3149 (0.2%)
1	F	0.94	0/2340	0.97	0/3176
2	B	0.87	0/860	0.99	1/1162 (0.1%)
2	G	0.92	0/860	0.99	2/1162 (0.2%)
3	C	1.09	0/87	1.13	0/119
3	H	1.08	0/87	1.17	0/119
4	D	0.89	0/1592	1.02	3/2154 (0.1%)
4	I	0.90	0/1592	1.06	7/2154 (0.3%)
5	E	1.01	1/2029 (0.0%)	1.03	5/2759 (0.2%)
5	J	0.91	0/2016	1.01	2/2741 (0.1%)
All	All	0.92	2/13783 (0.0%)	1.01	25/18695 (0.1%)

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
4	I	0	5
5	E	0	2
5	J	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	76	THR	N-CA	-5.18	1.39	1.46
1	A	114	HIS	N-CA	-5.11	1.40	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	41	ARG	N-CA-C	8.89	123.39	112.54
2	G	85	VAL	CB-CA-C	-8.44	100.98	112.04
5	J	181	GLU	N-CA-C	-7.53	98.52	109.59
4	I	189	ASN	N-CA-C	7.06	119.61	108.67
1	A	97	ARG	NE-CZ-NH2	6.76	125.28	119.20
2	G	85	VAL	N-CA-CB	6.54	118.64	110.47
2	B	48	LYS	CB-CA-C	6.19	120.15	111.86
5	J	209	HIS	CB-CA-C	6.11	120.30	110.16
5	E	40	MET	N-CA-C	-5.84	100.75	109.15
5	E	173	CYS	CA-CB-SG	5.83	127.81	114.40
4	D	190	ASN	N-CA-C	5.81	117.83	110.33
4	D	151	SER	N-CA-C	-5.78	106.17	113.23
5	E	76	THR	N-CA-CB	-5.73	100.63	111.00
4	I	160	VAL	N-CA-C	5.59	116.00	108.17
4	I	60	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	174	ASN	N-CA-C	-5.43	101.81	109.96
1	A	52	ILE	N-CA-CB	5.42	120.32	112.07
1	A	97	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	A	249	VAL	N-CA-CB	-5.40	105.87	111.64
5	E	209	HIS	CB-CA-C	5.32	119.44	109.71
4	I	137	THR	N-CA-C	-5.30	101.42	108.74
4	D	160	VAL	N-CA-C	5.11	115.20	107.80
4	I	137	THR	CA-C-O	-5.02	116.03	121.36
4	I	137	THR	CA-C-N	5.01	129.48	122.41
4	I	137	THR	C-N-CA	5.01	129.48	122.41

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	39	MET	Peptide
5	E	40	MET	Peptide
4	I	137	THR	Peptide
4	I	152	ASP	Peptide
4	I	176	TRP	Peptide
4	I	181	ASP	Peptide
4	I	188	PHE	Peptide
5	J	181	GLU	Peptide

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	2254	0	2103	41	0
1	F	2273	0	2116	32	0
2	B	837	0	803	7	0
2	G	837	0	803	10	0
3	C	83	0	80	3	0
3	H	83	0	80	3	0
4	D	1557	0	1469	23	0
4	I	1557	0	1469	17	0
5	E	1974	0	1887	30	0
5	J	1961	0	1875	24	0
6	A	8	0	12	9	0
6	D	8	0	12	1	0
6	E	4	0	6	2	0
6	F	12	0	18	2	0
6	H	8	0	12	2	0
6	I	4	0	6	0	0
6	J	8	0	12	6	0
7	A	5	0	0	0	0
7	D	5	0	0	1	0
7	E	15	0	0	0	0
7	F	5	0	0	0	0
7	G	5	0	0	0	0
7	J	5	0	0	0	0
8	B	6	0	8	0	0
8	F	12	0	16	2	0
8	G	6	0	8	0	0
8	J	6	0	8	1	0
9	A	18	0	0	0	0
9	B	6	0	0	0	0
9	C	4	0	0	0	0
9	D	8	0	0	0	0
9	E	32	0	0	0	0
9	F	48	0	0	2	0
9	G	12	0	0	0	0
9	H	8	0	0	0	0
9	I	16	0	0	0	0
9	J	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13708	0	12803	176	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 7.

