



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 02:32 PM EDT

PDB ID : 6EQB
Title : HLA class I histocompatibility antigen
Authors : Rizkallah, P.J.; Cole, D.K.
Deposited on : 2017-10-12
Resolution : 2.81 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

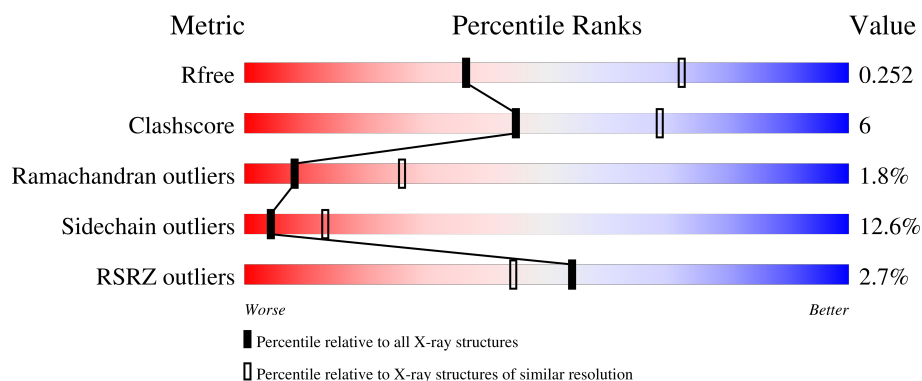
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	<div> <div>7%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
2	B	100	<div> <div>%</div> <div>73%</div> <div>27%</div> </div>
3	C	9	<div> <div>33%</div> <div>56%</div> <div>11%</div> </div>
4	D	196	<div> <div>%</div> <div>70%</div> <div>25%</div> <div>5%</div> </div>
5	E	244	<div> <div>78%</div> <div>20%</div> </div>

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	B	101	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6749 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			

- 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			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called ALA-ALA-GLY-ILE-GLY-ILE-LEU-THR-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	6	0
			91	59	15	17			

- Molecule 4 is a protein called High Affinity Mel5 TCR, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	196	Total	C	N	O	S	0	0	0
			1525	947	255	315	8			

- Molecule 5 is a protein called High Affinity Mel5 TCR, beta chain.

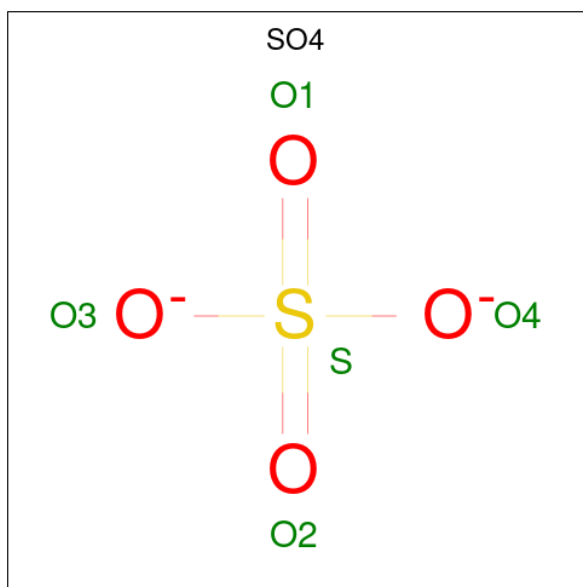
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	3	0
			1966	1247	342	371	6			

