



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 06:38 AM EDT

PDB ID : 4JFD
Title : Preservation of peptide specificity during TCR-MHC contact dominated affinity enhancement of a melanoma-specific TCR
Authors : Rizkallah, P.J.; Cole, D.K.; Madura, F.; Sewell, A.K.
Deposited on : 2013-02-28
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

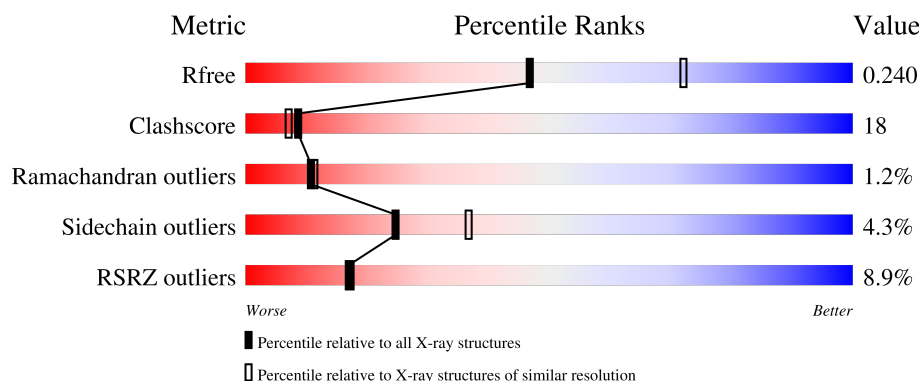
1 Overall quality at a glance

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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (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	<div> <div>18%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
2	B	100	<div> <div>5%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
3	C	10	<div> <div>60%</div> <div>40%</div> </div>
4	D	196	<div> <div>8%</div> <div>72%</div> <div>22%</div> <div>5%</div> <div>.</div> </div>
5	E	245	<div> <div>%</div> <div>71%</div> <div>27%</div> <div>.</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
6	TAM	A	301	-	X	-	-
7	SO4	A	303	-	-	X	-
7	SO4	A	304	-	-	X	-
7	SO4	A	305	-	-	X	-
7	SO4	E	305	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6820 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
			2253	1408	410	426	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 Melanoma peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			70	46	10	14			

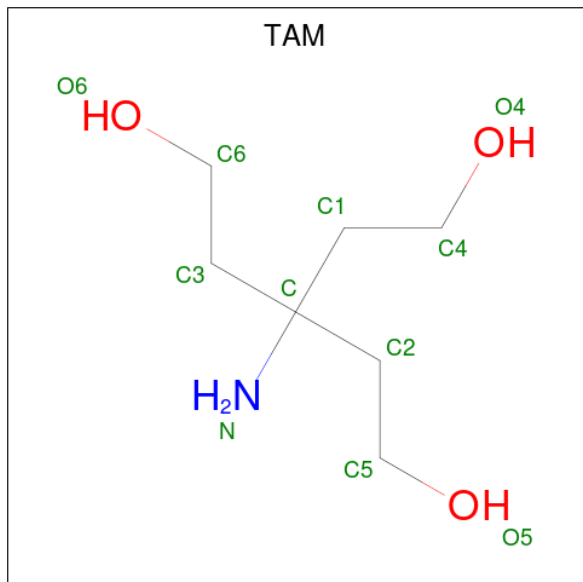
- Molecule 4 is a protein called High Affinity TCR Alpha Chain.

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 TCR Beta Chain.

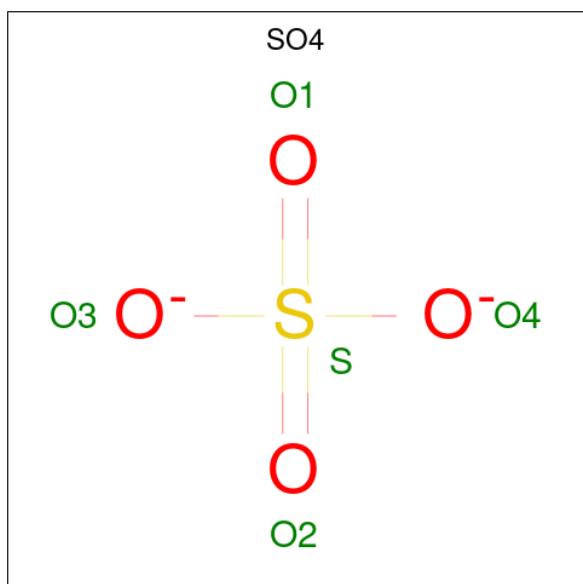
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1944	1235	334	368	7			

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	7	1	3		

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



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

Continued on next page...

Continued from previous page...