All (176) 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:40:ALA:HB3	6:A:302:EDO:H11	1.53	0.90
1:A:40:ALA:HB3	6:A:302:EDO:C1	2.03	0.88
1:F:189:MET:HE3	1:F:201:LEU:HG	1.63	0.79
3:H:5:PRO:HD2	6:H:102:EDO:H11	1.67	0.77
1:A:78:LEU:HD13	1:A:95:VAL:HG13	1.66	0.76
4:D:150:ASP:O	4:D:151:SER:OG	2.03	0.74
4:I:133:VAL:HG12	4:I:176:TRP:HB3	1.68	0.73
1:A:74:HIS:HE1	1:A:97:ARG:HH21	1.38	0.72
1:A:103:VAL:HG13	1:A:107:TRP:HA	1.72	0.71
1:F:82:ARG:HB2	8:F:302:GOL:H12	1.70	0.71
5:E:71:ASN:HD22	5:E:73:SER:H	1.39	0.71
1:F:103:VAL:HG13	1:F:107:TRP:HA	1.73	0.71
5:J:211:ARG:HH12	5:J:213:GLN:HE21	1.39	0.69
4:D:106:ARG:HH11	4:D:106:ARG:HG3	1.58	0.69
1:F:189:MET:CE	1:F:201:LEU:HG	2.21	0.69
4:I:123:LEU:HD12	4:I:133:VAL:O	1.91	0.69
1:A:107:TRP:O	1:A:169:ARG:NH1	2.26	0.69
5:J:181:GLU:O	5:J:188:SER:HB2	1.93	0.69
8:J:301:GOL:HO1	8:J:301:GOL:HO3	1.08	0.69
1:A:167:TRP:CZ2	3:C:1:MET:HE3	2.28	0.68
5:E:25:PRO:O	6:E:301:EDO:H12	1.95	0.67
4:I:3:GLU:OE1	4:I:3:GLU:HA	1.94	0.67
4:I:138:ASP:N	4:I:138:ASP:OD1	2.28	0.66
5:E:49:PHE:HB2	5:E:69:MET:HE1	1.77	0.66
1:F:167:TRP:CZ2	3:H:1:MET:HE3	2.30	0.66
5:J:64:ARG:NH1	5:J:86:ASP:OD2	2.29	0.65
1:A:275:GLU:HG3	1:A:276:PRO:HD3	1.79	0.65
5:E:49:PHE:CG	5:E:69:MET:CE	2.80	0.65
1:A:275:GLU:CG	1:A:276:PRO:HD3	2.28	0.64
5:E:64:ARG:NH2	5:E:86:ASP:OD2	2.31	0.64
1:A:40:ALA:HB3	6:A:302:EDO:H12	1.78	0.64
1:A:165:VAL:CG1	1:A:169:ARG:NH2	2.61	0.63
1:A:43:GLN:HA	6:A:302:EDO:O1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:HIS:HD2	1:F:29:ASP:OD2	1.81	0.62
5:E:35:TYR:HB3	5:E:43:LEU:HD22	1.82	0.62
2:G:4:THR:HG22	2:G:86:THR:CB	2.31	0.61
5:E:49:PHE:CB	5:E:69:MET:CE	2.78	0.61
1:A:37:ASP:O	6:A:302:EDO:H11	1.99	0.61
1:F:40:ALA:HB3	6:F:303:EDO:H12	1.83	0.61
5:J:51:ASN:HA	6:J:303:EDO:H11	1.83	0.61
5:E:49:PHE:CB	5:E:69:MET:HE3	2.32	0.60
1:A:171:TYR:O	1:A:174:ASN:O	2.20	0.60
5:J:188:SER:O	5:J:188:SER:OG	2.15	0.59
2:B:4:THR:HG22	2:B:86:THR:CB	2.32	0.59
1:A:74:HIS:CE1	1:A:97:ARG:HH21	2.20	0.59
4:D:149:LYS:HG3	4:D:150:ASP:O	2.02	0.59
4:D:186:ASN:HD22	4:D:186:ASN:C	2.11	0.59
1:A:165:VAL:HG12	1:A:169:ARG:NH2	2.19	0.57
2:B:73:THR:HG22	2:B:74:GLU:N	2.20	0.57
4:D:92:ARG:HE	5:E:103:ASN:HD21	1.52	0.57
5:E:49:PHE:CG	5:E:69:MET:HE3	2.40	0.57
1:F:6:ARG:NH2	1:F:113:TYR:OH	2.35	0.56
1:F:115[B]:GLN:HG3	2:G:60:TRP:CZ2	2.40	0.56
5:E:49:PHE:HB2	5:E:69:MET:CE	2.35	0.56
4:D:149:LYS:HE3	4:D:149:LYS:HA	1.87	0.56
1:F:74:HIS:HE1	1:F:97:ARG:HE	1.52	0.56
1:A:78:LEU:CD1	1:A:95:VAL:HG13	2.35	0.55