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



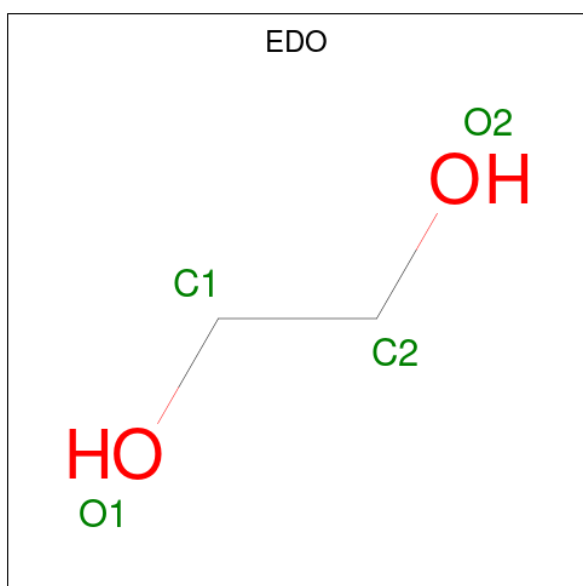
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0

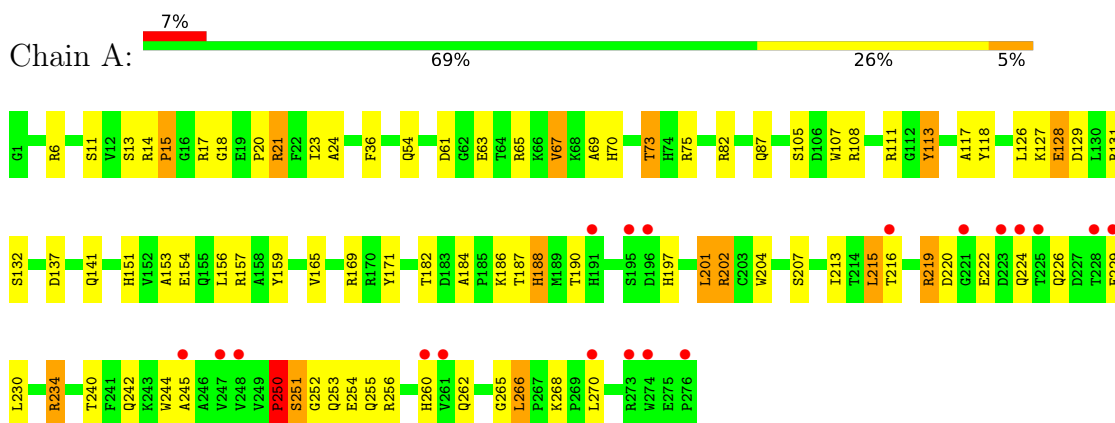
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	6	Total O 6 6	0	0
9	D	4	Total O 4 4	0	0
9	E	6	Total O 6 6	0	0

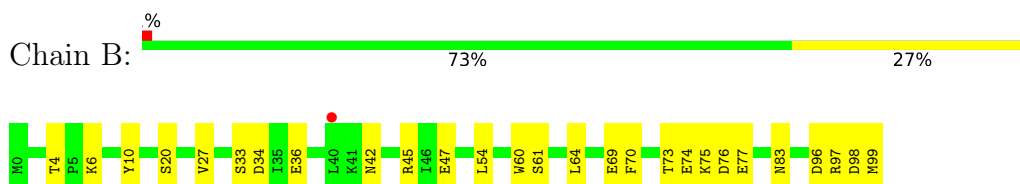
3 Residue-property plots [i](#)