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

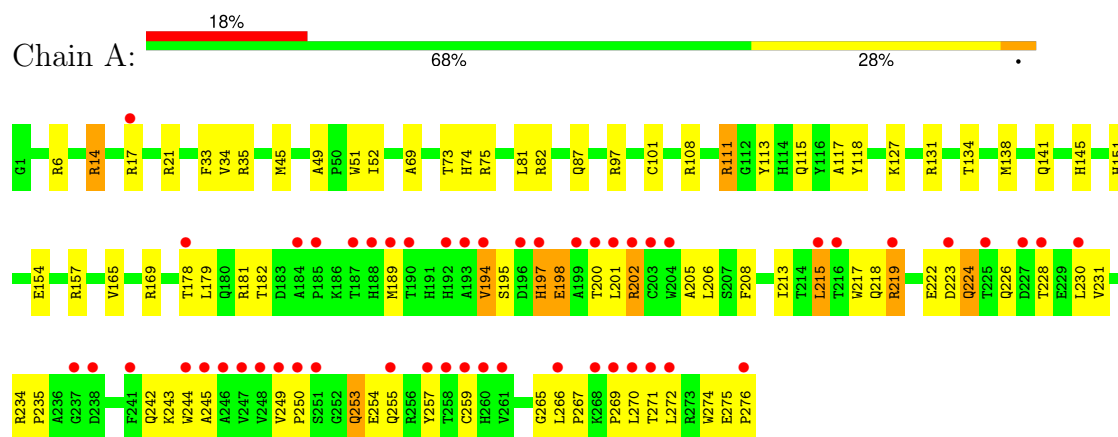
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	31	Total	O	0	0
			31	31		
8	B	13	Total	O	0	0
			13	13		
8	C	1	Total	O	0	0
			1	1		
8	D	32	Total	O	0	0
			32	32		
8	E	48	Total	O	0	0
			48	48		

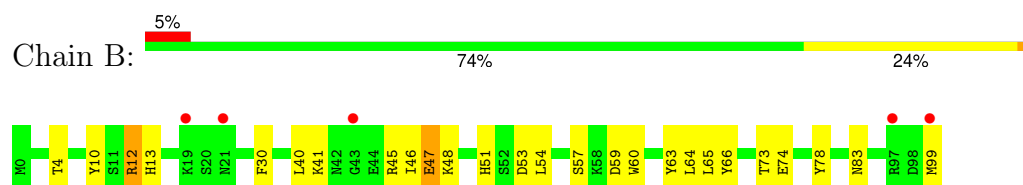
3 Residue-property plots [i](#)

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



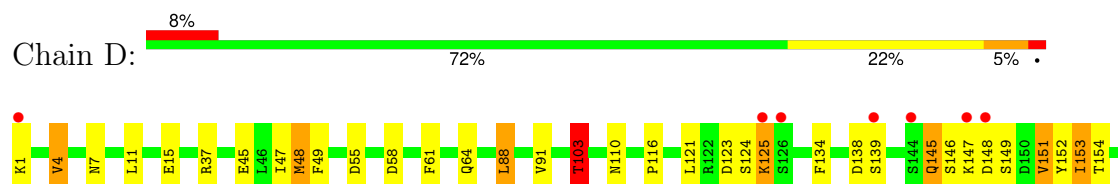
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Melanoma peptide

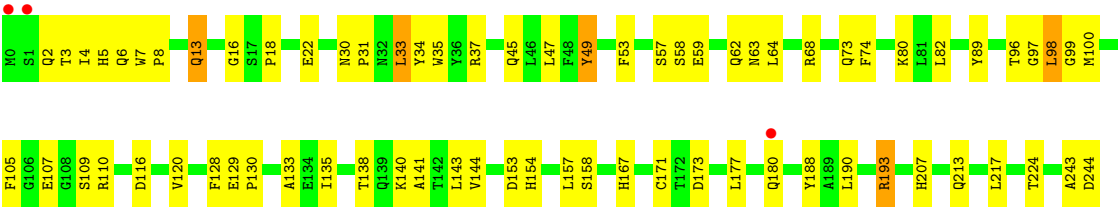


- Molecule 4: High Affinity TCR Alpha Chain





● Molecule 5: High Affinity TCR Beta Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	121.49Å 121.49Å 82.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.33 – 2.46 54.33 – 2.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.33-2.46) 100.0 (54.33-2.46)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.248 0.195 , 0.240	Depositor DCC
R_{free} test set	2220 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6820	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 3.00% 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: TAM, 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	0.98	2/2319 (0.1%)	0.54	0/3149
2	B	0.87	0/860	0.57	0/1162
3	C	1.09	0/69	0.60	0/92
4	D	1.04	5/1556 (0.3%)	0.61	0/2107
5	E	1.09	5/2003 (0.2%)	0.60	0/2732
All	All	1.02	12/6807 (0.2%)	0.58	0/9242

