



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 10:59 PM UTC

PDB ID : 6EQA / pdb_00006eqa
Title : HLA class I histocompatibility antigen
Authors : Rizkallah, P.J.; Cole, D.K.
Deposited on : 2017-10-12
Resolution : 3.16 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

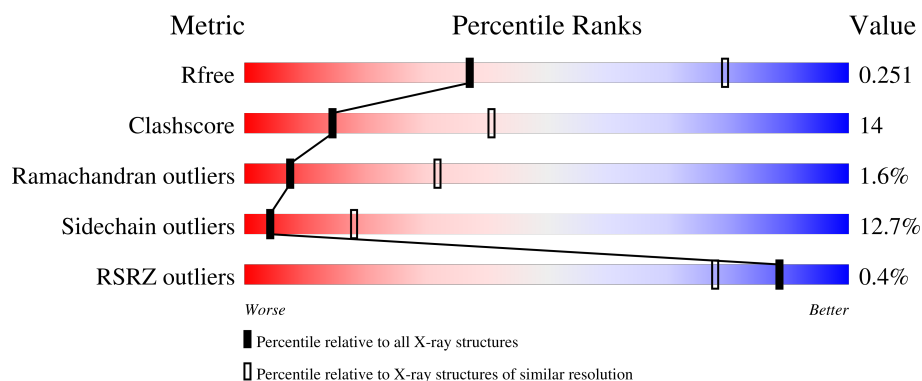
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	71% 23% 5%
2	B	100	64% 33% .
3	C	9	22% 56% 22%
4	D	194	% 60% 33% 7%
5	E	244	66% 29% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6627 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 Mel5 TCR, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	194	Total	C	N	O	S	0	0	0
			1498	927	249	314	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	0	0
			1926	1221	330	370	5			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		

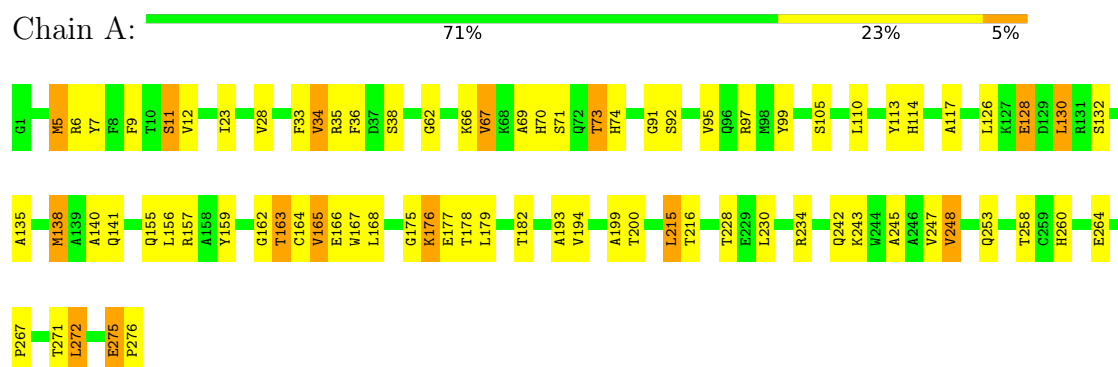
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		

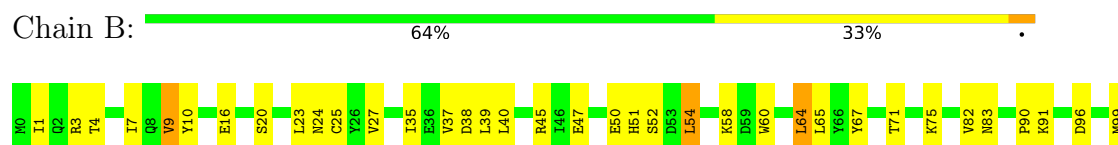
3 Residue-property plots

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.

