



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 5NME / pdb_00005nme
Title : 868 TCR in complex with HLA A02 presenting SLYNTVATL
Authors : Rizkallah, P.J.; Cole, D.K.; Fuller, A.; Sewell, A.K.
Deposited on : 2017-04-05
Resolution : 2.94 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

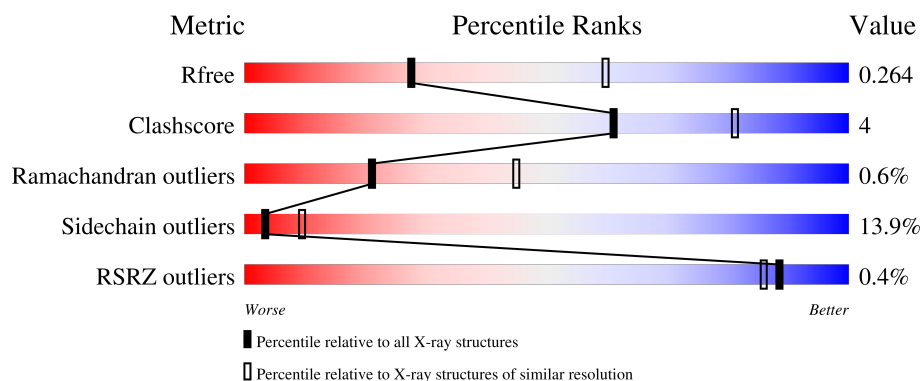
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

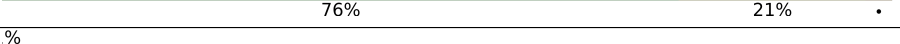
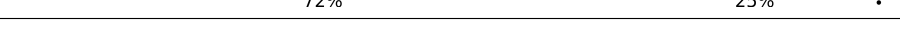
The reported resolution of this entry is 2.94 Å.

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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	
1	F	276	
2	B	100	
2	G	100	
3	C	9	

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Mol	Chain	Length	Quality of chain
3	H	9	 67% 22% 11%
4	D	201	 79% 19% •
4	I	201	 77% 19% •
5	E	242	 76% 21% •
5	J	242	 78% 20% •

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
7	SO4	J	305	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13441 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	1	0
			2264	1414	413	428	9			
1	F	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	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 Gag protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			69	44	10	15			
3	H	9	Total	C	N	O	0	0	0
			69	44	10	15			

- Molecule 4 is a protein called T-cell receptor Alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1567	981	260	318	8			

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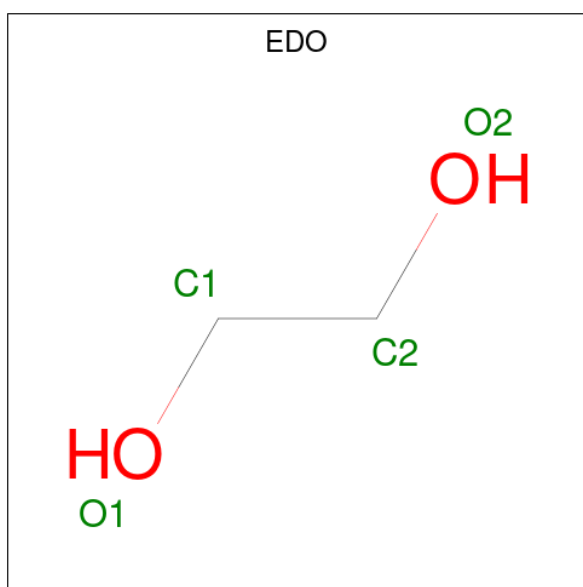
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	200	Total	C	N	O	S	0	0	0
			1560	976	259	317	8			

- Molecule 5 is a protein called Human T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1939	1219	337	378	5			
5	J	241	Total	C	N	O	S	0	0	0
			1930	1215	336	374	5			

- 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	E	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		
6	I	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	I	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	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	J	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: C₃H₈O₃).



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

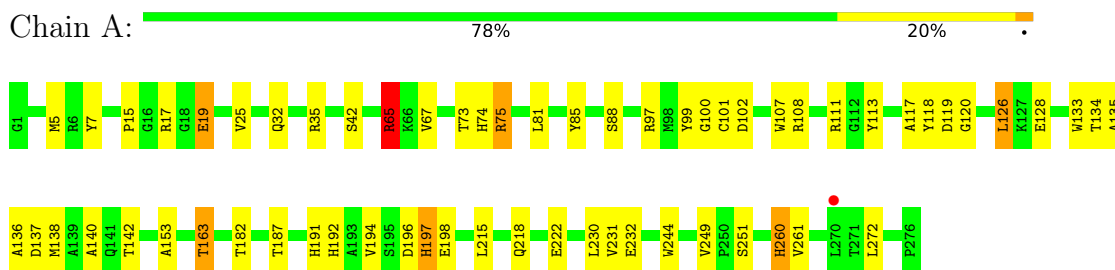
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	13	Total	O	0	0
			13	13		
9	B	4	Total	O	0	0
			4	4		
9	D	5	Total	O	0	0
			5	5		
9	E	4	Total	O	0	0
			4	4		
9	F	5	Total	O	0	0
			5	5		
9	G	1	Total	O	0	0
			1	1		
9	I	5	Total	O	0	0
			5	5		
9	J	5	Total	O	0	0
			5	5		

