



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:41 PM UTC

PDB ID : 3QEU / pdb_00003qeu
Title : The crystal structure of TCR DMF5
Authors : Borbulevych, O.Y.; Santhanagopalan, S.M.; Baker, B.M.
Deposited on : 2011-01-20
Resolution : 2.09 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

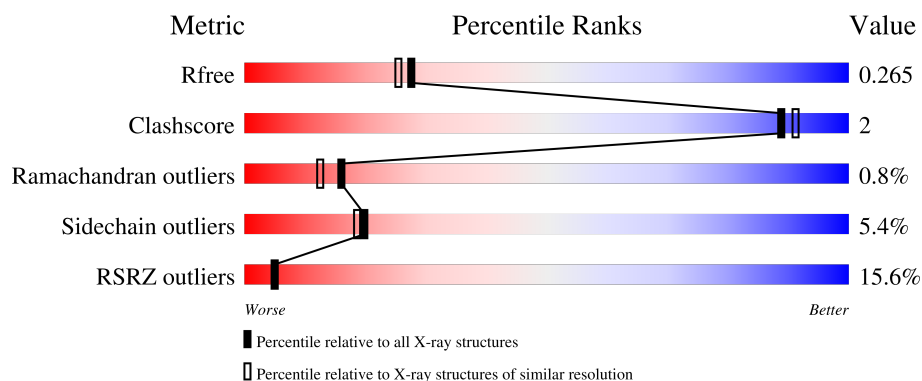
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	202	28% 82% 13% ..
1	D	202	4% 95% ..
2	B	243	27% 85% 12% ..
2	E	243	3% 91% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7373 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 DMF5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	202	Total	C	N	O	S	0	2	0
			1573	982	258	325	8			
1	A	195	Total	C	N	O	S	0	1	0
			1516	947	249	312	8			

- Molecule 2 is a protein called DMF5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	243	Total	C	N	O	S	0	0	0
			1905	1196	334	366	9			
2	B	238	Total	C	N	O	S	0	0	0
			1868	1176	326	358	8			

- Molecule 3 is LITHIUM ION (CCD ID: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Li	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	144	Total	O	0	0
			144	144		
5	E	208	Total	O	0	0
			208	208		
5	A	72	Total	O	0	0
			72	72		
5	B	74	Total	O	0	0
			74	74		

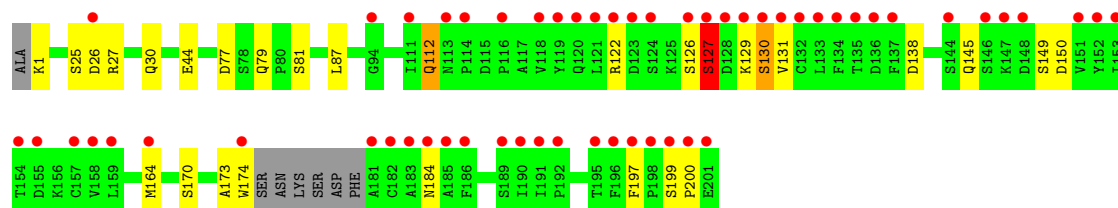
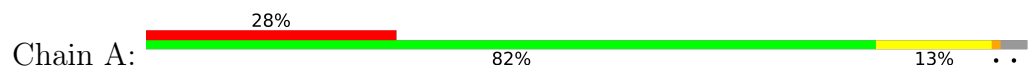
3 Residue-property plots

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.

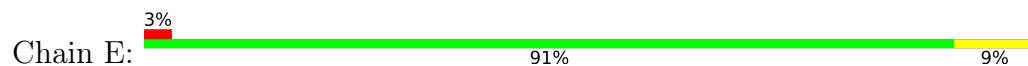
• Molecule 1: DMF5 alpha chain



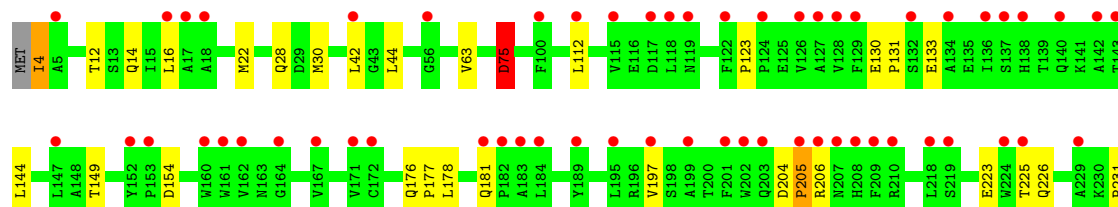
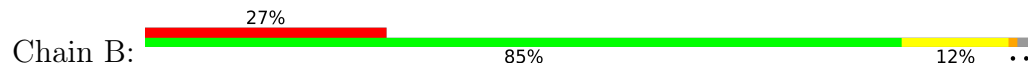
• Molecule 1: DMF5 alpha chain