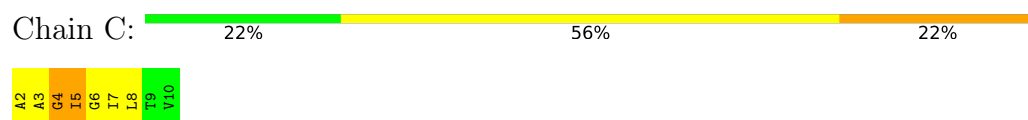
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



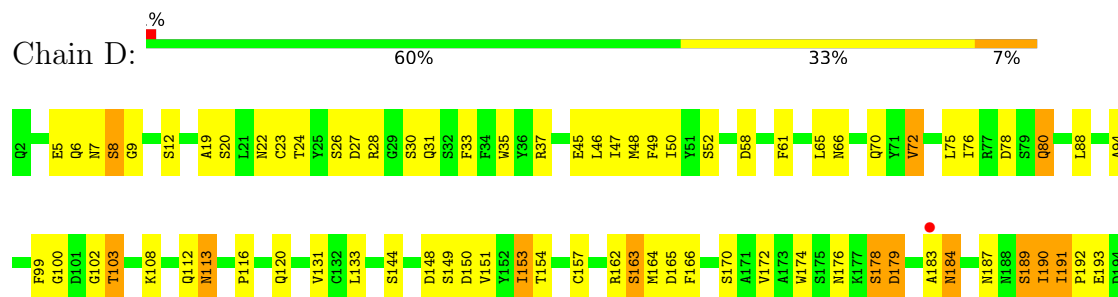
- Molecule 2: Beta-2-microglobulin



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



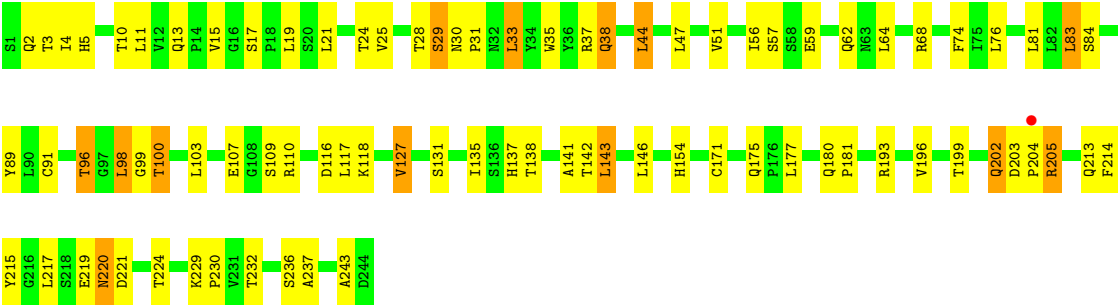
- Molecule 4: Mel5 TCR, alpha chain



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● Molecule 5: Mel5 TCR, beta chain

Chain E: 66% 29% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	121.40Å 121.40Å 82.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.13 – 3.16 68.13 – 3.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.13-3.16) 99.9 (68.13-3.16)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.263 0.188 , 0.251	Depositor DCC
R_{free} test set	1062 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6627	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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

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	0.74	0/2320	0.89	2/3149 (0.1%)
2	B	0.73	0/860	0.91	1/1162 (0.1%)
3	C	0.67	0/90	0.74	0/120
4	D	0.86	0/1527	1.03	5/2070 (0.2%)
5	E	0.80	0/1979	0.93	2/2698 (0.1%)
All	All	0.78	0/6776	0.94	10/9199 (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
3	C	0	1
4	D	0	3
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	100	THR	N-CA-C	-8.61	99.04	110.24
4	D	80	GLN	CA-C-N	6.96	127.25	119.32
4	D	80	GLN	C-N-CA	6.96	127.25	119.32
2	B	51	HIS	N-CA-C	5.99	118.03	107.61
4	D	108	LYS	CA-C-N	-5.53	114.56	120.03
4	D	108	LYS	C-N-CA	-5.53	114.56	120.03
1	A	73	THR	N-CA-C	-5.12	105.78	111.36
1	A	272	LEU	N-CA-C	5.11	116.91	108.13
4	D	150	ASP	N-CA-C	-5.07	106.51	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	E	116	ASP	N-CA-C	5.01	116.57	108.26

