



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:09 AM UTC

PDB ID : 1YOX / pdb_00001yox
Title : Structure of the conserved Protein of Unknown Function PA3696 from *Pseudomonas aeruginosa*
Authors : Walker, J.R.; Xu, X.; Gu, J.; Joachimiak, A.; Edwards, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2005-01-28
Resolution : 2.30 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

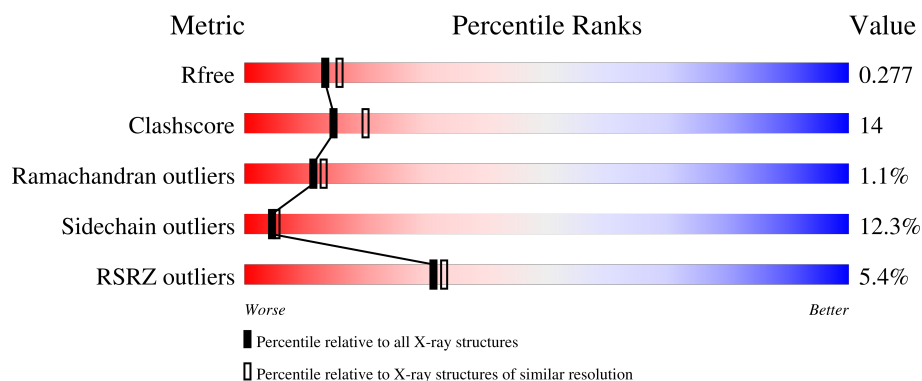
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	250	12% 49% 22% 5% 24%
1	B	250	3% 63% 13% • 22%
1	C	250	• 53% 21% • • 22%
1	D	250	2% 60% 19% • 16%
1	E	250	• 62% 16% • 19%

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Mol	Chain	Length	Quality of chain
1	F	250	6% 45% 26% • 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9193 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 hypothetical protein PA3696.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	Se	0	0	0
			1454	918	251	278	3	4			
1	B	195	Total	C	N	O	S	Se	0	0	0
			1474	933	253	281	3	4			
1	C	196	Total	C	N	O	S	Se	0	0	0
			1484	944	252	281	3	4			
1	D	209	Total	C	N	O	S	Se	0	0	0
			1576	1002	268	298	3	5			
1	E	203	Total	C	N	O	S	Se	0	0	0
			1541	980	261	292	3	5			
1	F	186	Total	C	N	O	S	Se	0	0	0
			1429	904	246	272	3	4			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q9HXU4
A	0	SER	-	cloning artifact	UNP Q9HXU4
A	1	MSE	MET	modified residue	UNP Q9HXU4
A	15	MSE	MET	modified residue	UNP Q9HXU4
A	35	MSE	MET	modified residue	UNP Q9HXU4
A	38	MSE	MET	modified residue	UNP Q9HXU4
A	48	MSE	MET	modified residue	UNP Q9HXU4
A	75	MSE	MET	modified residue	UNP Q9HXU4
A	200	MSE	MET	modified residue	UNP Q9HXU4
B	-1	GLY	-	cloning artifact	UNP Q9HXU4
B	0	SER	-	cloning artifact	UNP Q9HXU4
B	1	MSE	MET	modified residue	UNP Q9HXU4
B	15	MSE	MET	modified residue	UNP Q9HXU4
B	35	MSE	MET	modified residue	UNP Q9HXU4
B	38	MSE	MET	modified residue	UNP Q9HXU4
B	48	MSE	MET	modified residue	UNP Q9HXU4
B	75	MSE	MET	modified residue	UNP Q9HXU4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	200	MSE	MET	modified residue	UNP Q9HXU4
C	-1	GLY	-	cloning artifact	UNP Q9HXU4
C	0	SER	-	cloning artifact	UNP Q9HXU4
C	1	MSE	MET	modified residue	UNP Q9HXU4
C	15	MSE	MET	modified residue	UNP Q9HXU4
C	35	MSE	MET	modified residue	UNP Q9HXU4
C	38	MSE	MET	modified residue	UNP Q9HXU4
C	48	MSE	MET	modified residue	UNP Q9HXU4
C	75	MSE	MET	modified residue	UNP Q9HXU4
C	200	MSE	MET	modified residue	UNP Q9HXU4
D	-1	GLY	-	cloning artifact	UNP Q9HXU4
D	0	SER	-	cloning artifact	UNP Q9HXU4
D	1	MSE	MET	modified residue	UNP Q9HXU4
D	15	MSE	MET	modified residue	UNP Q9HXU4
D	35	MSE	MET	modified residue	UNP Q9HXU4
D	38	MSE	MET	modified residue	UNP Q9HXU4
D	48	MSE	MET	modified residue	UNP Q9HXU4
D	75	MSE	MET	modified residue	UNP Q9HXU4
D	200	MSE	MET	modified residue	UNP Q9HXU4
E	-1	GLY	-	cloning artifact	UNP Q9HXU4
E	0	SER	-	cloning artifact	UNP Q9HXU4
E	1	MSE	MET	modified residue	UNP Q9HXU4
E	15	MSE	MET	modified residue	UNP Q9HXU4
E	35	MSE	MET	modified residue	UNP Q9HXU4
E	38	MSE	MET	modified residue	UNP Q9HXU4
E	48	MSE	MET	modified residue	UNP Q9HXU4
E	75	MSE	MET	modified residue	UNP Q9HXU4
E	200	MSE	MET	modified residue	UNP Q9HXU4
F	-1	GLY	-	cloning artifact	UNP Q9HXU4
F	0	SER	-	cloning artifact	UNP Q9HXU4
F	1	MSE	MET	modified residue	UNP Q9HXU4
F	15	MSE	MET	modified residue	UNP Q9HXU4
F	35	MSE	MET	modified residue	UNP Q9HXU4
F	38	MSE	MET	modified residue	UNP Q9HXU4
F	48	MSE	MET	modified residue	UNP Q9HXU4
F	75	MSE	MET	modified residue	UNP Q9HXU4
F	200	MSE	MET	modified residue	UNP Q9HXU4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0