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	D	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	CYS	CB-SG	-17.85	1.51	1.82
4	D	103	THR	CB-CG2	-7.12	1.28	1.52
4	D	4	VAL	CB-CG1	-6.32	1.39	1.52
5	E	180	GLN	CB-CG	5.82	1.68	1.52
4	D	91	VAL	CB-CG1	-5.60	1.41	1.52
5	E	6	GLN	CB-CG	-5.27	1.38	1.52
5	E	13	GLN	CB-CG	-5.22	1.38	1.52
5	E	116	ASP	CB-CG	5.12	1.62	1.51
4	D	45	GLU	CB-CG	-5.10	1.42	1.52
5	E	105	PHE	CG-CD2	-5.04	1.31	1.38
1	A	154	GLU	CG-CD	5.01	1.59	1.51
4	D	88	LEU	CG-CD1	-5.01	1.33	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	48	MET	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2253	0	2103	99	0
2	B	837	0	803	25	0
3	C	70	0	81	5	0
4	D	1525	0	1439	60	0
5	E	1944	0	1848	74	0
6	A	11	0	17	2	0
7	A	25	0	0	9	0
7	E	30	0	0	5	0
8	A	31	0	0	0	0
8	B	13	0	0	1	0
8	C	1	0	0	0	0
8	D	32	0	0	0	0
8	E	48	0	0	3	0
All	All	6820	0	6291	240	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 18.