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	4[B]	GLY	Peptide
4	D	149	SER	Peptide
4	D	178	SER	Peptide
4	D	8	SER	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	55	0
2	B	837	0	803	19	0
3	C	91	0	100	30	0
4	D	1498	0	1410	50	0
5	E	1926	0	1845	52	0
6	B	5	0	0	0	0
6	D	5	0	0	0	0
6	E	10	0	0	0	0
7	B	1	0	0	0	0
All	All	6627	0	6261	181	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 14.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5[B]:ILE:HD12	3:C:6[B]:GLY:N	1.43	1.28
3:C:5[B]:ILE:CD1	3:C:6[B]:GLY:N	2.22	1.01
1:A:200:THR:HG22	1:A:248:VAL:HG23	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5[B]:ILE:CD1	3:C:6[B]:GLY:H	1.81	0.89
4:D:116:PRO:HB2	4:D:191:ILE:HG22	1.54	0.88
4:D:7:ASN:O	4:D:103:THR:HB	1.76	0.85
3:C:5[B]:ILE:HD12	3:C:6[B]:GLY:H	1.35	0.85
1:A:167:TRP:CD1	3:C:2[B]:ALA:HB2	2.17	0.79
4:D:23:CYS:HB3	4:D:72:VAL:HG23	1.65	0.78
4:D:6:GLN:CG	4:D:103:THR:HG22	2.14	0.77
3:C:7[B]:ILE:HG13	3:C:7[B]:ILE:O	1.83	0.77
1:A:138:MET:HE2	1:A:141:GLN:HG3	1.65	0.76
3:C:7[B]:ILE:C	3:C:7[B]:ILE:HD12	2.10	0.75
4:D:189:SER:O	4:D:191:ILE:HG23	1.87	0.74
3:C:7[B]:ILE:O	3:C:7[B]:ILE:CG1	2.35	0.74
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.23	0.74
4:D:116:PRO:HB2	4:D:191:ILE:CG2	2.17	0.73
2:B:9:VAL:HG23	2:B:23:LEU:HD11	1.71	0.73
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.70	0.72
3:C:5[B]:ILE:HD12	3:C:5[B]:ILE:C	2.14	0.71
5:E:30:ASN:O	5:E:96:THR:HB	1.90	0.71
4:D:131:VAL:HG12	4:D:174:TRP:CB	2.20	0.71
4:D:37:ARG:HB2	4:D:47:ILE:HD11	1.73	0.70
3:C:5[B]:ILE:HD12	3:C:6[B]:GLY:CA	2.21	0.70
4:D:6:GLN:HG3	4:D:103:THR:HG22	1.73	0.70
4:D:28:ARG:HG2	4:D:70:GLN:OE1	1.92	0.70
1:A:228:THR:HG22	1:A:247:VAL:HG23	1.74	0.68
1:A:66:LYS:NZ	3:C:3[B]:ALA:HB3	2.10	0.66
5:E:127:VAL:HG12	5:E:237:ALA:HB3	1.77	0.66
3:C:5[B]:ILE:O	3:C:6[B]:GLY:C	2.39	0.66
1:A:135:ALA:HB1	1:A:140:ALA:HB1	1.78	0.65
3:C:5[B]:ILE:O	3:C:7[B]:ILE:CG2	2.45	0.65
3:C:5[B]:ILE:O	3:C:7[B]:ILE:HG22	1.96	0.64
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.79	0.64
4:D:131:VAL:HG12	4:D:174:TRP:HB3	1.80	0.62
4:D:144:SER:O	4:D:153:ILE:HD11	2.00	0.62
1:A:155:GLN:OE1	3:C:6[B]:GLY:HA2	2.00	0.62
1:A:36:PHE:CD2	1:A:67:VAL:HG11	2.35	0.61
5:E:127:VAL:HG12	5:E:237:ALA:CB	2.30	0.61