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



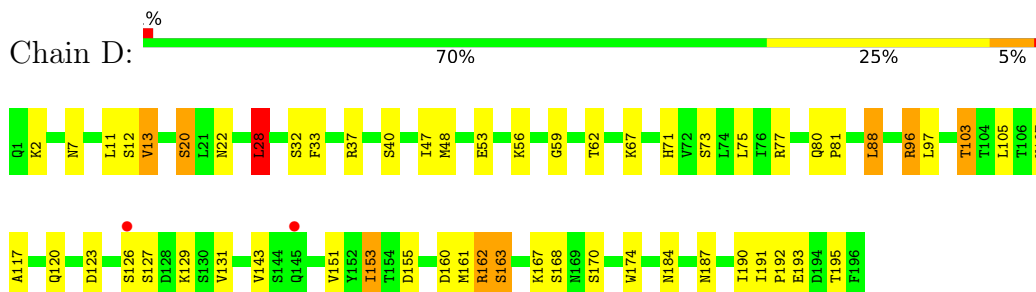
- Molecule 2: Beta-2-microglobulin



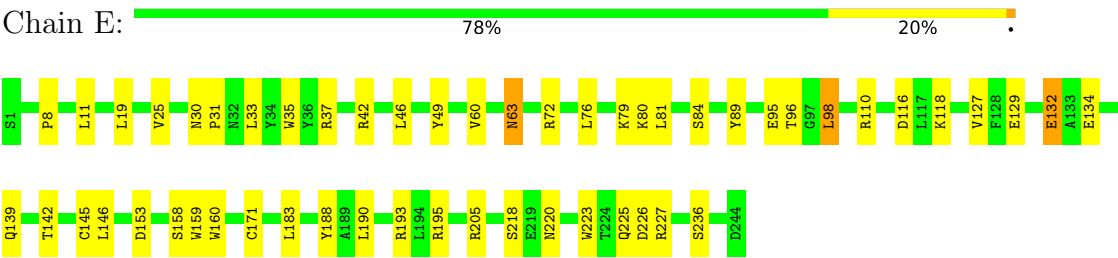
- Molecule 3: ALA-ALA-GLY-ILE-GLY-ILE-LEU-THR-VAL



- Molecule 4: High Affinity Mel5 TCR, alpha chain



● Molecule 5: High Affinity Mel5 TCR, beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	120.77Å 120.77Å 82.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	120.77 – 2.81 120.77 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (120.77-2.81) 100.0 (120.77-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.183 , 0.251 0.187 , 0.252	Depositor DCC
R_{free} test set	1478 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, SO4, EPE

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	0.98	1/2320 (0.0%)	1.05	9/3149 (0.3%)
2	B	0.96	0/860	0.99	1/1162 (0.1%)
3	C	0.75	0/90	0.89	0/120
4	D	1.08	0/1556	1.16	10/2107 (0.5%)
5	E	0.99	2/2026 (0.1%)	1.06	7/2763 (0.3%)
All	All	1.00	3/6852 (0.0%)	1.07	27/9301 (0.3%)

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	2
3	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CD-OE1	7.77	1.34	1.25
5	E	134	GLU	CD-OE1	6.48	1.32	1.25
5	E	132	GLU	CG-CD	5.09	1.59	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	96	ARG	NE-CZ-NH1	8.89	124.75	120.30
4	D	96	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	82	ARG	NE-CZ-NH1	-7.38	116.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	NE-CZ-NH2	-7.17	116.72	120.30
5	E	110	ARG	NE-CZ-NH2	-6.67	116.97	120.30
4	D	77	ARG	NE-CZ-NH1	6.36	123.48	120.30
5	E	227	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	61	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	21	ARG	NE-CZ-NH2	-5.99	117.31	120.30
4	D	37	ARG	NE-CZ-NH2	-5.97	117.32	120.30
5	E	42	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	B	61	SER	CB-CA-C	-5.89	98.91	110.10
4	D	123	ASP	CB-CG-OD1	5.87	123.58	118.30
5	E	116	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	111	ARG	NE-CZ-NH2	5.62	123.11	120.30
4	D	88	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	65	ARG	NE-CZ-NH2	-5.45	117.58	120.30
4	D	155	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	A	201	LEU	CA-CB-CG	5.31	127.52	115.30
5	E	110	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	108	ARG	NE-CZ-NH1	5.21	122.91	120.30
5	E	98	LEU	CA-CB-CG	5.21	127.28	115.30
4	D	155	ASP	CB-CG-OD1	5.14	122.92	118.30
4	D	28	LEU	CB-CG-CD2	5.13	119.73	111.00
4	D	88	LEU	CB-CG-CD1	5.09	119.66	111.00
5	E	205	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	137	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	LYS	Peptide
1	A	224	GLN	Peptide
3	C	4[B]	GLY	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	36	0
2	B	837	0	803	6	0
3	C	91	0	100	6	0
4	D	1525	0	1439	28	0
5	E	1966	0	1864	17	0
6	A	30	0	36	0	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
8	D	8	0	12	0	0
9	A	2	0	0	0	0
9	B	6	0	0	0	0
9	D	4	0	0	0	0
9	E	6	0	0	0	0
All	All	6749	0	6357	85	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 6.