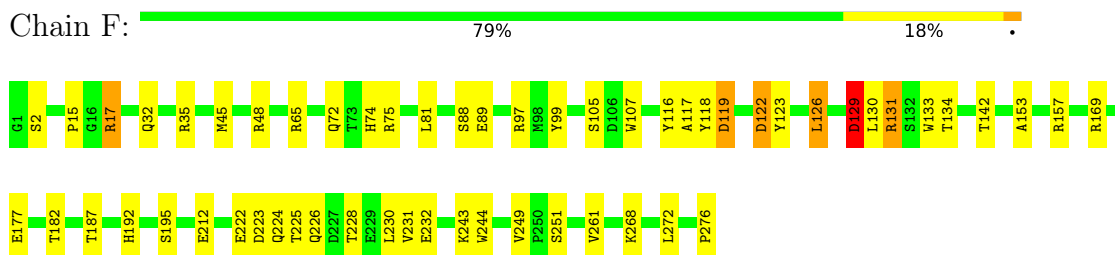
3 Residue-property plots

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.

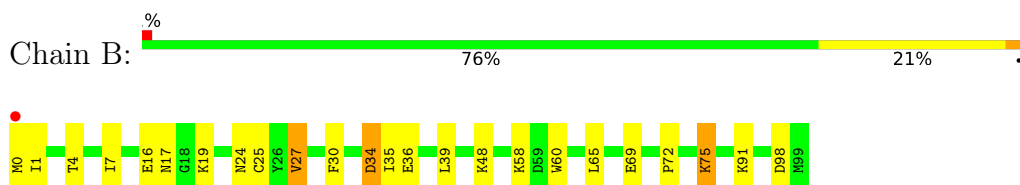
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



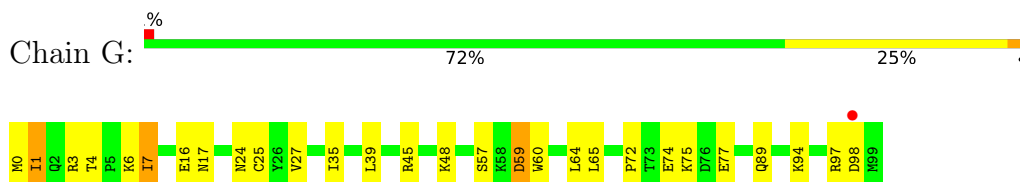
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin

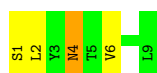


- Molecule 2: Beta-2-microglobulin



- Molecule 3: Gag protein

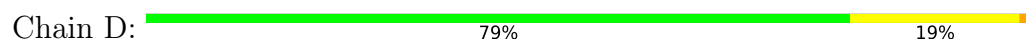




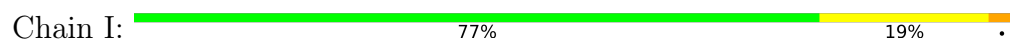
- Molecule 3: Gag protein



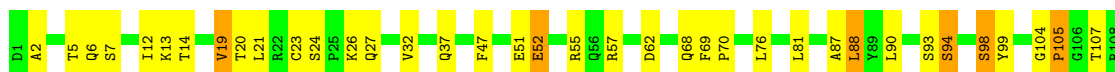
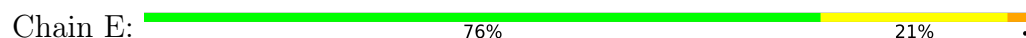
- Molecule 4: T-cell receptor Alpha chain



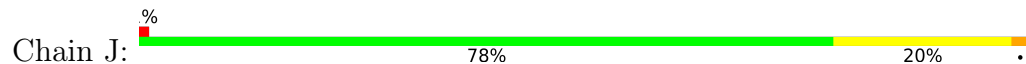
- Molecule 4: T-cell receptor Alpha chain