All (240) 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:201:LEU:HD12	1:A:217:TRP:CZ2	1.66	1.30
5:E:63:ASN:ND2	5:E:82:LEU:HD13	1.65	1.11
1:A:131:ARG:NH2	7:A:303:SO4:O3	1.87	1.08
1:A:201:LEU:CD1	1:A:217:TRP:CZ2	2.46	0.99
1:A:215:LEU:HD11	1:A:245:ALA:HB2	1.45	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:ASN:HD21	5:E:82:LEU:HD13	1.19	0.97
1:A:201:LEU:HD13	1:A:202:ARG:N	1.82	0.94
4:D:147:LYS:O	4:D:149:SER:N	2.02	0.93
5:E:135:ILE:HD11	5:E:141:ALA:HB2	1.50	0.92
5:E:63:ASN:HD21	5:E:82:LEU:CD1	1.82	0.91
5:E:58:SER:N	7:E:305:SO4:O1	2.03	0.91
1:A:215:LEU:HD12	1:A:215:LEU:O	1.73	0.88
1:A:182:THR:HG21	1:A:265:GLY:HA3	1.54	0.88
1:A:111:ARG:HD2	1:A:113:TYR:CZ	2.09	0.87
1:A:194:VAL:HG13	1:A:195:SER:H	1.38	0.87
5:E:130:PRO:HD3	5:E:143:LEU:HD23	1.58	0.85
2:B:47:GLU:OE2	2:B:48:LYS:N	2.12	0.83
1:A:217:TRP:O	1:A:218:GLN:HG3	1.77	0.82
1:A:270:LEU:HD23	1:A:271:THR:N	1.96	0.80
1:A:111:ARG:HD2	1:A:113:TYR:CE2	2.17	0.79
1:A:201:LEU:HD12	1:A:217:TRP:HZ2	1.36	0.79
4:D:7:ASN:O	4:D:103:THR:HB	1.81	0.79
1:A:69:ALA:O	1:A:73:THR:HG23	1.84	0.78
1:A:266:LEU:HD12	1:A:267:PRO:HD2	1.64	0.77
1:A:201:LEU:CD1	1:A:217:TRP:HZ2	1.92	0.77
4:D:48:MET:HE1	4:D:61:PHE:O	1.85	0.77
5:E:3:THR:HG21	5:E:5:HIS:CE1	2.21	0.76
1:A:73:THR:HG21	5:E:97:GLY:HA2	1.67	0.76
4:D:190:ILE:N	4:D:190:ILE:HD12	2.02	0.75
1:A:21:ARG:NH1	7:A:302:SO4:O4	2.20	0.75
1:A:49:ALA:O	1:A:52:ILE:HG22	1.87	0.75
2:B:30:PHE:HZ	2:B:64:LEU:HD13	1.51	0.74
1:A:157:ARG:NH1	7:A:303:SO4:O2	2.20	0.74
1:A:201:LEU:HD12	1:A:217:TRP:CH2	2.23	0.74
2:B:63:TYR:C	2:B:64:LEU:HD12	2.08	0.73
4:D:195:THR:HG21	5:E:133:ALA:HB1	1.71	0.73
2:B:63:TYR:O	2:B:64:LEU:HD12	1.89	0.73
4:D:47:ILE:HG22	4:D:48:MET:HG3	1.71	0.72
1:A:157:ARG:NH1	7:A:303:SO4:O3	2.24	0.71
1:A:73:THR:CG2	5:E:97:GLY:HA2	2.20	0.71
5:E:243:ALA:O	5:E:244:ASP:OD1	2.08	0.71
4:D:190:ILE:HG22	4:D:191:ILE:H	1.55	0.70
1:A:215:LEU:CD1	1:A:245:ALA:HB2	2.20	0.69
1:A:217:TRP:O	1:A:218:GLN:CG	2.40	0.69
5:E:37:ARG:HD2	8:E:448:HOH:O	1.93	0.69
5:E:3:THR:CG2	5:E:5:HIS:CE1	2.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:130:PRO:HD3	5:E:143:LEU:CD2	2.23	0.68
4:D:48:MET:HE3	4:D:58:ASP:HB3	1.75	0.68
5:E:129:GLU:HA	5:E:143:LEU:HD23	1.75	0.67
1:A:228:THR:O	1:A:228:THR:HG22	1.94	0.67
1:A:127:LYS:NZ	1:A:134:THR:OG1	2.26	0.66
4:D:146:SER:HB3	4:D:153:ILE:HG22	1.78	0.66
4:D:37:ARG:HB2	4:D:47:ILE:HD11	1.77	0.66
4:D:159:LEU:HB3	5:E:171:CYS:HB2	1.77	0.65
1:A:215:LEU:HD12	1:A:215:LEU:C	2.16	0.65
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.31	0.65
5:E:110:ARG:HD3	5:E:154:HIS:CD2	2.31	0.65
1:A:201:LEU:HD13	1:A:201:LEU:C	2.17	0.65
1:A:74:HIS:HE1	1:A:97:ARG:HH21	1.45	0.63
4:D:164:MET:SD	5:E:140:LYS:HD3	2.38	0.63
4:D:189:SER:C	4:D:190:ILE:HD12	2.19	0.63
3:C:9:THR:HG21	5:E:96:THR:HG21	1.81	0.63
4:D:161:MET:HE1	5:E:140:LYS:HD2	1.81	0.63
2:B:30:PHE:CZ	2:B:64:LEU:HD13	2.33	0.62
5:E:63:ASN:O	5:E:64:LEU:HD12	1.99	0.62
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.35	0.62
1:A:157:ARG:NH1	7:A:303:SO4:S	2.71	0.62
4:D:176:ASN:HD22	4:D:176:ASN:H	1.47	0.62
5:E:37:ARG:HB2	5:E:47:LEU:HD21	1.80	0.62
1:A:231:VAL:CG2	1:A:244:TRP:CZ2	2.84	0.61
1:A:275:GLU:N	1:A:276:PRO:CD	2.63	0.61
5:E:63:ASN:C	5:E:64:LEU:HD12	2.21	0.61
1:A:218:GLN:HE22	1:A:222:GLU:C	2.02	0.61
4:D:191:ILE:O	4:D:191:ILE:HG22	2.01	0.61
5:E:22:GLU:OE2	5:E:73:GLN:NE2	2.34	0.60
1:A:74:HIS:CE1	1:A:97:ARG:HH21	2.19	0.60
4:D:123:ASP:HB3	5:E:128:PHE:CD2	2.36	0.60
1:A:215:LEU:CD1	1:A:245:ALA:CB	2.79	0.60
1:A:218:GLN:NE2	1:A:222:GLU:O	2.34	0.60
4:D:189:SER:O	4:D:190:ILE:HG13	2.01	0.60
5:E:224:THR:O	5:E:224:THR:HG22	2.01	0.59
1:A:197:HIS:O	1:A:198:GLU:C	2.39	0.59
4:D:186:PHE:O	4:D:188:ASN:ND2	2.36	0.59
1:A:215:LEU:HD11	1:A:245:ALA:CB	2.26	0.59
2:B:54:LEU:CD1	2:B:64:LEU:HD11	2.32	0.59
4:D:48:MET:HE1	4:D:61:PHE:C	2.22	0.59
6:A:301:TAM:N	6:A:301:TAM:O4	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:O	1:A:181:ARG:HG2	2.03	0.59
5:E:45:GLN:NE2	8:E:414:HOH:O	2.33	0.58
1:A:75:ARG:HD2	5:E:53:PHE:CZ	2.38	0.58
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.86	0.58
4:D:195:THR:HG21	5:E:133:ALA:CB	2.33	0.58
4:D:187:ASN:ND2	4:D:187:ASN:O	2.37	0.58
5:E:13:GLN:NE2	5:E:18:PRO:O	2.38	0.56
1:A:205:ALA:C	1:A:206:LEU:HD22	2.25	0.56
1:A:253:GLN:H	1:A:253:GLN:NE2	2.03	0.56
4:D:1:LYS:HE2	8:E:414:HOH:O	2.03	0.56
1:A:201:LEU:CD1	1:A:217:TRP:CH2	2.84	0.56
1:A:231:VAL:HG23	1:A:244:TRP:CZ2	2.41	0.56
4:D:116:PRO:HB2	4:D:192:PRO:HB3	1.87	0.56
4:D:159:LEU:HD12	4:D:159:LEU:O	2.06	0.56
1:A:157:ARG:NH2	7:A:304:SO4:O1	2.39	0.56
5:E:138:THR:HG21	5:E:140:LYS:HE3	1.87	0.56
1:A:218:GLN:OE1	1:A:224:GLN:N	2.39	0.55
1:A:14:ARG:HB2	1:A:17:ARG:HD2	1.88	0.55
5:E:135:ILE:CD1	5:E:141:ALA:HB2	2.31	0.55
1:A:259:CYS:O	1:A:271:THR:HG22	2.06	0.55
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.42	0.55
1:A:208:PHE:CE2	1:A:242:GLN:HA	2.42	0.55
4:D:188:ASN:ND2	4:D:190:ILE:HD11	2.22	0.54
1:A:206:LEU:HD22	1:A:206:LEU:N	2.22	0.54
4:D:48:MET:CE	4:D:58:ASP:HB3	2.38	0.54
1:A:206:LEU:HD13	1:A:242:GLN:HB2	1.90	0.54
1:A:194:VAL:HG13	1:A:195:SER:N	2.17	0.53
1:A:231:VAL:HG21	1:A:244:TRP:CZ2	2.42	0.53
1:A:270:LEU:HD23	1:A:270:LEU:C	2.28	0.53
4:D:153:ILE:HD13	4:D:186:PHE:HE2	1.72	0.53
5:E:30:ASN:N	5:E:31:PRO:CD	2.71	0.53
4:D:153:ILE:HD13	4:D:186:PHE:CE2	2.44	0.53
4:D:153:ILE:HD12	4:D:154:THR:N	2.23	0.53
1:A:208:PHE:CD1	1:A:213:ILE:HD11	2.44	0.53
5:E:62:GLN:O	5:E:63:ASN:HB2	2.09	0.53
4:D:164:MET:O	4:D:164:MET:HG2	2.09	0.53
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.92	0.53
5:E:157:LEU:HD23	5:E:158:SER:N	2.24	0.53
1:A:249:VAL:HB	1:A:250:PRO:HD2	1.91	0.52
2:B:99:MET:OXT	2:B:99:MET:HG2	2.09	0.52