2:B:96:ASP:HB3	2:B:99:MET:HA	1.89	0.55
1:F:115[B]:GLN:CG	2:G:60:TRP:CZ2	2.91	0.54
1:A:43:GLN:N	6:A:302:EDO:O1	2.40	0.54
1:A:47:PRO:HB3	1:A:52:ILE:HD13	1.89	0.54
1:F:93:HIS:HE1	9:F:405:HOH:O	1.91	0.54
2:B:4:THR:HG22	2:B:86:THR:HB	1.89	0.54
2:G:4:THR:HG22	2:G:86:THR:HB	1.89	0.53
1:A:47:PRO:CB	1:A:52:ILE:CD1	2.86	0.53
1:F:115[B]:GLN:CG	2:G:60:TRP:HZ2	2.21	0.53
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.92	0.52
5:J:72:ALA:HB2	6:J:303:EDO:H12	1.90	0.52
5:J:29:HIS:HA	5:J:96:LEU:HD13	1.90	0.52
1:A:71:SER:HB2	6:A:301:EDO:H22	1.92	0.52
5:E:39:MET:N	5:E:39:MET:SD	2.83	0.51
1:A:253:GLN:N	1:A:253:GLN:OE1	2.43	0.51
1:F:234:ARG:HH11	2:G:8:GLN:NE2	2.08	0.51
4:D:147:GLN:CD	4:D:149:LYS:HB2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PRO:O	1:A:263:HIS:HE1	1.94	0.51
5:E:24:LYS:HE3	6:E:301:EDO:H11	1.92	0.50
1:F:40:ALA:HB3	6:F:303:EDO:C1	2.40	0.50
1:F:231:VAL:CG1	1:F:244:TRP:CZ2	2.95	0.50
1:A:11:SER:HB2	1:A:95:VAL:HG22	1.93	0.50
5:E:32:LEU:HB3	5:E:69:MET:HE1	1.93	0.50
1:A:66:LYS:O	1:A:70:HIS:HD2	1.95	0.49
4:D:147:GLN:HB3	4:D:155:ILE:HG12	1.94	0.49
5:E:38:THR:O	5:E:40:MET:O	2.30	0.49
1:F:66:LYS:O	1:F:70:HIS:HD2	1.96	0.49
5:J:240:GLU:OE1	5:J:242:TRP:CZ3	2.65	0.49
4:D:106:ARG:HH11	4:D:106:ARG:CG	2.24	0.49
4:D:133:VAL:HG23	4:D:176:TRP:HB3	1.94	0.49
5:E:10:HIS:HD2	5:E:156:HIS:ND1	2.11	0.49
1:A:97:ARG:HE	1:A:114:HIS:CE1	2.30	0.49
1:A:43:GLN:CA	6:A:302:EDO:O1	2.61	0.48
5:E:131:GLU:OE1	5:E:244:ARG:NH1	2.46	0.48
5:J:52:ASN:OD1	6:J:303:EDO:H22	2.13	0.48
4:I:187:ALA:O	4:I:189:ASN:N	2.45	0.48
5:E:88:ALA:HB3	5:E:90:TYR:CE1	2.48	0.48
1:F:93:HIS:HD2	1:F:119:ASP:OD2	1.97	0.48
1:F:189:MET:HE2	1:F:274:TRP:HB2	1.95	0.48
1:F:68:LYS:NZ	9:F:403:HOH:O	2.41	0.47
4:D:113:ILE:HG23	4:D:113:ILE:O	2.14	0.47
1:A:274:TRP:CE2	1:A:276:PRO:HD2	2.50	0.47
1:A:232:GLU:OE1	1:A:232:GLU:N	2.45	0.47
1:F:165:VAL:CG1	1:F:169:ARG:NH2	2.78	0.47
1:A:44:ARG:O	6:A:302:EDO:H21	2.13	0.47
5:E:64:ARG:HH22	5:E:86:ASP:CG	2.23	0.47
4:I:118:PRO:HB2	4:I:195:GLU:HB3	1.97	0.47
5:J:51:ASN:HA	6:J:303:EDO:C1	2.45	0.46
4:I:92:ARG:HE	5:J:103:ASN:HD21	1.64	0.46
4:D:147:GLN:OE1	4:D:148:SER:N	2.48	0.46
1:A:194:VAL:HG13	1:A:200:THR:OG1	2.15	0.46
4:D:22:ASN:C	4:D:22:ASN:HD22	2.24	0.46
5:E:112:ARG:HG2	5:E:156:HIS:CE1	2.50	0.46
5:E:157:VAL:HA	5:E:215:GLN:O	2.16	0.46
5:J:64:ARG:HH12	5:J:86:ASP:CG	2.23	0.46
5:J:99:LYS:HE3	5:J:106:TYR:OH	2.15	0.46
4:D:147:GLN:OE1	4:D:149:LYS:HB2	2.16	0.46