All (85) 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:188:HIS:HB2	1:A:204:TRP:HB2	1.53	0.90
5:E:63:ASN:ND2	5:E:80:LYS:O	2.17	0.76
4:D:7:ASN:O	4:D:103:THR:HB	1.89	0.72
1:A:171:TYR:HH	3:C:2[B]:ALA:N	1.90	0.70
1:A:6:ARG:NE	1:A:113:TYR:OH	2.25	0.69
1:A:202:ARG:NH2	2:B:98:ASP:O	2.26	0.68
1:A:69:ALA:O	1:A:73:THR:HG22	1.93	0.68
1:A:14:ARG:O	1:A:15:PRO:C	2.33	0.67
4:D:116:PRO:O	4:D:192:PRO:CD	2.42	0.67
4:D:116:PRO:O	4:D:192:PRO:HD2	1.94	0.67
2:B:42:ASN:HA	2:B:77:GLU:HB2	1.77	0.66
1:A:215:LEU:HD11	1:A:245:ALA:HB3	1.78	0.65
4:D:47:ILE:HG22	4:D:48:MET:HG2	1.79	0.64
4:D:117:ALA:HA	4:D:192:PRO:HD2	1.81	0.61
1:A:197:HIS:O	1:A:251:SER:HB2	2.01	0.61
4:D:112:GLN:HE21	4:D:112:GLN:HA	1.66	0.61
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.37	0.60
5:E:19:LEU:HB2	5:E:81:LEU:HD11	1.84	0.59
5:E:8:PRO:HG2	5:E:11:LEU:HD21	1.85	0.58
4:D:33:PHE:CD1	4:D:33:PHE:N	2.73	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:VAL:HG23	4:D:174:TRP:HB3	1.87	0.57
1:A:159:TYR:CD1	3:C:4[B]:GLY:HA2	2.40	0.57
5:E:8:PRO:CG	5:E:11:LEU:HD21	2.36	0.56
3:C:7[A]:ILE:C	3:C:8:LEU:HD23	2.27	0.56
4:D:53:GLU:OE2	4:D:67:LYS:N	2.40	0.55
4:D:143:VAL:CG1	4:D:153:ILE:HD11	2.37	0.54
4:D:20:SER:HB2	4:D:75:LEU:CD2	2.37	0.54
3:C:7[B]:ILE:C	3:C:8:LEU:HD23	2.28	0.54
1:A:250:PRO:O	1:A:252:GLY:N	2.42	0.53
1:A:151:HIS:HB3	1:A:154:GLU:HG2	1.90	0.53
1:A:213:ILE:HG23	1:A:213:ILE:O	2.09	0.52
5:E:158:SER:HG	5:E:160:TRP:HE1	1.57	0.52
4:D:153:ILE:HD13	4:D:153:ILE:O	2.09	0.52
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.45	0.51
4:D:96:ARG:HD2	5:E:46:LEU:HD22	1.93	0.50
1:A:107:TRP:O	1:A:169:ARG:NH1	2.41	0.50
4:D:191:ILE:CG2	4:D:193:GLU:O	2.60	0.50
5:E:25:VAL:HG11	5:E:31:PRO:HG3	1.93	0.50
4:D:32:SER:C	4:D:33:PHE:CD1	2.86	0.49
4:D:81:PRO:HA	4:D:107:VAL:HB	1.95	0.49
1:A:184:ALA:HB2	1:A:265:GLY:O	2.12	0.49
1:A:156:LEU:HD21	3:C:6[B]:GLY:O	2.13	0.48
5:E:145:CYS:HB2	5:E:159:TRP:CZ2	2.48	0.48
4:D:187:ASN:OD1	4:D:187:ASN:C	2.51	0.48
4:D:153:ILE:HD13	4:D:153:ILE:C	2.34	0.48
4:D:20:SER:HB2	4:D:75:LEU:HD23	1.95	0.48