- Molecule 5: Human T-cell receptor beta chain



- Molecule 5: Human T-cell receptor beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	211.14Å 85.14Å 113.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.76 – 2.94 64.76 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (64.76-2.94) 99.0 (64.76-2.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.263 0.199 , 0.264	Depositor DCC
R_{free} test set	2212 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13441	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: SO4, GOL, EDO

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	1.15	5/2331 (0.2%)	1.20	7/3164 (0.2%)
1	F	0.98	0/2320	1.09	3/3149 (0.1%)
2	B	1.05	0/860	1.15	2/1162 (0.2%)
2	G	0.90	0/860	1.09	0/1162
3	C	1.59	0/69	1.47	0/93
3	H	1.08	0/69	1.38	1/93 (1.1%)
4	D	1.20	2/1601 (0.1%)	1.20	4/2167 (0.2%)
4	I	1.24	1/1593 (0.1%)	1.24	10/2155 (0.5%)
5	E	1.19	4/1994 (0.2%)	1.23	11/2717 (0.4%)
5	J	1.14	0/1985	1.19	7/2706 (0.3%)
All	All	1.13	12/13682 (0.1%)	1.18	45/18568 (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
1	F	0	1
4	I	0	2
5	E	0	1
5	J	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ASP	C-O	7.83	1.33	1.24
4	D	47	ILE	C-O	-6.28	1.18	1.24
4	D	192	ILE	CA-CB	6.03	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	7	SER	CA-C	5.67	1.58	1.52
4	I	78	ASP	CB-CG	5.59	1.66	1.52
1	A	67	VAL	C-O	-5.43	1.17	1.24
5	E	99	TYR	N-CA	5.39	1.52	1.46
1	A	198	GLU	N-CA	5.22	1.52	1.46
1	A	197	HIS	CA-C	5.22	1.59	1.52
1	A	136	ALA	N-CA	5.18	1.52	1.46
5	E	6	GLN	C-O	-5.15	1.17	1.23
5	E	87	ALA	C-O	-5.11	1.18	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	98	SER	CA-C-N	-9.62	108.15	122.86
5	E	98	SER	C-N-CA	-9.62	108.15	122.86
1	A	249	VAL	N-CA-C	8.48	116.14	109.19
5	E	105	PRO	CA-C-N	-8.20	115.17	122.47
5	E	105	PRO	C-N-CA	-8.20	115.17	122.47
4	I	186	ASN	CB-CA-C	-8.20	95.70	110.70
5	J	71	ASN	N-CA-C	-8.07	99.88	110.53
5	J	105	PRO	CA-C-N	-7.46	115.55	121.82
5	J	105	PRO	C-N-CA	-7.46	115.55	121.82
1	A	119	ASP	CB-CA-C	7.35	125.04	110.42
5	E	98	SER	N-CA-C	-7.29	98.43	110.17
1	A	196	ASP	N-CA-C	-7.18	101.02	110.43
1	F	249	VAL	N-CA-C	7.17	115.06	109.19
1	A	101	CYS	CB-CA-C	-6.85	95.83	109.33
4	I	166	MET	N-CA-C	-6.71	102.16	110.41
4	D	192	ILE	N-CA-CB	6.34	118.75	111.90
5	E	94	SER	CA-CB-OG	6.16	123.42	111.10
1	A	100	GLY	N-CA-C	6.01	118.68	110.69
5	J	146	THR	N-CA-C	6.00	118.41	108.99
5	E	146	THR	N-CA-C	5.97	118.36	108.99
3	H	6	VAL	CB-CA-C	-5.97	103.04	111.28
4	I	28	ARG	N-CA-C	-5.84	101.84	110.48
4	I	110	THR	N-CA-C	5.84	117.00	109.65
2	B	75	LYS	N-CA-C	5.81	117.61	111.28
5	J	52	GLU	CA-CB-CG	5.79	125.69	114.10
1	A	65	ARG	CG-CD-NE	5.79	124.73	112.00
1	A	19	GLU	CB-CA-C	5.76	118.59	109.96
5	E	2	ALA	N-CA-C	5.75	118.78	109.86
4	I	13	VAL	CA-C-N	-5.58	114.22	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	13	VAL	C-N-CA	-5.58	114.22	119.85
5	J	71	ASN	CA-C-O	-5.56	115.42	121.87
2	B	34	ASP	N-CA-CB	5.49	118.56	109.88
5	E	152	HIS	CA-CB-CG	5.49	119.29	113.80
4	I	187	ALA	N-CA-C	-5.45	102.21	110.28
5	E	98	SER	O-C-N	-5.42	116.87	123.10
5	J	152	HIS	CB-CA-C	-5.38	103.85	111.76
1	F	122	ASP	N-CA-C	5.32	119.26	112.34
5	E	57	ARG	NE-CZ-NH2	5.27	123.94	119.20
4	I	32	SER	N-CA-C	5.26	118.01	108.69
4	I	52	SER	N-CA-C	5.24	118.03	109.59
4	D	13	VAL	CA-C-N	-5.13	114.67	119.85
4	D	13	VAL	C-N-CA	-5.13	114.67	119.85
1	F	129	ASP	N-CA-C	-5.10	99.48	108.20
4	I	200	PRO	N-CA-C	5.09	122.97	112.47
4	D	7	ASN	N-CA-CB	5.01	117.62	110.06