• Molecule 2: DMF5 beta chain



• Molecule 2: DMF5 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.16Å 86.50Å 66.47Å 90.00° 103.97° 90.00°	Depositor
Resolution (Å)	29.79 – 2.09 29.79 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.79-2.09) 99.0 (29.79-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.266 0.205 , 0.265	Depositor DCC
R_{free} test set	2977 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7373	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LI

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	0.81	1/1552 (0.1%)	1.04	7/2099 (0.3%)
1	D	0.88	0/1613	1.02	3/2182 (0.1%)
2	B	0.72	1/1917 (0.1%)	1.01	8/2614 (0.3%)
2	E	0.90	0/1954	1.04	6/2661 (0.2%)
All	All	0.83	2/7036 (0.0%)	1.03	24/9556 (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	3
2	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	SER	CB-OG	10.95	1.64	1.42
2	B	63	VAL	CA-C	5.52	1.58	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	N-CA-C	-8.76	100.52	114.09
2	B	181	GLN	CA-C-N	7.54	129.26	119.84
2	B	181	GLN	C-N-CA	7.54	129.26	119.84
2	E	7	ILE	CB-CA-C	-7.10	102.10	110.91
2	E	42	LEU	N-CA-C	6.32	118.98	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	SER	CA-C-N	6.28	127.69	119.84
1	A	199	SER	C-N-CA	6.28	127.69	119.84
1	A	127	SER	N-CA-C	6.27	124.16	110.80
1	D	111	ILE	CA-C-N	6.24	129.47	120.79
1	D	111	ILE	C-N-CA	6.24	129.47	120.79
2	B	226	GLN	N-CA-C	6.20	116.26	108.45
1	D	159	LEU	CA-CB-CG	6.04	137.42	116.30
2	B	75	ASP	N-CA-C	5.87	120.44	113.28
2	B	205	PRO	N-CA-C	5.56	123.92	112.47
2	E	118	LEU	N-CA-C	5.47	119.21	112.54
1	A	149	SER	N-CA-C	5.46	117.01	109.15
1	A	197	PHE	CA-C-N	5.39	126.58	119.84
1	A	197	PHE	C-N-CA	5.39	126.58	119.84
2	E	221	ASN	N-CA-C	5.39	117.91	111.71
2	E	118	LEU	CA-C-N	-5.17	114.41	122.73
2	E	118	LEU	C-N-CA	-5.17	114.41	122.73
2	B	206	ARG	N-CA-C	-5.14	105.75	112.23
2	B	130	GLU	CA-C-N	5.13	125.13	119.90
2	B	130	GLU	C-N-CA	5.13	125.13	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	SER	Peptide
1	A	127	SER	Peptide
1	A	173	ALA	Peptide
2	B	204	ASP	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	1516	0	1433	8	0
1	D	1573	0	1488	3	0
2	B	1868	0	1783	8	0
2	E	1905	0	1817	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	B	6	0	8	1	0
4	E	6	0	8	0	0
5	A	72	0	0	0	0
5	B	74	0	0	0	0
5	D	144	0	0	0	0
5	E	208	0	0	1	0
All	All	7373	0	6537	26	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 2.