3:C:7[B]:ILE:O	3:C:7[B]:ILE:CD1	2.47	0.61
1:A:175:GLY:O	1:A:176:LYS:C	2.42	0.61
1:A:135:ALA:HB1	1:A:140:ALA:CB	2.30	0.60
4:D:27:ASP:O	4:D:30:SER:OG	2.19	0.60
3:C:7[B]:ILE:O	3:C:7[B]:ILE:HD12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:GLN:NE2	4:D:100:GLY:HA3	2.17	0.59
4:D:131:VAL:HG12	4:D:174:TRP:HB2	1.81	0.59
1:A:23:ILE:HG21	2:B:54:LEU:HD23	1.84	0.59
4:D:6:GLN:HE21	4:D:100:GLY:HA3	1.68	0.59
5:E:117:LEU:HD13	5:E:217:LEU:CD2	2.32	0.59
4:D:8:SER:OG	4:D:9:GLY:N	2.36	0.58
4:D:116:PRO:O	4:D:192:PRO:HD2	2.03	0.58
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.50	0.58
2:B:83:ASN:HD22	2:B:90:PRO:HG3	1.68	0.57
5:E:37:ARG:HD2	5:E:89:TYR:CZ	2.39	0.57
4:D:37:ARG:CB	4:D:47:ILE:HD11	2.34	0.57
5:E:15:VAL:CG2	5:E:83:LEU:HD23	2.35	0.57
1:A:62:GLY:HA2	4:D:94:ALA:HB1	1.87	0.56
1:A:228:THR:HG22	1:A:247:VAL:CG2	2.36	0.56
5:E:19:LEU:HD11	5:E:21:LEU:HG	1.88	0.56
1:A:167:TRP:CG	3:C:2[B]:ALA:HB2	2.41	0.55
4:D:133:LEU:CD2	5:E:142:THR:HG21	2.36	0.55
5:E:203:ASP:OD1	5:E:203:ASP:C	2.49	0.55
4:D:48:MET:HE3	4:D:61:PHE:HB2	1.88	0.55
5:E:38:GLN:HG3	5:E:44:LEU:HD22	1.88	0.55
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.54	0.55
5:E:214:PHE:O	5:E:232:THR:HG23	2.07	0.55
1:A:162:GLY:O	1:A:165:VAL:HG13	2.08	0.54
1:A:97:ARG:NH1	1:A:114:HIS:NE2	2.55	0.54
4:D:112:GLN:HE21	4:D:113:ASN:HD21	1.55	0.54
1:A:159:TYR:CZ	1:A:164:CYS:HB2	2.43	0.53
4:D:6:GLN:HG2	4:D:103:THR:HG22	1.89	0.53
1:A:73:THR:HG21	3:C:7[B]:ILE:HD11	1.90	0.53
5:E:117:LEU:HD13	5:E:217:LEU:HD22	1.89	0.53
5:E:17:SER:HB3	5:E:81:LEU:HD12	1.90	0.53
1:A:66:LYS:HD2	3:C:3[B]:ALA:HB3	1.91	0.53
2:B:20:SER:HA	2:B:71:THR:HG22	1.90	0.53
4:D:48:MET:HE2	4:D:58:ASP:HB3	1.91	0.52
5:E:110:ARG:HE	5:E:154:HIS:CD2	2.28	0.52
2:B:23:LEU:HD12	2:B:24:ASN:N	2.25	0.52
3:C:5[B]:ILE:HD13	3:C:6[B]:GLY:H	1.73	0.52
5:E:10:THR:HG21	5:E:215:TYR:CG	2.45	0.52
1:A:5:MET:HE1	3:C:2[B]:ALA:N	2.24	0.52
4:D:133:LEU:HD21	5:E:142:THR:HG21	1.92	0.52
5:E:202:GLN:O	5:E:204:PRO:HD3	2.10	0.51
4:D:157:CYS:C	5:E:171:CYS:SG	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:PHE:CD1	4:D:49:PHE:C	2.89	0.51
5:E:10:THR:HG21	5:E:215:TYR:CB	2.40	0.51
1:A:7:TYR:HH	3:C:2[B]:ALA:N	2.07	0.51
4:D:35:TRP:O	4:D:46:LEU:HD12	2.12	0.50