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	GLY	Peptide
5	E	168	VAL	Peptide
1	F	129	ASP	Peptide
4	I	167	ASP	Peptide
4	I	29	GLY	Peptide
5	J	168	VAL	Peptide

5.2 Too-close contacts [i](#)

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	2264	0	2109	24	0
1	F	2254	0	2103	22	0
2	B	837	0	803	8	0
2	G	837	0	803	13	0
3	C	69	0	72	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	69	0	72	1	0
4	D	1567	0	1493	12	0
4	I	1560	0	1486	11	0
5	E	1939	0	1814	16	0
5	J	1930	0	1810	10	0
6	A	8	0	12	2	0
6	D	4	0	6	0	0
6	E	4	0	6	0	0
6	I	12	0	18	0	0
6	J	4	0	6	0	0
7	A	5	0	0	0	0
7	E	10	0	0	0	0
7	J	20	0	0	1	5
8	F	6	0	8	0	0
9	A	13	0	0	0	0
9	B	4	0	0	0	0
9	D	5	0	0	1	0
9	E	4	0	0	0	0
9	F	5	0	0	0	0
9	G	1	0	0	0	0
9	I	5	0	0	0	0
9	J	5	0	0	0	0
All	All	13441	0	12621	110	5

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 4.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:GLN:HE22	5:E:37:GLN:HE22	1.12	0.96
5:E:21:LEU:HD22	5:E:107:THR:HG21	1.57	0.85
3:C:4:ASN:H	3:C:4:ASN:HD22	1.23	0.85
4:I:38:GLN:HE22	5:J:37:GLN:HE22	1.23	0.83
4:I:50:ILE:HD11	4:I:52:SER:O	1.81	0.80
1:A:7:TYR:CZ	3:C:1:SER:O	2.35	0.79
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.05	0.75
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.38	0.70
2:B:27:VAL:HG21	2:B:35:ILE:HD13	1.72	0.70
1:F:131:ARG:HH21	1:F:153:ALA:HB3	1.55	0.69
2:G:7:ILE:HD13	2:G:7:ILE:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:HIS:HE1	1:F:97:ARG:HE	1.39	0.68
4:D:7:ASN:ND2	9:D:401:HOH:O	2.27	0.66
5:J:21:LEU:HD22	5:J:107:THR:HG21	1.78	0.66
4:I:182:PHE:HA	4:I:186:ASN:HD22	1.62	0.65
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.15	0.64
3:C:4:ASN:HD22	3:C:4:ASN:N	1.92	0.64
4:D:93:THR:HG23	4:D:95:SER:H	1.63	0.63
5:J:84:GLY:N	7:J:305:SO4:O1	2.24	0.63
1:F:74:HIS:CE1	1:F:97:ARG:HE	2.16	0.63
5:E:182:ASN:C	5:E:182:ASN:HD22	2.07	0.63
1:F:230:LEU:HD12	1:F:243:LYS:HE3	1.81	0.61
4:D:10:PRO:HB3	4:D:108:LEU:HD23	1.82	0.61
2:B:7:ILE:HD12	2:B:91:LYS:HE3	1.82	0.61
2:G:35:ILE:HD11	2:G:64:LEU:HD12	1.83	0.59
1:F:129:ASP:OD2	1:F:129:ASP:N	2.36	0.59
1:F:130:LEU:HB2	1:F:157:ARG:HG3	1.84	0.59
4:D:60:ARG:NH2	4:D:83:ASP:OD2	2.36	0.58
5:J:155:LEU:C	5:J:155:LEU:HD23	2.30	0.57
4:I:182:PHE:HA	4:I:186:ASN:ND2	2.19	0.57
5:E:155:LEU:C	5:E:155:LEU:HD23	2.29	0.56
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.41	0.56
1:F:119:ASP:OD1	2:G:0:MET:HE2	2.06	0.55
4:D:110:THR:HG23	4:D:141:SER:HB3	1.89	0.55
1:F:224:GLN:O	1:F:228:THR:OG1	2.25	0.55
3:C:4:ASN:H	3:C:4:ASN:ND2	1.99	0.54
1:A:7:TYR:OH	3:C:1:SER:O	2.22	0.53
1:A:7:TYR:CE1	3:C:1:SER:O	2.61	0.53
5:J:104:GLY:C	5:J:105:PRO:O	2.49	0.53
5:J:21:LEU:HD12	5:J:76:LEU:HD23	1.91	0.53
5:E:205:HIS:HB2	5:E:238:TRP:CE3	2.45	0.52
4:I:111:PRO:HG3	4:I:160:VAL:HG21	1.91	0.52
5:E:52:GLU:H	5:E:68:GLN:NE2	2.07	0.52
1:A:135:ALA:HB1	1:A:140:ALA:HB1	1.92	0.51
5:J:88:LEU:HD13	5:J:90:LEU:HD21	1.93	0.51