1:A:253:GLN:NE2	1:A:253:GLN:N	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:CD1	1:A:201:LEU:C	2.77	0.52
1:A:253:GLN:H	1:A:253:GLN:HE21	1.58	0.52
2:B:54:LEU:HD12	2:B:64:LEU:HD11	1.92	0.51
4:D:158:VAL:HG22	4:D:169:ASN:OD1	2.10	0.51
4:D:190:ILE:HB	4:D:192:PRO:HD3	1.92	0.51
5:E:57:SER:HB2	5:E:59:GLU:OE1	2.10	0.51
5:E:37:ARG:CB	5:E:47:LEU:HD21	2.40	0.51
5:E:138:THR:HG21	5:E:140:LYS:CE	2.41	0.51
1:A:111:ARG:CD	1:A:113:TYR:CZ	2.88	0.50
5:E:3:THR:HG21	5:E:5:HIS:HE1	1.71	0.50
1:A:189:MET:HG2	1:A:272:LEU:HD23	1.94	0.50
5:E:35:TRP:CD1	5:E:74:PHE:CE2	2.99	0.50
5:E:177:LEU:HD12	5:E:177:LEU:O	2.12	0.49
2:B:12:ARG:NH1	2:B:13:HIS:ND1	2.61	0.49
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.13	0.49
1:A:234:ARG:HD2	2:B:10:TYR:CE2	2.48	0.49
5:E:120:VAL:HG21	5:E:217:LEU:HD21	1.95	0.49
5:E:157:LEU:HD23	5:E:157:LEU:C	2.33	0.49
4:D:188:ASN:ND2	4:D:189:SER:H	2.11	0.48
5:E:177:LEU:HD12	5:E:177:LEU:C	2.34	0.48
1:A:254:GLU:OE1	1:A:274:TRP:CD1	2.67	0.48
2:B:12:ARG:HG2	2:B:12:ARG:HH11	1.77	0.48
4:D:152:TYR:O	4:D:173:ALA:HA	2.14	0.48
4:D:176:ASN:HD22	4:D:176:ASN:N	2.06	0.48
5:E:16:GLY:HA2	5:E:80:LYS:HG3	1.95	0.48
4:D:138:ASP:OD1	4:D:139:SER:N	2.46	0.47
4:D:176:ASN:H	4:D:176:ASN:ND2	2.09	0.47
5:E:33:LEU:HD23	5:E:74:PHE:HB2	1.96	0.47
1:A:219:ARG:O	1:A:219:ARG:HG2	2.15	0.47
4:D:49:PHE:C	4:D:49:PHE:CD2	2.87	0.47
1:A:219:ARG:O	1:A:219:ARG:CG	2.62	0.47
5:E:34:TYR:CE1	5:E:49:TYR:CD1	3.03	0.47
1:A:215:LEU:CD1	1:A:215:LEU:C	2.82	0.47
4:D:124:SER:O	4:D:125:LYS:C	2.53	0.47
1:A:75:ARG:HD2	5:E:53:PHE:CE1	2.51	0.46
1:A:226:GLN:O	1:A:226:GLN:HG3	2.15	0.46
2:B:12:ARG:NH1	2:B:12:ARG:HG2	2.31	0.46
4:D:123:ASP:HB3	5:E:128:PHE:HD2	1.79	0.46
1:A:255:GLN:HB2	1:A:257:TYR:HE2	1.79	0.46
4:D:195:THR:CG2	5:E:133:ALA:HB1	2.43	0.46
4:D:191:ILE:N	4:D:192:PRO:HD3	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:224:THR:O	5:E:224:THR:CG2	2.63	0.46
4:D:189:SER:C	4:D:190:ILE:CD1	2.85	0.45
5:E:167:HIS:N	7:E:304:SO4:O1	2.48	0.45
1:A:255:GLN:HB2	1:A:257:TYR:CE2	2.52	0.45
1:A:202:ARG:HA	1:A:245:ALA:O	2.17	0.45
5:E:171:CYS:HB3	5:E:193:ARG:HD3	1.99	0.45
5:E:99:GLY:O	5:E:100:MET:HE2	2.17	0.44
5:E:207:HIS:CE1	7:E:303:SO4:O4	2.71	0.44
1:A:219:ARG:H	1:A:219:ARG:HD2	1.83	0.44
4:D:121:LEU:HD21	5:E:144:VAL:HG23	1.98	0.44
1:A:51:TRP:CE2	1:A:179:LEU:HD11	2.52	0.44
5:E:8:PRO:O	5:E:109:SER:OG	2.26	0.44
5:E:49:TYR:HB3	5:E:57:SER:HB3	1.99	0.44
5:E:153:ASP:HB3	5:E:188:TYR:CE2	2.51	0.44
2:B:30:PHE:HZ	2:B:64:LEU:CD1	2.28	0.44
4:D:190:ILE:HG22	4:D:191:ILE:N	2.29	0.44
5:E:33:LEU:HD22	5:E:68:ARG:CZ	2.47	0.44
1:A:169:ARG:NH2	7:A:305:SO4:O3	2.50	0.44
1:A:222:GLU:O	1:A:224:GLN:N	2.50	0.44
4:D:151:VAL:HG12	4:D:177:LYS:NZ	2.33	0.44
1:A:200:THR:O	1:A:201:LEU:HB2	2.18	0.43
5:E:3:THR:CG2	5:E:4:ILE:N	2.81	0.43
1:A:141:GLN:O	1:A:145:HIS:CD2	2.71	0.43
1:A:138:MET:HA	1:A:138:MET:CE	2.48	0.43
1:A:194:VAL:HG22	1:A:195:SER:N	2.33	0.43
5:E:30:ASN:N	5:E:31:PRO:HD3	2.33	0.43
3:C:9:THR:CG2	5:E:96:THR:CG2	2.97	0.43
5:E:63:ASN:ND2	5:E:82:LEU:CD1	2.49	0.43
4:D:15:GLU:OE2	4:D:167:LYS:NZ	2.52	0.43
5:E:58:SER:CB	7:E:305:SO4:O1	2.67	0.43
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.54	0.43
5:E:7:TRP:HB2	5:E:8:PRO:HA	2.00	0.43
6:A:301:TAM:H42	6:A:301:TAM:O5	2.18	0.43
1:A:230:LEU:HD23	1:A:230:LEU:N	2.34	0.43
4:D:134:PHE:HZ	4:D:190:ILE:HG21	1.84	0.43
1:A:73:THR:HG22	5:E:97:GLY:HA2	2.00	0.42
1:A:235:PRO:CG	2:B:65:LEU:HD22	2.48	0.42
4:D:48:MET:CE	4:D:61:PHE:O	2.61	0.42
2:B:59:ASP:O	2:B:60:TRP:HB2	2.18	0.42
5:E:98:LEU:HD22	5:E:98:LEU:N	2.33	0.42
4:D:190:ILE:N	4:D:190:ILE:CD1	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:HIS:HA	7:A:304:SO4:O4	2.19	0.42
1:A:243:LYS:HG2	1:A:244:TRP:N	2.34	0.42
4:D:195:THR:O	4:D:196:PHE:HB2	2.20	0.42
2:B:46:ILE:HG22	2:B:47:GLU:O	2.18	0.42
1:A:215:LEU:HD13	1:A:245:ALA:HB3	2.02	0.42
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.55	0.42
1:A:165:VAL:O	1:A:169:ARG:HG3	2.19	0.42
5:E:37:ARG:HD3	5:E:89:TYR:CZ	2.55	0.42
2:B:73:THR:OG1	2:B:74:GLU:N	2.53	0.41
3:C:7:ILE:C	3:C:8:LEU:HD12	2.40	0.41
2:B:41:LYS:HD3	2:B:78:TYR:CE1	2.55	0.41
5:E:2:GLN:H	5:E:2:GLN:HG2	1.74	0.41
5:E:173:ASP:HB2	5:E:190:LEU:HD12	2.00	0.41
1:A:45:MET:CE	3:C:2:LEU:HD11	2.50	0.41
3:C:9:THR:CG2	5:E:96:THR:HG21	2.49	0.41
4:D:48:MET:HE2	4:D:58:ASP:N	2.35	0.41
4:D:189:SER:C	4:D:190:ILE:CG1	2.88	0.41
4:D:55:ASP:OD1	4:D:64:GLN:HG2	2.20	0.41
4:D:159:LEU:HD11	4:D:168:SER:HB3	2.03	0.41
5:E:58:SER:HB2	7:E:305:SO4:O1	2.21	0.41
1:A:208:PHE:CE1	1:A:213:ILE:CD1	3.04	0.41
4:D:145:GLN:H	4:D:145:GLN:NE2	2.20	0.41
4:D:159:LEU:HD12	4:D:159:LEU:C	2.42	0.41
1:A:108:ARG:HA	7:A:305:SO4:O3	2.21	0.40
1:A:208:PHE:CE1	1:A:213:ILE:HD11	2.56	0.40
4:D:187:ASN:N	4:D:187:ASN:HD22	2.19	0.40
4:D:161:MET:CE	5:E:140:LYS:HD2	2.49	0.40
1:A:242:GLN:NE2	2:B:10:TYR:CD1	2.90	0.40
1:A:82:ARG:HA	1:A:87:GLN:HG2	2.04	0.40
2:B:57:SER:HB2	8:B:110:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	250 (91%)	19 (7%)	5 (2%)	7	6
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4	2
5	E	243/245 (99%)	229 (94%)	14 (6%)	0	100	100
All	All	817/827 (99%)	760 (93%)	47 (6%)	10 (1%)	11	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
4	D	148	ASP
1	A	194	VAL
1	A	198	GLU
1	A	197	HIS
4	D	125	LYS
4	D	190	ILE
4	D	162	ARG
4	D	188	ASN
1	A	269	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	232/232 (100%)	223 (96%)	9 (4%)	27	41
2	B	95/95 (100%)	91 (96%)	4 (4%)	25	38
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	174/174 (100%)	162 (93%)	12 (7%)	13	16
5	E	211/211 (100%)	205 (97%)	6 (3%)	38	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	719/719 (100%)	688 (96%)	31 (4%)	25	37