4:D:160:ASP:HB2	4:D:162:ARG:HH11	1.79	0.47
1:A:234:ARG:NH1	1:A:242:GLN:HE21	2.11	0.47
4:D:13:VAL:HG13	4:D:105:LEU:HD11	1.96	0.47
1:A:87:GLN:OE1	1:A:118:TYR:OH	2.25	0.46
4:D:161:MET:O	4:D:163:SER:N	2.49	0.46
4:D:143:VAL:HG12	4:D:153:ILE:HD11	1.96	0.46
1:A:67:VAL:O	1:A:70:HIS:HB2	2.16	0.45
1:A:127:LYS:O	1:A:129:ASP:O	2.34	0.45
1:A:220:ASP:HB2	1:A:256:ARG:HG2	1.99	0.45
5:E:37[A]:ARG:HD3	5:E:89:TYR:CE1	2.50	0.45
1:A:207:SER:HA	1:A:240:THR:CB	2.46	0.45
1:A:21:ARG:NH2	1:A:23:ILE:HD11	2.32	0.45
1:A:219:ARG:HB2	1:A:222:GLU:HB3	1.99	0.45
1:A:234:ARG:HH11	1:A:242:GLN:HE21	1.65	0.45
4:D:22:ASN:OD1	4:D:71:HIS:CE1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HA	1:A:20:PRO:HB3	1.99	0.44
1:A:219:ARG:O	1:A:220:ASP:C	2.55	0.44
4:D:160:ASP:OD1	4:D:167:LYS:HG2	2.17	0.44
1:A:128:GLU:C	1:A:129:ASP:O	2.52	0.43
2:B:73:THR:OG1	2:B:76:ASP:HB3	2.19	0.43
5:E:95:GLU:O	5:E:96:THR:C	2.57	0.43
5:E:30:ASN:N	5:E:31:PRO:CD	2.82	0.43
1:A:204:TRP:CH2	1:A:244:TRP:CD1	3.08	0.42
5:E:25:VAL:HG13	5:E:72:ARG:HD2	2.02	0.42
1:A:234:ARG:HD3	1:A:242:GLN:HG3	2.02	0.42
5:E:142:THR:OG1	5:E:195:ARG:HG3	2.19	0.42
1:A:182:THR:O	1:A:182:THR:HG23	2.20	0.41
1:A:131:ARG:HA	1:A:153:ALA:HB1	2.01	0.41
1:A:23:ILE:HG21	2:B:54:LEU:HB3	2.01	0.41
4:D:56:LYS:O	4:D:62:THR:HA	2.21	0.41
4:D:191:ILE:HG22	4:D:193:GLU:O	2.20	0.41
5:E:223:TRP:CE2	5:E:225:GLN:HB2	2.56	0.41
1:A:24:ALA:HB3	1:A:36:PHE:HB3	2.03	0.41
4:D:191:ILE:HD13	4:D:191:ILE:HG21	1.89	0.41
5:E:35:TRP:CE2	5:E:76:LEU:HB2	2.56	0.41
1:A:266:LEU:HD22	1:A:268:LYS:O	2.21	0.40
5:E:19:LEU:HD22	5:E:81:LEU:HD21	2.03	0.40
3:C:6[B]:GLY:C	3:C:7[B]:ILE:HG12	2.41	0.40
5:E:153:ASP:HB3	5:E:188:TYR:CE2	2.56	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%)	247 (90%)	21 (8%)	6 (2%)	6 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	7	23
3	C	12/9 (133%)	6 (50%)	6 (50%)	0	100	100
4	D	194/196 (99%)	174 (90%)	14 (7%)	6 (3%)	4	13
5	E	245/244 (100%)	233 (95%)	11 (4%)	1 (0%)	34	64
All	All	823/825 (100%)	746 (91%)	62 (8%)	15 (2%)	8	26