5:E:104:GLY:C	5:E:105:PRO:O	2.52	0.51
1:A:218:GLN:OE1	1:A:260:HIS:ND1	2.44	0.51
5:E:182:ASN:C	5:E:182:ASN:ND2	2.68	0.51
1:F:116:TYR:O	1:F:122:ASP:O	2.29	0.50
2:B:27:VAL:HG21	2:B:35:ILE:CD1	2.42	0.50
5:E:21:LEU:HD12	5:E:76:LEU:HD23	1.94	0.50
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:205:HIS:HB2	5:E:238:TRP:CZ3	2.48	0.49
2:B:27:VAL:HG23	2:B:30:PHE:CE1	2.49	0.48
1:F:117:ALA:HB2	2:G:60:TRP:CZ2	2.49	0.48
1:A:163:THR:HG23	4:D:31:GLN:HE21	1.77	0.48
5:J:54:GLU:OE1	5:J:57:ARG:NH2	2.46	0.47
4:I:50:ILE:HD12	4:I:51:TYR:N	2.28	0.47
2:G:57:SER:O	2:G:59:ASP:O	2.32	0.47
5:E:13:LYS:HD2	5:E:19:VAL:HG23	1.96	0.47
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.96	0.47
1:A:126:LEU:HD13	1:A:133:TRP:CZ3	2.50	0.47
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.98	0.46
1:F:32:GLN:HE21	1:F:48:ARG:HG3	1.80	0.46
4:I:13:VAL:HG21	4:I:107:LEU:HD11	1.98	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.51	0.46
2:B:17:ASN:HA	2:B:72:PRO:O	2.15	0.46
4:I:157:ASP:OD1	4:I:157:ASP:N	2.47	0.46
4:D:81:LEU:HD21	4:D:111:PRO:HB3	1.98	0.46
1:F:272:LEU:N	1:F:272:LEU:HD12	2.31	0.46
1:A:153:ALA:HB3	6:A:301:EDO:C1	2.47	0.45
1:A:102:ASP:OD2	1:A:111:ARG:NH1	2.50	0.45
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.97	0.45
1:A:25:VAL:HB	1:A:32:GLN:HE21	1.82	0.45
2:G:7:ILE:N	2:G:7:ILE:CD1	2.76	0.45
2:G:17:ASN:HA	2:G:72:PRO:O	2.17	0.44
1:A:272:LEU:HD12	1:A:272:LEU:N	2.33	0.44
4:I:48:MET:HE1	4:I:56:LYS:O	2.17	0.44
5:E:88:LEU:HD13	5:E:90:LEU:HD21	2.00	0.44
5:J:57:ARG:NH1	5:J:64:PHE:O	2.42	0.44
1:A:231:VAL:HG11	1:A:244:TRP:CZ2	2.53	0.43
1:F:231:VAL:HG11	1:F:244:TRP:CZ2	2.53	0.43
1:F:187:THR:HG21	1:F:261:VAL:HG21	2.00	0.43
4:I:30:SER:HA	4:I:93:THR:HG22	2.01	0.43
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.54	0.43
2:G:1:ILE:HD11	2:G:3:ARG:NH1	2.33	0.43
2:G:25:CYS:HB2	2:G:39:LEU:HD21	1.99	0.43
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.53	0.43
5:E:23:CYS:SG	5:E:24:SER:N	2.92	0.43
3:C:6:VAL:HG13	3:C:6:VAL:O	2.20	0.42
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.32	0.42
1:A:163:THR:CG2	4:D:31:GLN:HE21	2.32	0.42
4:D:93:THR:CG2	4:D:95:SER:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:HB3	6:A:301:EDO:H12	2.01	0.42
1:F:45:MET:CE	3:H:2:LEU:HD11	2.49	0.42
1:F:65:ARG:NH1	4:I:95:SER:O	2.53	0.42
4:D:94:ASN:O	4:D:94:ASN:CG	2.63	0.42
1:F:107:TRP:HB2	1:F:169:ARG:HD3	2.02	0.42
1:F:72:GLN:HG2	1:F:75:ARG:HH11	1.84	0.42
2:G:6:LYS:C	2:G:7:ILE:HD13	2.44	0.42
1:F:126:LEU:HD13	1:F:133:TRP:CZ3	2.56	0.41
4:D:188:PHE:HB3	4:D:193:ILE:HD11	2.02	0.41
1:F:99:TYR:C	1:F:99:TYR:CD1	2.97	0.41
5:E:69:PHE:HB3	5:E:70:PRO:HD2	2.03	0.41
1:A:99:TYR:CD1	1:A:99:TYR:C	2.98	0.40
5:J:18:GLN:HE21	5:J:77:ASN:HD21	1.69	0.40
1:A:75:ARG:HH12	5:E:51:GLU:HG2	1.86	0.40
5:E:52:GLU:H	5:E:68:GLN:HE21	1.68	0.40
2:G:7:ILE:HD12	2:G:27:VAL:HG13	2.04	0.40
1:A:74:HIS:HE1	1:A:97:ARG:NE	2.14	0.40