4:D:112:GLN:HE21	4:D:113:ASN:ND2	2.09	0.50
5:E:35:TRP:CD1	5:E:74:PHE:CE2	3.00	0.49
1:A:260:HIS:CD2	1:A:271:THR:HG22	2.47	0.49
5:E:202:GLN:HG3	5:E:243:ALA:HA	1.95	0.49
1:A:5:MET:HE3	1:A:7:TYR:HE1	1.77	0.49
1:A:66:LYS:HZ1	3:C:3[B]:ALA:HB3	1.76	0.49
5:E:10:THR:O	5:E:11:LEU:HD23	2.12	0.49
5:E:56:ILE:HG22	5:E:57:SER:N	2.28	0.49
3:C:5[B]:ILE:O	3:C:7[B]:ILE:HG23	2.13	0.49
5:E:33:LEU:HD22	5:E:68:ARG:CZ	2.42	0.49
2:B:96:ASP:HB3	2:B:99:MET:HB3	1.95	0.48
5:E:219:GLU:O	5:E:220:ASN:OD1	2.32	0.48
2:B:50:GLU:HB2	2:B:67:TYR:CE1	2.49	0.48
1:A:138:MET:CE	1:A:141:GLN:HG3	2.40	0.48
5:E:143:LEU:HD12	5:E:143:LEU:N	2.29	0.47
2:B:1:ILE:HD13	2:B:3:ARG:NH1	2.29	0.47
5:E:30:ASN:N	5:E:31:PRO:HD3	2.29	0.47
5:E:177:LEU:C	5:E:177:LEU:HD12	2.40	0.47
5:E:199:THR:HG22	5:E:199:THR:O	2.15	0.47
2:B:7:ILE:HG12	2:B:27:VAL:HG12	1.95	0.47
5:E:33:LEU:HD22	5:E:68:ARG:NH1	2.30	0.47
1:A:69:ALA:O	1:A:73:THR:HG23	2.15	0.46
1:A:215:LEU:HD13	1:A:245:ALA:HB2	1.97	0.46
4:D:162:ARG:O	4:D:163:SER:C	2.58	0.46
1:A:23:ILE:HG21	2:B:54:LEU:CD2	2.45	0.46
1:A:126:LEU:HD12	1:A:132:SER:O	2.16	0.46
1:A:11:SER:HB2	1:A:95:VAL:HG12	1.98	0.46
5:E:203:ASP:OD1	5:E:205:ARG:N	2.48	0.46
2:B:38:ASP:OD2	2:B:45:ARG:HG3	2.16	0.46
4:D:6:GLN:NE2	4:D:102:GLY:H	2.14	0.46
4:D:20:SER:HB2	4:D:75:LEU:CD2	2.46	0.46
4:D:52:SER:C	4:D:65:LEU:HD23	2.41	0.45
5:E:131:SER:O	5:E:135:ILE:HD12	2.17	0.45
5:E:21:LEU:HD13	5:E:109:SER:HB2	1.98	0.45
3:C:2[B]:ALA:O	3:C:3[B]:ALA:HB2	2.15	0.45
1:A:62:GLY:CA	4:D:94:ALA:HB1	2.47	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:GLY:C	5:E:100:THR:O	2.56	0.45
3:C:4[A]:GLY:O	5:E:98:LEU:HB3	2.17	0.45
4:D:88:LEU:CD1	4:D:88:LEU:N	2.80	0.45
1:A:33:PHE:CD2	1:A:34:VAL:CG1	2.99	0.45
1:A:159:TYR:CE2	1:A:164:CYS:HB2	2.52	0.45
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.99	0.45
5:E:217:LEU:HD12	5:E:230:PRO:HG2	1.99	0.44
4:D:192:PRO:HG3	5:E:137:HIS:NE2	2.32	0.44
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.98	0.44
1:A:70:HIS:O	1:A:71:SER:C	2.61	0.44
5:E:21:LEU:HD13	5:E:109:SER:CB	2.48	0.44
4:D:78:ASP:O	4:D:80:GLN:NE2	2.50	0.44
5:E:56:ILE:CG2	5:E:57:SER:N	2.81	0.44
1:A:6:ARG:HD3	1:A:113:TYR:HE1	1.83	0.44
1:A:156:LEU:O	1:A:157:ARG:C	2.60	0.44
1:A:138:MET:HE3	1:A:138:MET:HA	2.00	0.43