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:153:VAL:HA	4:I:176:TRP:O	2.15	0.46
5:J:88:ALA:HB3	5:J:90:TYR:CE1	2.51	0.46
5:E:69:MET:HE2	5:E:69:MET:HB2	1.76	0.45
5:E:49:PHE:CD2	5:E:69:MET:CE	2.99	0.45
3:C:4:GLY:HA2	3:C:5:PRO:C	2.41	0.45
4:I:133:VAL:HG22	5:J:130:PHE:CD2	2.52	0.45
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.52	0.45
5:E:99:LYS:HE3	5:E:106:TYR:OH	2.17	0.45
4:I:193:ILE:HB	4:I:194:PRO:HD3	1.98	0.45
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.52	0.44
1:F:115[B]:GLN:HG3	2:G:60:TRP:CH2	2.52	0.44
5:E:182:GLN:HG3	5:E:185:LEU:HD12	1.99	0.44
5:J:182:GLN:C	5:J:182:GLN:HE21	2.24	0.44
2:B:73:THR:CG2	2:B:74:GLU:N	2.81	0.44
1:A:47:PRO:CB	1:A:52:ILE:HD13	2.46	0.44
5:J:157:VAL:HA	5:J:215:GLN:O	2.18	0.44
2:B:7:ILE:HD13	2:B:82:VAL:CG1	2.48	0.44
4:D:147:GLN:OE1	4:D:149:LYS:N	2.50	0.44
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.53	0.43
1:F:231:VAL:HG11	1:F:244:TRP:CZ2	2.53	0.43
5:J:182:GLN:O	5:J:182:GLN:HG3	2.18	0.43
6:D:201:EDO:HO2	5:E:103:ASN:HD22	1.62	0.43
2:B:51:HIS:HA	2:B:65:LEU:O	2.19	0.43
4:D:11:LEU:HD22	7:D:203:SO4:O1	2.19	0.43
5:J:112:ARG:HG2	5:J:156:HIS:CE1	2.53	0.43
1:F:110:LEU:HD13	1:F:111:ARG:NH2	2.34	0.43
5:J:51:ASN:HA	6:J:303:EDO:C2	2.49	0.43
1:A:180:GLN:HE21	1:A:180:GLN:HB3	1.68	0.42
1:F:107:TRP:CH2	1:F:172:LEU:HB3	2.54	0.42
4:I:123:LEU:CD1	4:I:133:VAL:HG23	2.49	0.42
5:J:72:ALA:CB	6:J:303:EDO:H12	2.49	0.42
1:F:74:HIS:CE1	1:F:97:ARG:HE	2.36	0.42
1:F:82:ARG:HB2	8:F:302:GOL:C1	2.44	0.42
5:E:49:PHE:CD2	5:E:69:MET:HE2	2.55	0.42
2:G:39:LEU:HD23	2:G:68:THR:HG22	2.02	0.42
1:A:47:PRO:HB3	1:A:52:ILE:CD1	2.49	0.42
1:A:156:LEU:HD13	3:C:3:TRP:CZ2	2.55	0.42
1:F:231:VAL:HG13	1:F:244:TRP:CZ2	2.55	0.42
1:A:176:LYS:HA	1:A:180:GLN:HG3	2.01	0.42
5:J:211:ARG:HH12	5:J:213:GLN:NE2	2.13	0.41
1:A:186:LYS:N	1:A:186:LYS:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:O	1:A:223:ASP:C	2.63	0.41
1:F:115[B]:GLN:HG3	2:G:60:TRP:HZ2	1.83	0.41
4:I:154:TYR:O	4:I:175:ALA:HA	2.20	0.41
4:I:155:ILE:HD12	4:I:155:ILE:O	2.21	0.41
4:D:163:MET:O	4:D:166:MET:O	2.38	0.41
5:E:8:PRO:O	5:E:111:THR:HG23	2.21	0.41
4:D:92:ARG:NE	5:E:103:ASN:HD21	2.17	0.41
4:D:145:VAL:HG13	4:D:190:ASN:ND2	2.36	0.41
1:F:222:GLU:O	1:F:223:ASP:C	2.63	0.41
4:I:123:LEU:HD12	4:I:133:VAL:HG23	2.03	0.41
4:D:118:PRO:HB2	4:D:195:GLU:HB3	2.03	0.41
4:I:166:MET:HG3	4:I:168:PHE:HB2	2.02	0.41
4:D:155:ILE:C	4:D:155:ILE:HD12	2.46	0.41
4:I:143:THR:HG22	4:I:192:ILE:HD11	2.03	0.41
4:D:186:ASN:C	4:D:186:ASN:ND2	2.78	0.40