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	251	SER
4	D	195	THR
1	A	18	GLY
4	D	126	SER
1	A	253	GLN
2	B	74	GLU
4	D	28	LEU
4	D	162	ARG
5	E	84	SER
1	A	15	PRO
2	B	97	ARG
4	D	40	SER
1	A	250	PRO
4	D	59	GLY

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%)	201 (87%)	31 (13%)	4	11
2	B	95/95 (100%)	79 (83%)	16 (17%)	2	6
3	C	7/5 (140%)	5 (71%)	2 (29%)	0	1
4	D	174/174 (100%)	152 (87%)	22 (13%)	4	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	213/210 (101%)	193 (91%)	20 (9%)	8	25
All	All	721/716 (101%)	630 (87%)	91 (13%)	4	13

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	54	GLN
1	A	67	VAL
1	A	73	THR
1	A	75	ARG
1	A	105	SER
1	A	113	TYR
1	A	126	LEU
1	A	128	GLU
1	A	132	SER
1	A	141	GLN
1	A	165	VAL
1	A	187	THR
1	A	188	HIS
1	A	190	THR
1	A	201	LEU
1	A	202	ARG
1	A	215	LEU
1	A	216	THR
1	A	219	ARG
1	A	226	GLN
1	A	229	GLU
1	A	230	LEU
1	A	234	ARG
1	A	250	PRO
1	A	254	GLU
1	A	255	GLN
1	A	260	HIS
1	A	262	GLN
1	A	266	LEU
1	A	270	LEU
2	B	4	THR
2	B	6	LYS
2	B	20	SER
2	B	27	VAL
2	B	33	SER

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Mol	Chain	Res	Type
2	B	34	ASP
2	B	36	GLU
2	B	45	ARG
2	B	47	GLU
2	B	64	LEU
2	B	69	GLU
2	B	70	PHE
2	B	75	LYS
2	B	83	ASN
2	B	96	ASP
2	B	99	MET
3	C	5[A]	ILE
3	C	5[B]	ILE
4	D	2	LYS
4	D	11	LEU
4	D	12	SER
4	D	13	VAL
4	D	20	SER
4	D	28	LEU
4	D	73	SER
4	D	80	GLN
4	D	88	LEU
4	D	97	LEU
4	D	103	THR
4	D	112	GLN
4	D	120	GLN
4	D	127	SER
4	D	129	LYS
4	D	151	VAL
4	D	153	ILE
4	D	163	SER
4	D	168	SER
4	D	170	SER
4	D	184	ASN
4	D	190	ILE
5	E	33	LEU
5	E	49	TYR
5	E	60	VAL
5	E	63	ASN
5	E	79	LYS
5	E	98	LEU
5	E	118	LYS