All (5) 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)
7:J:305:SO4:O2	7:J:305:SO4:O2[2_655]	1.18	1.02
7:J:305:SO4:O4	7:J:305:SO4:O4[2_655]	1.41	0.79
7:J:305:SO4:S	7:J:305:SO4:O4[2_655]	1.65	0.55
7:J:305:SO4:O3	7:J:305:SO4:O4[2_655]	1.71	0.49
7:J:305:SO4:S	7:J:305:SO4:O2[2_655]	2.11	0.09

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	275/276 (100%)	263 (96%)	10 (4%)	2 (1%)	18	40
1	F	274/276 (99%)	258 (94%)	12 (4%)	4 (2%)	8	23
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	G	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	5 (71%)	1 (14%)	1 (14%)	0	0
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
4	I	198/201 (98%)	188 (95%)	10 (5%)	0	100	100
5	E	240/242 (99%)	231 (96%)	7 (3%)	2 (1%)	16	36
5	J	239/242 (99%)	231 (97%)	7 (3%)	1 (0%)	30	54
All	All	1635/1656 (99%)	1558 (95%)	67 (4%)	10 (1%)	21	45

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	123	TYR
1	A	17	ARG
5	E	52	GLU
1	F	17	ARG
1	F	119	ASP
3	C	2	LEU
5	E	223	GLN
5	J	223	GLN
1	A	15	PRO
1	F	15	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	233/232 (100%)	205 (88%)	28 (12%)	5	14
1	F	232/232 (100%)	208 (90%)	24 (10%)	7	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	95/95 (100%)	82 (86%)	13 (14%)	3	10
2	G	95/95 (100%)	81 (85%)	14 (15%)	3	8
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	12
3	H	8/8 (100%)	6 (75%)	2 (25%)	0	1
4	D	179/179 (100%)	152 (85%)	27 (15%)	3	8
4	I	178/179 (99%)	153 (86%)	25 (14%)	3	9
5	E	211/211 (100%)	178 (84%)	33 (16%)	2	8
5	J	210/211 (100%)	176 (84%)	34 (16%)	2	7
All	All	1449/1450 (100%)	1248 (86%)	201 (14%)	3	9

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	19	GLU
1	A	35	ARG
1	A	42	SER
1	A	65	ARG
1	A	73	THR
1	A	75	ARG
1	A	88	SER
1	A	107	TRP
1	A	108	ARG
1	A	113	TYR
1	A	126	LEU
1	A	128	GLU
1	A	134	THR
1	A	138	MET
1	A	142	THR
1	A	163	THR
1	A	182	THR
1	A	191	HIS
1	A	192	HIS
1	A	194	VAL
1	A	197	HIS
1	A	215	LEU
1	A	222	GLU
1	A	230	LEU
1	A	232	GLU

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Mol	Chain	Res	Type
1	A	251	SER
1	A	260	HIS
2	B	0	MET
2	B	1	ILE
2	B	4	THR
2	B	16	GLU
2	B	19	LYS
2	B	27	VAL
2	B	34	ASP
2	B	36	GLU
2	B	48	LYS
2	B	58	LYS
2	B	69	GLU
2	B	75	LYS
2	B	98	ASP
3	C	4	ASN
4	D	2	LYS
4	D	8	SER
4	D	10	PRO
4	D	11	LEU
4	D	20	SER
4	D	40	SER
4	D	45	GLU
4	D	50	ILE
4	D	52	SER
4	D	72	ILE
4	D	91	VAL
4	D	93	THR
4	D	99	LEU
4	D	114	GLN
4	D	115	LYS
4	D	127	LYS
4	D	132	SER
4	D	140	ASP
4	D	144	ASN
4	D	149	LYS
4	D	150	ASP
4	D	158	LYS
4	D	160	VAL
4	D	172	SER
4	D	181	ASP
4	D	192	ILE