3:H:9:TYR:CZ	6:H:101:EDO:H22	2.56	0.40
5:J:181:GLU:O	5:J:183:PRO:HD2	2.21	0.40
4:D:92:ARG:HE	5:E:103:ASN:ND2	2.17	0.40
4:I:188:PHE:HB3	4:I:189:ASN:ND2	2.36	0.40
5:J:240:GLU:OE1	5:J:242:TRP:CH2	2.75	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	274/276 (99%)	267 (97%)	7 (3%)	0	100	100
1	F	276/276 (100%)	270 (98%)	6 (2%)	0	100	100
2	B	98/100 (98%)	97 (99%)	0	1 (1%)	12	14
2	G	98/100 (98%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	H	8/10 (80%)	8 (100%)	0	0	100	100
4	D	195/197 (99%)	181 (93%)	14 (7%)	0	100	100
4	I	195/197 (99%)	174 (89%)	20 (10%)	1 (0%)	24	32
5	E	244/246 (99%)	235 (96%)	9 (4%)	0	100	100
5	J	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	37
All	All	1638/1658 (99%)	1567 (96%)	68 (4%)	3 (0%)	43	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	188	PHE
2	B	97	ARG
5	J	39	MET

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	232/232 (100%)	213 (92%)	19 (8%)	10	13
1	F	234/232 (101%)	220 (94%)	14 (6%)	17	26
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	16
2	G	95/95 (100%)	89 (94%)	6 (6%)	16	23
3	C	9/9 (100%)	9 (100%)	0	100	100
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	178/178 (100%)	155 (87%)	23 (13%)	4	3
4	I	178/178 (100%)	147 (83%)	31 (17%)	2	1
5	E	216/216 (100%)	190 (88%)	26 (12%)	5	4
5	J	215/216 (100%)	193 (90%)	22 (10%)	7	6
All	All	1461/1460 (100%)	1313 (90%)	148 (10%)	7	7

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	52	ILE
1	A	55	GLU
1	A	78	LEU
1	A	103	VAL
1	A	121	LYS
1	A	152	VAL
1	A	156	LEU
1	A	180	GLN
1	A	181	ARG
1	A	200	THR
1	A	201	LEU
1	A	206	LEU
1	A	214	THR
1	A	215	LEU
1	A	224	GLN
1	A	228	THR
1	A	231	VAL
1	A	264	GLU
2	B	48	LYS
2	B	70	PHE
2	B	71	THR
2	B	82	VAL
2	B	87	LEU
2	B	89	GLN
2	B	97	ARG
4	D	22	ASN
4	D	26	SER
4	D	42	LYS
4	D	67	LYS
4	D	73	SER
4	D	88	LEU
4	D	99	LEU
4	D	100	ILE
4	D	106	ARG
4	D	114	GLN
4	D	127	LYS
4	D	129	SER
4	D	131	LYS
4	D	132	SER
4	D	149	LYS
4	D	155	ILE

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Mol	Chain	Res	Type
4	D	161	LEU
4	D	172	SER
4	D	186	ASN
4	D	189	ASN
4	D	192	ILE
4	D	193	ILE
4	D	195	GLU
5	E	21	LEU
5	E	39	MET
5	E	40	MET
5	E	41	ARG
5	E	52	ASN
5	E	69	MET
5	E	73	SER
5	E	76	THR
5	E	80	GLN
5	E	100	LEU
5	E	102	LYS
5	E	115	VAL
5	E	116	LEU
5	E	120	LYS
5	E	126	GLU
5	E	145	LEU
5	E	146	VAL
5	E	163	VAL
5	E	166	LYS
5	E	174	THR
5	E	177	GLN
5	E	182	GLN
5	E	196	LEU
5	E	221	GLU
5	E	222	ASN
5	E	244	ARG
1	F	78	LEU
1	F	103	VAL
1	F	111	ARG