All (26) 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:130:SER:OG	1:A:130:SER:CB	1.64	1.43
2:E:210:ARG:NH2	2:E:212:GLN:OE1	2.22	0.73
2:B:28:GLN:O	2:B:75:ASP:HB3	1.92	0.68
1:A:130:SER:CB	1:A:130:SER:HG	2.07	0.58
2:E:222:ASP:OD1	2:E:222:ASP:N	2.38	0.57
1:A:122:ARG:HD2	1:A:129:LYS:HD3	1.87	0.57
2:E:16:LEU:HD12	2:E:112:LEU:HD11	1.87	0.56
2:E:98:LEU:HD22	4:B:246:GOL:H11	1.89	0.54
1:A:130:SER:OG	1:A:130:SER:CA	2.52	0.54
2:E:113:THR:OG1	2:E:155:HIS:NE2	2.41	0.53
1:D:164:MET:HE1	2:E:198:SER:HB3	1.93	0.51
2:E:186:ASP:OD1	2:E:186:ASP:N	2.43	0.51
1:A:127:SER:HA	1:A:129:LYS:HG3	1.93	0.50
2:E:179:LYS:NZ	5:E:391:HOH:O	2.35	0.50
1:A:122:ARG:HA	1:A:129:LYS:HB3	1.94	0.50
1:D:121:LEU:HB3	2:E:130:GLU:O	2.16	0.45
2:B:131:PRO:HD3	2:B:144:LEU:HG	1.99	0.44
1:D:112:GLN:H	1:D:112:GLN:HG3	1.18	0.44
2:B:4:ILE:HD13	2:B:30:MET:HG2	1.99	0.44
2:B:14:GLN:HB3	2:B:112:LEU:HD13	2.00	0.43
2:B:16:LEU:HD12	2:B:112:LEU:HD11	2.00	0.43
2:B:154:ASP:HB2	2:B:177:PRO:HG2	2.01	0.43
1:A:112:GLN:H	1:A:112:GLN:HG2	1.53	0.42
2:B:16:LEU:HD21	2:B:22:MET:HB2	2.03	0.41
1:A:131:VAL:HG12	1:A:174:TRP:HB3	2.02	0.41
2:B:123:PRO:HD3	2:B:231:PRO:HB3	2.02	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	192/202 (95%)	171 (89%)	16 (8%)	5 (3%)	4	1
1	D	202/202 (100%)	200 (99%)	1 (0%)	1 (0%)	24	22
2	B	236/243 (97%)	227 (96%)	8 (3%)	1 (0%)	30	28
2	E	241/243 (99%)	239 (99%)	2 (1%)	0	100	100
All	All	871/890 (98%)	837 (96%)	27 (3%)	7 (1%)	16	12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	145	GLN
2	B	205	PRO
1	A	27	ARG
1	A	200	PRO
1	A	184	ASN
1	D	1	LYS

5.3.2 Protein sidechains [i](#)

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	173/178 (97%)	160 (92%)	13 (8%)	12	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	180/178 (101%)	172 (96%)	8 (4%)	25	26
2	B	202/205 (98%)	189 (94%)	13 (6%)	16	14
2	E	205/205 (100%)	198 (97%)	7 (3%)	32	35
All	All	760/766 (99%)	719 (95%)	41 (5%)	20	18

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	20	LEU
1	D	26	ASP
1	D	30	GLN
1	D	56	GLU
1	D	112	GLN
1	D	121	LEU
1	D	144	SER
1	D	159	LEU
2	E	4	ILE
2	E	12	THR
2	E	44	LEU
2	E	176	GLN
2	E	194	ARG
2	E	219	SER
2	E	222	ASP
1	A	1	LYS
1	A	25	SER
1	A	26	ASP
1	A	30	GLN
1	A	44	GLU
1	A	77	ASP
1	A	79	GLN
1	A	81	SER
1	A	87	LEU
1	A	112	GLN
1	A	138	ASP
1	A	164	MET
1	A	170	SER
2	B	4	ILE
2	B	12	THR
2	B	42	LEU
2	B	44	LEU
2	B	75	ASP