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	14	ARG
1	A	111	ARG
1	A	115	GLN
1	A	202	ARG
1	A	215	LEU
1	A	219	ARG
1	A	224	GLN
1	A	253	GLN
2	B	4	THR
2	B	12	ARG
2	B	47	GLU
2	B	83	ASN
4	D	4	VAL
4	D	11	LEU
4	D	88	LEU
4	D	103	THR
4	D	110	ASN
4	D	145	GLN
4	D	151	VAL
4	D	153	ILE
4	D	176	ASN
4	D	187	ASN
4	D	188	ASN
4	D	190	ILE
5	E	33	LEU
5	E	49	TYR
5	E	98	LEU
5	E	107	GLU
5	E	193	ARG
5	E	213	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	74	HIS
1	A	86	ASN
1	A	93	HIS
1	A	115	GLN
1	A	141	GLN
1	A	145	HIS
1	A	174	ASN
1	A	224	GLN
1	A	242	GLN
1	A	253	GLN
1	A	262	GLN
2	B	17	ASN
2	B	83	ASN
4	D	38	GLN
4	D	110	ASN
4	D	145	GLN
4	D	176	ASN
4	D	187	ASN
4	D	188	ASN
5	E	5	HIS
5	E	6	GLN
5	E	13	GLN
5	E	38	GLN
5	E	63	ASN
5	E	119	ASN
5	E	154	HIS
5	E	207	HIS