1	F	121	LYS
1	F	172	LEU
1	F	197	HIS
1	F	200	THR
1	F	201	LEU
1	F	206	LEU

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Mol	Chain	Res	Type
1	F	214	THR
1	F	215	LEU
1	F	226	GLN
1	F	228	THR
1	F	230	LEU
2	G	0	MET
2	G	64	LEU
2	G	70	PHE
2	G	71	THR
2	G	85	VAL
2	G	89	GLN
4	I	3	GLU
4	I	5	GLU
4	I	11	LEU
4	I	19	VAL
4	I	31	GLN
4	I	49	TYR
4	I	53	SER
4	I	73	SER
4	I	88	LEU
4	I	99	LEU
4	I	109	VAL
4	I	120	VAL
4	I	121	TYR
4	I	123	LEU
4	I	127	LYS
4	I	131	LYS
4	I	132	SER
4	I	133	VAL
4	I	135	LEU
4	I	136	PHE
4	I	138	ASP
4	I	143	THR
4	I	147	GLN
4	I	155	ILE
4	I	177	SER
4	I	178	ASN
4	I	182	PHE
4	I	191	SER
4	I	193	ILE
4	I	195	GLU
4	I	199	PHE

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Mol	Chain	Res	Type
5	J	7	SER
5	J	38	THR
5	J	40	MET
5	J	41	ARG
5	J	52	ASN
5	J	80	GLN
5	J	96	LEU
5	J	141	GLN
5	J	163	VAL
5	J	173	CYS
5	J	174	THR
5	J	177	GLN
5	J	179	LEU
5	J	181	GLU
5	J	185	LEU
5	J	192	LEU
5	J	195	ARG
5	J	196	LEU
5	J	209	HIS
5	J	221	GLU
5	J	244	ARG
5	J	246	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	70	HIS
1	A	74	HIS
1	A	86	ASN
1	A	87	GLN
1	A	93	HIS
1	A	114	HIS
1	A	115	GLN
1	A	174	ASN
1	A	180	GLN
1	A	191	HIS
1	A	226	GLN
1	A	242	GLN
1	A	255	GLN
1	A	263	HIS
2	B	8	GLN

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Mol	Chain	Res	Type
2	B	13	HIS
2	B	17	ASN
2	B	24	ASN
2	B	42	ASN
2	B	51	HIS
2	B	84	HIS
2	B	89	GLN
4	D	22	ASN
4	D	55	ASN
4	D	80	GLN
4	D	186	ASN
5	E	10	HIS
5	E	50	ASN
5	E	51	ASN
5	E	71	ASN
5	E	103	ASN
5	E	105	GLN
5	E	141	GLN
5	E	208	ASN
5	E	209	HIS
1	F	3	HIS
1	F	70	HIS
1	F	74	HIS
1	F	174	ASN
1	F	191	HIS
1	F	224	GLN
1	F	255	GLN
1	F	262	GLN
2	G	8	GLN
2	G	51	HIS
2	G	84	HIS
2	G	89	GLN
4	I	31	GLN
4	I	55	ASN
4	I	171	ASN
4	I	186	ASN
4	I	189	ASN
5	J	50	ASN
5	J	103	ASN
5	J	141	GLN
5	J	177	GLN
5	J	182	GLN

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Mol	Chain	Res	Type
5	J	213	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

26 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	$\# Z > 2$
7	SO4	G	102	-	4,4,4	0.54	0	6,6,6	0.41	0
8	GOL	B	101	-	5,5,5	0.41	0	5,5,5	0.59	0
6	EDO	A	302	-	3,3,3	0.23	0	2,2,2	0.45	0
6	EDO	E	301	-	3,3,3	0.26	0	2,2,2	0.50	0
6	EDO	D	202	-	3,3,3	0.48	0	2,2,2	0.57	0
7	SO4	D	203	-	4,4,4	0.36	0	6,6,6	0.61	0
6	EDO	F	305	-	3,3,3	0.77	0	2,2,2	0.37	0
8	GOL	F	302	-	5,5,5	0.92	0	5,5,5	2.29	3 (60%)
6	EDO	D	201	-	3,3,3	0.36	0	2,2,2	0.32	0
7	SO4	E	302	-	4,4,4	0.47	0	6,6,6	0.17	0
6	EDO	I	201	-	3,3,3	0.55	0	2,2,2	0.19	0