3:C:5[A]:ILE:HG22	5:E:99:GLY:O	2.17	0.43
4:D:99:PHE:CG	5:E:44:LEU:HB2	2.53	0.43
4:D:184:ASN:O	4:D:184:ASN:CG	2.61	0.43
1:A:33:PHE:O	1:A:34:VAL:HG12	2.18	0.43
4:D:164:MET:O	4:D:166:PHE:N	2.50	0.43
4:D:33:PHE:HB2	4:D:50:ILE:HG23	2.01	0.43
1:A:163:THR:O	1:A:164:CYS:C	2.62	0.43
5:E:3:THR:O	5:E:25:VAL:HG23	2.18	0.43
5:E:177:LEU:HD12	5:E:177:LEU:O	2.18	0.43
4:D:66:ASN:OD1	4:D:66:ASN:C	2.62	0.43
5:E:146:LEU:HD12	5:E:146:LEU:HA	1.80	0.43
1:A:275:GLU:N	1:A:276:PRO:HD2	2.33	0.43
4:D:19:ALA:HB3	4:D:76:ILE:HB	2.01	0.42
5:E:180:GLN:O	5:E:181:PRO:C	2.62	0.42
2:B:64:LEU:HD12	2:B:64:LEU:HA	1.86	0.42
1:A:9:PHE:CD1	1:A:9:PHE:N	2.87	0.42
1:A:234:ARG:HD2	2:B:10:TYR:CE2	2.55	0.42
5:E:4:ILE:HD11	5:E:91:CYS:SG	2.59	0.42
3:C:8:LEU:HD22	3:C:8:LEU:N	2.35	0.42
5:E:35:TRP:CE2	5:E:76:LEU:HB2	2.55	0.42
1:A:156:LEU:HD23	3:C:6[A]:GLY:HA3	2.01	0.42
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.01	0.41
1:A:165:VAL:O	1:A:166:GLU:C	2.63	0.41
5:E:141:ALA:HB3	5:E:196:VAL:O	2.20	0.41
1:A:33:PHE:C	1:A:34:VAL:CG1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:O	1:A:177:GLU:N	2.53	0.41
4:D:6:GLN:HG3	4:D:103:THR:CG2	2.48	0.41
4:D:47:ILE:HD12	4:D:47:ILE:HG23	1.68	0.41
4:D:8:SER:O	4:D:9:GLY:O	2.37	0.41
1:A:5:MET:HB3	1:A:168:LEU:HD13	2.02	0.41
5:E:137:HIS:HB3	5:E:138:THR:HG23	2.02	0.41
1:A:70:HIS:CE1	1:A:99:TYR:OH	2.74	0.41
4:D:133:LEU:HD22	5:E:142:THR:HG21	2.03	0.41
4:D:190:ILE:H	4:D:190:ILE:CD1	2.33	0.40
5:E:29:SER:O	5:E:30:ASN:C	2.64	0.40
1:A:128:GLU:O	1:A:130:LEU:HD13	2.21	0.40
1:A:193:ALA:HA	1:A:199:ALA:HA	2.03	0.40
4:D:154:THR:OG1	4:D:172:VAL:HG12	2.22	0.40
5:E:224:THR:HG22	5:E:224:THR:O	2.21	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%)	249 (91%)	21 (8%)	4 (2%)	8	33
2	B	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	6	27
3	C	12/9 (133%)	5 (42%)	5 (42%)	2 (17%)	0	0
4	D	192/194 (99%)	175 (91%)	13 (7%)	4 (2%)	5	26
5	E	242/244 (99%)	219 (90%)	21 (9%)	2 (1%)	16	46
All	All	818/823 (99%)	736 (90%)	68 (8%)	14 (2%)	7	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	163	SER
5	E	205	ARG
1	A	253	GLN
2	B	52	SER
1	A	176	LYS
4	D	165	ASP
4	D	179	ASP
4	D	183	ALA
5	E	220	ASN
1	A	91	GLY
1	A	267	PRO
3	C	5[A]	ILE
3	C	5[B]	ILE
2	B	35	ILE