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

12 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	A	304	-	4,4,4	0.17	0	6,6,6	0.25	0
7	SO4	E	305	-	4,4,4	0.19	0	6,6,6	0.21	0
7	SO4	A	302	-	4,4,4	0.38	0	6,6,6	0.15	0
7	SO4	E	301	-	4,4,4	0.37	0	6,6,6	0.17	0
7	SO4	E	302	-	4,4,4	0.43	0	6,6,6	0.12	0
7	SO4	E	303	-	4,4,4	0.35	0	6,6,6	0.09	0
6	TAM	A	301	-	10,10,10	1.72	3 (30%)	12,12,12	2.39	9 (75%)
7	SO4	E	304	-	4,4,4	0.18	0	6,6,6	0.11	0
7	SO4	A	303	-	4,4,4	0.43	0	6,6,6	0.13	0
7	SO4	A	306	-	4,4,4	0.22	0	6,6,6	0.07	0
7	SO4	E	306	-	4,4,4	0.31	0	6,6,6	0.15	0
7	SO4	A	305	-	4,4,4	0.45	0	6,6,6	0.13	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	TAM	A	301	-	-	8/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	301	TAM	C1-C	-3.07	1.49	1.53
6	A	301	TAM	C3-C	-2.62	1.49	1.53
6	A	301	TAM	C2-C	-2.21	1.50	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	TAM	C2-C-C1	3.20	116.15	110.50
6	A	301	TAM	C3-C-C1	3.06	115.90	110.50
6	A	301	TAM	C6-C3-C	-2.91	112.54	115.97
6	A	301	TAM	C4-C1-C	-2.78	112.70	115.97
6	A	301	TAM	C3-C-N	-2.70	101.44	108.22
6	A	301	TAM	C3-C-C2	2.70	115.27	110.50
6	A	301	TAM	C5-C2-C	-2.51	113.01	115.97
6	A	301	TAM	C1-C-N	-2.44	102.10	108.22
6	A	301	TAM	C2-C-N	-2.26	102.55	108.22