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Mol	Chain	Res	Type
2	B	133	GLU
2	B	149	THR
2	B	176	GLN
2	B	178	LEU
2	B	197	VAL
2	B	223	GLU
2	B	225	THR
2	B	239	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	30	GLN
1	D	37	GLN
1	D	69	GLN
1	D	91	ASN
2	E	14	GLN
2	E	40	GLN
2	E	108	GLN
1	A	69	GLN
1	A	120	GLN
1	A	169	ASN
2	B	119	ASN
2	B	140	GLN
2	B	176	GLN
2	B	226	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	GOL	B	246	-	5,5,5	0.16	0	5,5,5	1.25	1 (20%)
4	GOL	E	2	-	5,5,5	0.38	0	5,5,5	0.36	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
4	GOL	B	246	-	-	3/4/4/4	-
4	GOL	E	2	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	246	GOL	C3-C2-C1	-2.07	104.19	111.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	246	GOL	C1-C2-C3-O3
4	B	246	GOL	O2-C2-C3-O3
4	E	2	GOL	O1-C1-C2-C3
4	B	246	GOL	O1-C1-C2-O2
4	E	2	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	246	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	195/202 (96%)	1.37	56 (28%) ⓘ ⓘ	23, 45, 118, 119	1 (0%)
1	D	202/202 (100%)	0.11	8 (3%) 42 44	14, 29, 45, 53	2 (0%)
2	B	238/243 (97%)	1.32	65 (27%) ⓘ ⓘ	22, 54, 78, 90	0
2	E	243/243 (100%)	-0.02	8 (3%) 49 51	17, 27, 47, 60	0
All	All	878/890 (98%)	0.68	137 (15%) ⓘ ⓘ	14, 35, 83, 119	3 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	TRP	9.1
1	A	183	ALA	6.7
1	A	185	ALA	6.2
1	A	186	PHE	5.7
1	A	196	PHE	5.5
1	A	200	PRO	5.3
1	A	181	ALA	5.0
2	B	134	ALA	4.9
1	A	197	PHE	4.8
1	A	190	ILE	4.8
2	B	184	LEU	4.7
1	A	158	VAL	4.6
1	A	192	PRO	4.5
2	B	241	TRP	4.5
1	A	124	SER	4.4
1	A	130	SER	4.4
1	A	121	LEU	4.3
1	A	131	VAL	4.1
2	B	126	VAL	3.9
1	A	157	CYS	3.9
2	B	219	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	236	VAL	3.8
1	A	137	PHE	3.8
2	B	136	ILE	3.8
1	A	134	PHE	3.8
1	A	184	ASN	3.7
1	A	116	PRO	3.7
1	D	128	ASP	3.6
2	B	128	VAL	3.6
2	B	210	ARG	3.5
1	A	182	CYS	3.5
1	A	118	VAL	3.5
1	A	195	THR	3.5
1	A	191	ILE	3.5
2	B	205	PRO	3.4
1	A	189	SER	3.4
2	E	42	LEU	3.4
2	B	118	LEU	3.4
1	A	153	ILE	3.4
2	B	142	ALA	3.4
1	A	114	PRO	3.3
1	A	198	PRO	3.3
2	B	5	ALA	3.3
1	A	133	LEU	3.3
1	D	179	ASP	3.3
1	A	123	ASP	3.3
1	A	152	TYR	3.2
2	B	209	PHE	3.2
1	A	144	SER	3.2
1	D	0	ALA	3.2
2	B	183	ALA	3.2
1	A	113	ASN	3.2
1	A	132	CYS	3.1
2	B	16	LEU	3.1
2	B	129	PHE	3.1
2	E	245	ASP	3.1
2	B	137	SER	3.1
2	B	140	GLN	3.1
2	B	233	THR	3.0
2	B	164	GLY	3.0
1	A	26	ASP	3.0
2	B	127	ALA	3.0
1	D	126	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	199	ALA	2.9
1	A	155	ASP	2.9
2	E	225	THR	2.9
1	A	146	SER	2.9
2	B	202	TRP	2.9
2	B	143	THR	2.8
2	B	161	TRP	2.7
2	B	240	ALA	2.7
2	B	225	THR	2.7
1	A	151	VAL	2.7
1	A	128	ASP	2.7
2	B	207	ASN	2.6
2	B	224	TRP	2.6
2	B	18	ALA	2.6
2	B	122	PHE	2.6
1	A	136	ASP	2.6
2	B	138	HIS	2.6
2	B	124	PRO	2.6
2	B	181	GLN	2.6
2	B	172	CYS	2.6
2	E	3	MET	2.6
1	A	159	LEU	2.6
1	A	154	THR	2.5
2	B	42	LEU	2.5
1	A	135	THR	2.5
2	B	234	GLN	2.5
2	B	201	PHE	2.5
1	A	129	LYS	2.5
2	B	197	VAL	2.5
1	A	199	SER	2.5
2	B	147	LEU	2.5
2	B	100	PHE	2.5
1	D	26	ASP	2.4
1	A	147	LYS	2.4
2	B	218	LEU	2.4
2	B	208	HIS	2.4
2	E	100	PHE	2.4
1	A	148	ASP	2.4
2	B	17	ALA	2.4
2	B	56	GLY	2.4
1	A	127	SER	2.4
2	E	220	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	126	SER	2.4
2	B	229	ALA	2.3
2	E	185	ASN	2.3
2	B	195	LEU	2.3
1	A	164	MET	2.3
1	D	112	GLN	2.3
2	B	153	PRO	2.3
1	A	119	TYR	2.3
1	A	111	ILE	2.3
2	B	162	VAL	2.3
2	B	152	TYR	2.3
2	B	237	SER	2.2
2	B	235	ILE	2.2
2	B	115	VAL	2.2
2	B	206	ARG	2.2
2	B	171	VAL	2.2
1	D	67	ALA	2.2
2	E	119	ASN	2.2
2	B	182	PRO	2.2
1	A	94	GLY	2.2
2	B	203	GLN	2.2
1	A	201	GLU	2.1
2	B	189	TYR	2.1
2	B	160	TRP	2.1
1	D	63	GLN	2.1
1	A	120	GLN	2.1
1	A	122	ARG	2.1
2	B	167	VAL	2.1
2	B	132	SER	2.1
2	B	112	LEU	2.0
2	B	119	ASN	2.0
2	B	117	ASP	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
4	GOL	B	246	6/6	0.88	0.14	34,40,41,41	0
4	GOL	E	2	6/6	0.91	0.10	53,54,54,55	6
3	LI	D	202	1/1	0.99	0.12	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.