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Mol	Chain	Res	Type
4	D	195	GLU
5	E	5	THR
5	E	12	ILE
5	E	14	THR
5	E	19	VAL
5	E	20	THR
5	E	26	LYS
5	E	27	GLN
5	E	32	VAL
5	E	47	PHE
5	E	55	ARG
5	E	62	ASP
5	E	81	LEU
5	E	88	LEU
5	E	93	SER
5	E	94	SER
5	E	98	SER
5	E	109	LEU
5	E	110	THR
5	E	113	GLU
5	E	116	LYS
5	E	134	SER
5	E	142	VAL
5	E	144	LEU
5	E	152	HIS
5	E	154	GLU
5	E	175	LEU
5	E	182	ASN
5	E	191	ARG
5	E	197	THR
5	E	209	GLN
5	E	222	THR
5	E	223	GLN
5	E	242	ASP
1	F	2	SER
1	F	17	ARG
1	F	35	ARG
1	F	88	SER
1	F	89	GLU
1	F	105	SER
1	F	126	LEU
1	F	129	ASP

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Mol	Chain	Res	Type
1	F	131	ARG
1	F	134	THR
1	F	142	THR
1	F	177	GLU
1	F	182	THR
1	F	192	HIS
1	F	195	SER
1	F	212	GLU
1	F	222	GLU
1	F	223	ASP
1	F	225	THR
1	F	226	GLN
1	F	232	GLU
1	F	251	SER
1	F	268	LYS
1	F	276	PRO
2	G	1	ILE
2	G	4	THR
2	G	7	ILE
2	G	16	GLU
2	G	45	ARG
2	G	48	LYS
2	G	59	ASP
2	G	74	GLU
2	G	75	LYS
2	G	77	GLU
2	G	89	GLN
2	G	94	LYS
2	G	97	ARG
2	G	98	ASP
3	H	6	VAL
3	H	9	LEU
4	I	2	LYS
4	I	5	GLU
4	I	8	SER
4	I	11	LEU
4	I	40	SER
4	I	42	LYS
4	I	45	GLU
4	I	48	MET
4	I	50	ILE
4	I	52	SER

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Mol	Chain	Res	Type
4	I	72	ILE
4	I	75	LEU
4	I	80	LYS
4	I	91	VAL
4	I	99	LEU
4	I	124	ARG
4	I	126	SER
4	I	128	SER
4	I	131	LYS
4	I	132	SER
4	I	140	ASP
4	I	147	GLN
4	I	157	ASP
4	I	160	VAL
4	I	172	SER
5	J	5	THR
5	J	6	GLN
5	J	14	THR
5	J	15	ARG
5	J	20	THR
5	J	32	VAL
5	J	47	PHE
5	J	52	GLU
5	J	55	ARG
5	J	62	ASP
5	J	73	SER
5	J	79	ASN
5	J	81	LEU
5	J	83	LEU
5	J	88	LEU
5	J	93	SER
5	J	94	SER
5	J	97	VAL
5	J	98	SER
5	J	109	LEU
5	J	110	THR
5	J	113	GLU
5	J	134	SER
5	J	138	LYS
5	J	142	VAL
5	J	144	LEU
5	J	154	GLU

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Mol	Chain	Res	Type
5	J	178	GLN
5	J	183	ASP
5	J	191	ARG
5	J	197	THR
5	J	209	GLN
5	J	217	GLU
5	J	223	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	74	HIS
1	A	174	ASN
1	A	197	HIS
1	A	218	GLN
1	A	224	GLN
1	A	263	HIS
2	B	13	HIS
3	C	4	ASN
4	D	6	GLN
4	D	7	ASN
4	D	31	GLN
4	D	64	GLN
5	E	18	GLN
5	E	36	GLN
5	E	37	GLN
5	E	68	GLN
5	E	117	ASN
5	E	135	HIS
5	E	182	ASN
5	E	205	HIS
1	F	32	GLN
1	F	43	GLN
1	F	74	HIS
1	F	93	HIS
1	F	260	HIS
1	F	263	HIS
4	I	31	GLN
4	I	122	GLN
4	I	186	ASN