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Mol	Chain	Res	Type
5	E	127	VAL
5	E	129	GLU
5	E	132	GLU
5	E	139	GLN
5	E	146	LEU
5	E	171	CYS
5	E	183	LEU
5	E	190	LEU
5	E	193	ARG
5	E	218	SER
5	E	220	ASN
5	E	226	ASP
5	E	236	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	54	GLN
1	A	70	HIS
1	A	74	HIS
1	A	93	HIS
1	A	141	GLN
1	A	180	GLN
1	A	218	GLN
1	A	242	GLN
1	A	255	GLN
1	A	262	GLN
2	B	17	ASN
2	B	83	ASN
4	D	71	HIS
4	D	80	GLN
4	D	112	GLN
5	E	225	GLN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	EDO	D	301	-	3,3,3	0.63	0	2,2,2	0.30	0
6	EPE	A	301	-	15,15,15	2.08	1 (6%)	18,20,20	1.50	1 (5%)
7	SO4	A	304	-	4,4,4	0.44	0	6,6,6	0.41	0
7	SO4	D	303	-	4,4,4	0.34	0	6,6,6	0.36	0
7	SO4	A	303	-	4,4,4	0.46	0	6,6,6	0.87	0
6	EPE	A	302	-	15,15,15	1.75	1 (6%)	18,20,20	1.53	2 (11%)
7	SO4	B	101	-	4,4,4	0.41	0	6,6,6	0.27	0
8	EDO	D	302	-	3,3,3	0.45	0	2,2,2	0.29	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	EPE	A	302	-	-	5/9/19/19	0/1/1/1
8	EDO	D	302	-	-	0/1/1/1	-
8	EDO	D	301	-	-	0/1/1/1	-
6	EPE	A	301	-	-	3/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	301	EPE	C10-S	-7.63	1.66	1.77
6	A	302	EPE	C10-S	-6.21	1.68	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	EPE	O2S-S-C10	4.83	112.74	106.92
6	A	302	EPE	O2S-S-C10	4.38	112.19	106.92
6	A	302	EPE	O3S-S-C10	2.38	109.62	105.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	EPE	N4-C7-C8-O8
6	A	302	EPE	C10-C9-N1-C2
6	A	302	EPE	C9-C10-S-O1S
6	A	302	EPE	C9-C10-S-O3S
6	A	302	EPE	S-C10-C9-N1
6	A	301	EPE	C9-C10-S-O2S
6	A	302	EPE	C9-C10-S-O2S
6	A	301	EPE	C9-C10-S-O3S

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 [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%)	0.29	19 (6%) 16 10	40, 73, 155, 170	0
2	B	100/100 (100%)	-0.08	1 (1%) 82 77	50, 88, 139, 158	0
3	C	9/9 (100%)	0.59	0 100 100	32, 38, 50, 56	0
4	D	196/196 (100%)	0.06	2 (1%) 82 77	36, 62, 123, 145	0
5	E	244/244 (100%)	-0.10	0 100 100	37, 60, 100, 125	0
All	All	825/825 (100%)	0.08	22 (2%) 54 44	32, 66, 142, 170	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	7.0
1	A	228	THR	4.0
1	A	221	GLY	3.7
1	A	223	ASP	3.7
1	A	224	GLN	3.2
1	A	245	ALA	2.9
1	A	195	SER	2.8
1	A	216	THR	2.7
4	D	126	SER	2.6
1	A	276	PRO	2.5
1	A	248	VAL	2.4
1	A	261	VAL	2.3
1	A	229	GLU	2.3
1	A	191	HIS	2.2
1	A	260	HIS	2.2
1	A	225	THR	2.1
1	A	196	ASP	2.1
2	B	40	LEU	2.1
1	A	273	ARG	2.1
1	A	270	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	145	GLN	2.0
1	A	274	TRP	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EPE	A	302	15/15	0.71	0.28	103,131,203,206	0
7	SO4	B	101	5/5	0.78	0.47	134,148,152,155	0
7	SO4	A	304	5/5	0.85	0.20	118,122,133,133	0
7	SO4	A	303	5/5	0.93	0.27	84,85,88,96	0
8	EDO	D	301	4/4	0.93	0.20	56,59,61,64	0
7	SO4	D	303	5/5	0.94	0.17	100,101,104,115	0
8	EDO	D	302	4/4	0.95	0.19	66,67,71,72	0
6	EPE	A	301	15/15	0.96	0.20	58,90,113,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.