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%)	205 (88%)	27 (12%)	5	21
2	B	95/95 (100%)	86 (90%)	9 (10%)	8	29
3	C	7/5 (140%)	7 (100%)	0	100	100
4	D	172/172 (100%)	147 (86%)	25 (14%)	3	14
5	E	211/211 (100%)	181 (86%)	30 (14%)	3	15
All	All	717/715 (100%)	626 (87%)	91 (13%)	4	18

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

Mol	Chain	Res	Type
1	A	5	MET
1	A	11	SER
1	A	12	VAL
1	A	34	VAL
1	A	35	ARG
1	A	38	SER

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Mol	Chain	Res	Type
1	A	67	VAL
1	A	92	SER
1	A	105	SER
1	A	110	LEU
1	A	128	GLU
1	A	130	LEU
1	A	138	MET
1	A	163	THR
1	A	165	VAL
1	A	178	THR
1	A	182	THR
1	A	194	VAL
1	A	215	LEU
1	A	216	THR
1	A	230	LEU
1	A	243	LYS
1	A	248	VAL
1	A	258	THR
1	A	264	GLU
1	A	272	LEU
1	A	275	GLU
2	B	4	THR
2	B	9	VAL
2	B	16	GLU
2	B	47	GLU
2	B	54	LEU
2	B	58	LYS
2	B	64	LEU
2	B	75	LYS
2	B	91	LYS
4	D	5	GLU
4	D	12	SER
4	D	22	ASN
4	D	24	THR
4	D	26	SER
4	D	31	GLN
4	D	45	GLU
4	D	72	VAL
4	D	103	THR
4	D	113	ASN
4	D	120	GLN
4	D	148	ASP

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Mol	Chain	Res	Type
4	D	151	VAL
4	D	153	ILE
4	D	170	SER
4	D	176	ASN
4	D	178	SER
4	D	179	ASP
4	D	184	ASN
4	D	187	ASN
4	D	189	SER
4	D	190	ILE
4	D	191	ILE
4	D	193	GLU
4	D	195	THR
5	E	2	GLN
5	E	5	HIS
5	E	13	GLN
5	E	24	THR
5	E	28	THR
5	E	29	SER
5	E	33	LEU
5	E	38	GLN
5	E	44	LEU
5	E	47	LEU
5	E	51	VAL
5	E	59	GLU
5	E	62	GLN
5	E	64	LEU
5	E	83	LEU
5	E	84	SER
5	E	96	THR
5	E	98	LEU
5	E	103	LEU
5	E	107	GLU
5	E	118	LYS
5	E	127	VAL
5	E	143	LEU
5	E	175	GLN
5	E	193	ARG
5	E	202	GLN
5	E	213	GLN
5	E	221	ASP
5	E	229	LYS

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Mol	Chain	Res	Type
5	E	236	SER

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

Mol	Chain	Res	Type
1	A	70	HIS
1	A	72	GLN
1	A	74	HIS
1	A	93	HIS
1	A	141	GLN
1	A	174	ASN
1	A	242	GLN
1	A	255	GLN
2	B	31	HIS
4	D	2	GLN
4	D	6	GLN
4	D	38	GLN
4	D	80	GLN
4	D	112	GLN
4	D	113	ASN
4	D	187	ASN
4	D	188	ASN
5	E	38	GLN
5	E	55	GLN
5	E	70	GLN
5	E	139	GLN
5	E	154	HIS
5	E	175	GLN
5	E	233	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	E	301	-	4,4,4	0.28	0	6,6,6	0.13	0
6	SO4	E	302	-	4,4,4	0.26	0	6,6,6	0.34	0
6	SO4	B	101	-	4,4,4	0.24	0	6,6,6	0.23	0
6	SO4	D	201	-	4,4,4	0.25	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.33	0 100 100	35, 63, 124, 149	0
2	B	100/100 (100%)	-0.32	0 100 100	37, 70, 123, 139	0
3	C	9/9 (100%)	-0.17	0 100 100	15, 15, 39, 43	6 (66%)
4	D	194/194 (100%)	-0.12	2 (1%) 79 62	31, 56, 119, 133	0
5	E	244/244 (100%)	-0.39	1 (0%) 88 78	31, 55, 101, 123	0
All	All	823/823 (100%)	-0.29	3 (0%) 88 78	15, 59, 119, 149	6 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	183	ALA	2.3
4	D	195	THR	2.3
5	E	204	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	E	301	5/5	0.84	0.25	125,125,126,126	0
6	SO4	D	201	5/5	0.87	0.19	127,127,127,127	0
6	SO4	E	302	5/5	0.89	0.19	125,125,125,125	0
6	SO4	B	101	5/5	0.94	0.28	132,132,132,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.