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	TAM	C2-C-C1-C4
6	A	301	TAM	C3-C-C1-C4
6	A	301	TAM	N-C-C1-C4
6	A	301	TAM	C3-C-C2-C5
6	A	301	TAM	N-C-C2-C5
6	A	301	TAM	C1-C-C3-C6
6	A	301	TAM	N-C-C3-C6
6	A	301	TAM	C-C2-C5-O5

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	304	SO4	2	0
7	E	305	SO4	3	0
7	A	302	SO4	1	0
7	E	303	SO4	1	0
6	A	301	TAM	2	0
7	E	304	SO4	1	0
7	A	303	SO4	4	0
7	A	305	SO4	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.55	51 (18%) 4 4	26, 59, 196, 217	0
2	B	100/100 (100%)	0.32	5 (5%) 35 35	26, 66, 153, 169	0
3	C	10/10 (100%)	-0.82	0 100 100	25, 28, 34, 38	0
4	D	196/196 (100%)	0.14	15 (7%) 21 21	21, 49, 135, 163	0
5	E	245/245 (100%)	-0.18	3 (1%) 76 77	24, 44, 107, 151	0
All	All	827/827 (100%)	0.19	74 (8%) 17 17	21, 52, 164, 217	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	191	ILE	6.3
1	A	230	LEU	4.9
1	A	261	VAL	4.6
1	A	270	LEU	4.4
1	A	201	LEU	4.3
2	B	99	MET	4.2
4	D	196	PHE	4.2
1	A	249	VAL	4.2
2	B	43	GLY	4.0
1	A	272	LEU	3.9
1	A	227	ASP	3.8
1	A	269	PRO	3.8
4	D	190	ILE	3.7
1	A	188	HIS	3.6
1	A	250	PRO	3.6
1	A	187	THR	3.6
1	A	247	VAL	3.5
4	D	160	ASP	3.4
1	A	246	ALA	3.3
1	A	251	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	248	VAL	3.3
1	A	193	ALA	3.3
4	D	144	SER	3.2
1	A	178	THR	3.1
1	A	199	ALA	3.1
1	A	228	THR	3.1
1	A	245	ALA	3.1
1	A	215	LEU	3.0
1	A	258	THR	3.0
1	A	266	LEU	2.9
1	A	259	CYS	2.9
1	A	203	CYS	2.8
1	A	276	PRO	2.7
1	A	225	THR	2.7
1	A	185	PRO	2.7
1	A	192	HIS	2.7
1	A	204	TRP	2.7
1	A	196	ASP	2.6
1	A	200	THR	2.6
4	D	147	LYS	2.6
4	D	126	SER	2.5
1	A	194	VAL	2.5
4	D	1	LYS	2.5
1	A	184	ALA	2.5
1	A	244	TRP	2.5
4	D	139	SER	2.5
1	A	255	GLN	2.4
5	E	180	GLN	2.4
1	A	271	THR	2.4
1	A	223	ASP	2.4
1	A	189	MET	2.4
5	E	0	MET	2.4
1	A	268	LYS	2.4
1	A	260	HIS	2.4
4	D	166	PHE	2.3
1	A	241	PHE	2.3
1	A	190	THR	2.3
1	A	237	GLY	2.3
1	A	17	ARG	2.3
1	A	257	TYR	2.3
1	A	197	HIS	2.2
2	B	97	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	238	ASP	2.2
5	E	1	SER	2.2
2	B	21	ASN	2.1
4	D	148	ASP	2.1
4	D	188	ASN	2.1
4	D	167	LYS	2.1
1	A	202	ARG	2.1
2	B	19	LYS	2.1
1	A	219	ARG	2.1
1	A	216	THR	2.0
4	D	125	LYS	2.0
4	D	178	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 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
7	SO4	E	303	5/5	0.67	0.20	47,53,67,73	5
7	SO4	E	304	5/5	0.73	0.18	46,53,65,73	5
6	TAM	A	301	11/11	0.75	0.15	66,80,80,80	0
7	SO4	E	302	5/5	0.79	0.17	36,44,52,62	5
7	SO4	A	306	5/5	0.83	0.10	40,41,53,62	5
7	SO4	A	302	5/5	0.86	0.14	67,74,80,80	0
7	SO4	E	301	5/5	0.89	0.20	63,76,80,80	1
7	SO4	A	305	5/5	0.93	0.11	33,41,44,52	5
7	SO4	E	305	5/5	0.93	0.13	35,39,47,53	5
7	SO4	E	306	5/5	0.93	0.10	31,34,46,54	5
7	SO4	A	303	5/5	0.96	0.12	41,64,76,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SO4	A	304	5/5	0.99	0.08	37,40,48,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.