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Mol	Chain	Res	Type
5	J	18	GLN
5	J	36	GLN
5	J	37	GLN
5	J	117	ASN
5	J	178	GLN
5	J	218	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
8	GOL	F	301	-	5,5,5	0.30	0	5,5,5	0.30	0
6	EDO	D	301	-	3,3,3	0.57	0	2,2,2	0.25	0
6	EDO	I	303	-	3,3,3	0.43	0	2,2,2	0.45	0
6	EDO	A	302	-	3,3,3	0.53	0	2,2,2	0.23	0
7	SO4	E	303	-	4,4,4	0.51	0	6,6,6	0.30	0
7	SO4	J	302	-	4,4,4	0.43	0	6,6,6	0.39	0
6	EDO	I	302	-	3,3,3	0.44	0	2,2,2	0.43	0
7	SO4	J	304	-	4,4,4	0.48	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	J	303	-	4,4,4	0.47	0	6,6,6	0.28	0
6	EDO	I	301	-	3,3,3	0.45	0	2,2,2	0.46	0
6	EDO	J	301	-	3,3,3	0.48	0	2,2,2	0.40	0
6	EDO	A	301	-	3,3,3	0.40	0	2,2,2	0.56	0
6	EDO	E	301	-	3,3,3	0.46	0	2,2,2	0.55	0
7	SO4	J	305	-	4,4,4	0.43	0	6,6,6	0.64	0
7	SO4	A	303	-	4,4,4	0.43	0	6,6,6	0.31	0
7	SO4	E	302	-	4,4,4	0.46	0	6,6,6	0.59	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	F	301	-	-	1/4/4/4	-
6	EDO	D	301	-	-	1/1/1/1	-
6	EDO	I	303	-	-	0/1/1/1	-
6	EDO	A	302	-	-	0/1/1/1	-
6	EDO	I	302	-	-	1/1/1/1	-
6	EDO	I	301	-	-	0/1/1/1	-
6	EDO	J	301	-	-	0/1/1/1	-
6	EDO	A	301	-	-	1/1/1/1	-
6	EDO	E	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	EDO	O1-C1-C2-O2
6	I	302	EDO	O1-C1-C2-O2
6	D	301	EDO	O1-C1-C2-O2
8	F	301	GOL	O1-C1-C2-C3
6	E	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	EDO	2	0
7	J	305	SO4	1	5

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%)	-0.21	1 (0%) 88 86	33, 66, 112, 147	1 (0%)
1	F	276/276 (100%)	0.08	0 100 100	59, 92, 125, 144	0
2	B	100/100 (100%)	-0.37	1 (1%) 79 74	43, 61, 89, 107	0
2	G	100/100 (100%)	0.14	1 (1%) 79 74	71, 101, 130, 154	0
3	C	9/9 (100%)	-0.27	0 100 100	41, 43, 59, 64	0
3	H	9/9 (100%)	-0.20	0 100 100	62, 66, 79, 95	0
4	D	201/201 (100%)	-0.13	1 (0%) 87 83	37, 66, 114, 137	0
4	I	200/201 (99%)	-0.25	1 (0%) 87 83	41, 64, 103, 136	0
5	E	242/242 (100%)	-0.31	0 100 100	35, 59, 92, 126	0
5	J	241/242 (99%)	-0.23	2 (0%) 82 77	45, 63, 97, 149	0
All	All	1654/1656 (99%)	-0.16	7 (0%) 88 86	33, 69, 117, 154	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	192	ILE	2.8
5	J	2	ALA	2.6
5	J	238	TRP	2.5
4	I	127	LYS	2.5
2	G	98	ASP	2.2
2	B	0	MET	2.1
1	A	270	LEU	2.1

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	EDO	D	301	4/4	0.64	0.21	69,75,75,77	0
6	EDO	I	303	4/4	0.75	0.13	84,85,87,91	0
6	EDO	I	302	4/4	0.78	0.17	70,71,73,74	0
6	EDO	I	301	4/4	0.80	0.18	71,75,80,82	0
6	EDO	A	302	4/4	0.81	0.12	72,72,72,74	0
8	GOL	F	301	6/6	0.81	0.13	75,90,93,98	0
7	SO4	J	304	5/5	0.82	0.17	89,91,97,98	0
6	EDO	E	301	4/4	0.83	0.10	66,73,74,81	0
6	EDO	J	301	4/4	0.84	0.20	64,66,71,72	0
6	EDO	A	301	4/4	0.86	0.13	61,62,62,65	0
7	SO4	A	303	5/5	0.88	0.13	96,99,102,103	0
7	SO4	E	303	5/5	0.91	0.10	93,94,96,104	0
7	SO4	E	302	5/5	0.93	0.07	72,78,82,84	0
7	SO4	J	303	5/5	0.94	0.08	67,69,69,70	0
7	SO4	J	302	5/5	0.95	0.10	63,69,71,84	0
7	SO4	J	305	5/5	0.98	0.06	48,75,153,165	1

6.5 Other polymers [i](#)

There are no such residues in this entry.