6	EDO	H	101	-	3,3,3	0.41	0	2,2,2	0.15	0
6	EDO	A	301	-	3,3,3	1.13	0	2,2,2	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	303	-	4,4,4	0.43	0	6,6,6	0.50	0
8	GOL	J	301	-	5,5,5	0.43	0	5,5,5	0.65	0
8	GOL	F	301	-	5,5,5	0.52	0	5,5,5	0.29	0
6	EDO	J	303	-	3,3,3	0.69	0	2,2,2	0.27	0
6	EDO	J	302	-	3,3,3	0.51	0	2,2,2	0.16	0
8	GOL	G	101	-	5,5,5	0.32	0	5,5,5	0.43	0
6	EDO	F	303	-	3,3,3	0.33	0	2,2,2	0.37	0
7	SO4	F	306	-	4,4,4	0.53	0	6,6,6	0.19	0
7	SO4	J	304	-	4,4,4	0.50	0	6,6,6	0.20	0
7	SO4	E	304	-	4,4,4	0.62	0	6,6,6	0.89	0
7	SO4	E	303	-	4,4,4	0.54	0	6,6,6	0.10	0
6	EDO	H	102	-	3,3,3	0.36	0	2,2,2	0.45	0
6	EDO	F	304	-	3,3,3	0.50	0	2,2,2	0.55	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
8	GOL	J	301	-	-	4/4/4/4	-
6	EDO	F	305	-	-	1/1/1/1	-
6	EDO	F	304	-	-	1/1/1/1	-
6	EDO	J	303	-	-	0/1/1/1	-
8	GOL	F	301	-	-	4/4/4/4	-
8	GOL	F	302	-	-	0/4/4/4	-
6	EDO	H	102	-	-	0/1/1/1	-
6	EDO	H	101	-	-	0/1/1/1	-
6	EDO	J	302	-	-	1/1/1/1	-
8	GOL	G	101	-	-	2/4/4/4	-
6	EDO	F	303	-	-	0/1/1/1	-
8	GOL	B	101	-	-	2/4/4/4	-
6	EDO	I	201	-	-	1/1/1/1	-
6	EDO	A	302	-	-	0/1/1/1	-
6	EDO	E	301	-	-	1/1/1/1	-
6	EDO	D	202	-	-	1/1/1/1	-
6	EDO	D	201	-	-	1/1/1/1	-
6	EDO	A	301	-	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	302	GOL	O3-C3-C2	3.04	124.06	110.38
8	F	302	GOL	O1-C1-C2	2.81	123.03	110.38
8	F	302	GOL	O2-C2-C3	-2.14	100.33	109.18

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	301	GOL	C1-C2-C3-O3
8	G	101	GOL	C1-C2-C3-O3
8	J	301	GOL	O1-C1-C2-C3
8	J	301	GOL	C1-C2-C3-O3
8	G	101	GOL	O2-C2-C3-O3
8	J	301	GOL	O1-C1-C2-O2
8	B	101	GOL	C1-C2-C3-O3
8	F	301	GOL	O1-C1-C2-C3
8	J	301	GOL	O2-C2-C3-O3
6	D	201	EDO	O1-C1-C2-O2
8	B	101	GOL	O2-C2-C3-O3
8	F	301	GOL	O1-C1-C2-O2
8	F	301	GOL	O2-C2-C3-O3
6	E	301	EDO	O1-C1-C2-O2
6	F	304	EDO	O1-C1-C2-O2
6	F	305	EDO	O1-C1-C2-O2
6	J	302	EDO	O1-C1-C2-O2
6	D	202	EDO	O1-C1-C2-O2
6	A	301	EDO	O1-C1-C2-O2
6	I	201	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	EDO	8	0
6	E	301	EDO	2	0
7	D	203	SO4	1	0
8	F	302	GOL	2	0
6	D	201	EDO	1	0
6	H	101	EDO	1	0
6	A	301	EDO	1	0
8	J	301	GOL	1	0
6	J	303	EDO	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	303	EDO	2	0
6	H	102	EDO	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	276/276 (100%)	0.06	2 (0%) 84 86	34, 68, 112, 124	0
1	F	276/276 (100%)	-0.14	4 (1%) 73 75	19, 55, 117, 140	2 (0%)
2	B	100/100 (100%)	-0.05	1 (1%) 79 80	41, 65, 89, 102	0
2	G	100/100 (100%)	-0.17	0 100 100	34, 57, 86, 108	0
3	C	10/10 (100%)	-0.44	0 100 100	36, 43, 51, 61	0
3	H	10/10 (100%)	-0.52	0 100 100	33, 37, 43, 46	0
4	D	197/197 (100%)	0.36	11 (5%) 30 27	37, 69, 133, 152	0
4	I	197/197 (100%)	0.40	16 (8%) 18 16	34, 70, 152, 179	0
5	E	246/246 (100%)	-0.10	6 (2%) 59 62	27, 57, 103, 130	0
5	J	244/246 (99%)	0.14	5 (2%) 65 66	30, 67, 132, 176	0
All	All	1656/1658 (99%)	0.06	45 (2%) 56 57	19, 62, 128, 179	2 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	193	ILE	4.7
4	D	165	SER	4.1
5	J	185	LEU	3.7
5	E	40	MET	3.3
5	J	135	ALA	3.3
4	I	193	ILE	3.3
4	D	198	PHE	3.3
5	J	184	ALA	3.3
4	I	136	PHE	3.2
4	D	199	PHE	3.1
5	J	137	ILE	3.0
4	D	134	CYS	3.0
4	I	187	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
4	I	198	PHE	2.8
4	D	163	MET	2.8
4	I	192	ILE	2.7
4	I	199	PHE	2.6
1	F	193	ALA	2.6
4	I	194	PRO	2.6
4	I	155	ILE	2.5
4	I	134	CYS	2.4
4	D	192	ILE	2.4
5	E	184	ALA	2.4
4	D	194	PRO	2.4
4	D	166	MET	2.4
4	D	145	VAL	2.4
4	I	188	PHE	2.3
4	I	153	VAL	2.3
4	I	120	VAL	2.3
5	J	245	ALA	2.2
2	B	18	GLY	2.2
5	E	179	LEU	2.2
1	F	247	VAL	2.2
1	F	265	GLY	2.2
4	I	165	SER	2.2
4	I	145	VAL	2.2
5	E	246	ASP	2.2
5	E	39	MET	2.1
4	I	184	CYS	2.1
4	D	162	ASP	2.1
1	A	228	THR	2.1
1	A	197	HIS	2.1
1	F	201	LEU	2.1
5	E	131	GLU	2.0
4	I	128	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 ⓘ

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
7	SO4	E	303	5/5	0.57	0.11	105,107,112,114	0
7	SO4	G	102	5/5	0.68	0.14	107,112,132,134	0
7	SO4	J	304	5/5	0.72	0.10	115,117,133,140	0
7	SO4	E	302	5/5	0.76	0.09	114,115,127,129	0
7	SO4	A	303	5/5	0.80	0.13	66,104,108,113	0
7	SO4	F	306	5/5	0.82	0.14	107,116,121,126	0
8	GOL	F	301	6/6	0.83	0.14	62,74,81,84	0
8	GOL	G	101	6/6	0.84	0.13	73,78,92,95	0
7	SO4	D	203	5/5	0.85	0.12	78,92,100,115	0
6	EDO	I	201	4/4	0.85	0.13	76,81,83,84	0
6	EDO	F	304	4/4	0.86	0.17	57,57,58,61	0
6	EDO	A	301	4/4	0.87	0.19	62,69,69,75	0
8	GOL	J	301	6/6	0.89	0.13	54,78,88,90	0
6	EDO	F	305	4/4	0.90	0.14	65,72,78,80	0
6	EDO	F	303	4/4	0.92	0.30	44,65,67,69	0
6	EDO	A	302	4/4	0.93	0.18	44,48,51,54	0
8	GOL	F	302	6/6	0.93	0.18	43,55,59,60	0
6	EDO	J	303	4/4	0.93	0.11	50,56,57,57	0
7	SO4	E	304	5/5	0.93	0.09	58,59,63,66	0
6	EDO	H	102	4/4	0.94	0.14	45,53,54,55	0
6	EDO	D	202	4/4	0.94	0.12	65,66,68,69	0
6	EDO	H	101	4/4	0.94	0.12	44,46,51,54	0
6	EDO	E	301	4/4	0.95	0.15	55,58,59,60	0
6	EDO	J	302	4/4	0.95	0.09	46,49,52,53	0
6	EDO	D	201	4/4	0.95	0.09	42,44,46,47	0
8	GOL	B	101	6/6	0.96	0.09	73,77,79,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.