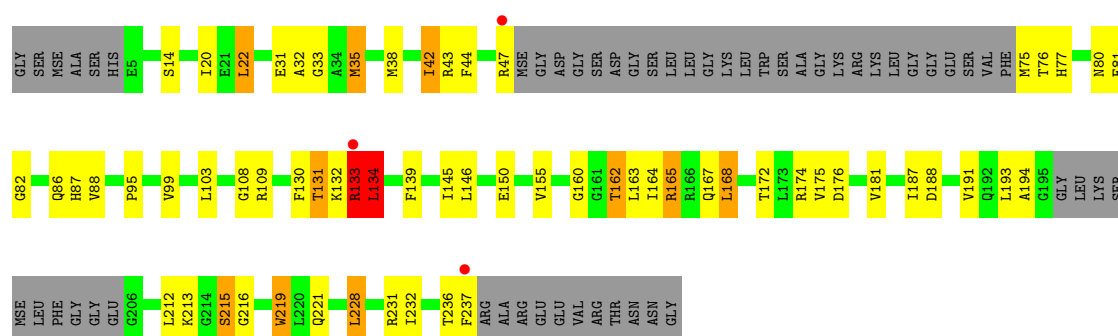
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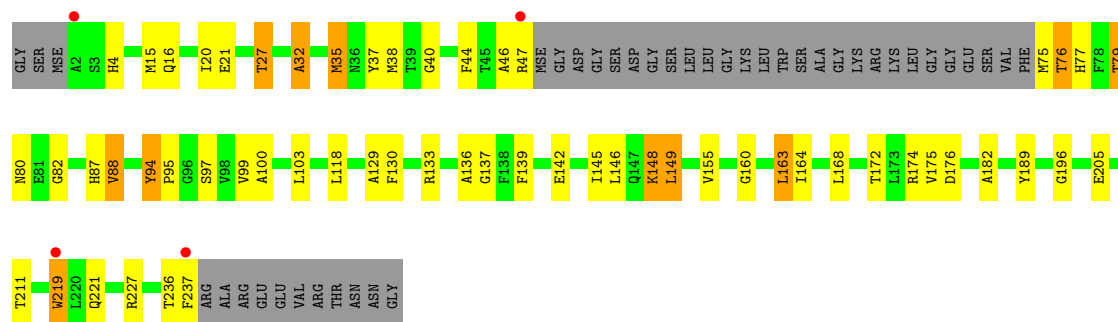
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	43	Total 43	O 43	0	0
2	C	35	Total 35	O 35	0	0
2	D	64	Total 64	O 64	0	0
2	E	52	Total 52	O 52	0	0
2	F	26	Total 26	O 26	0	0

- Molecule 1: hypothetical protein PA3696

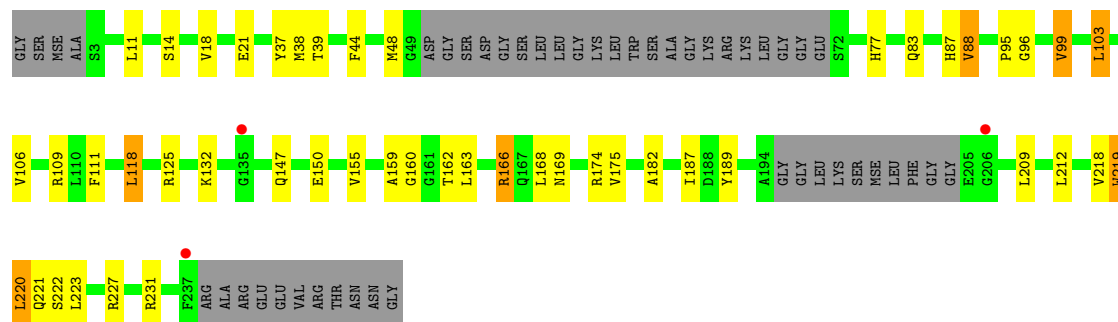




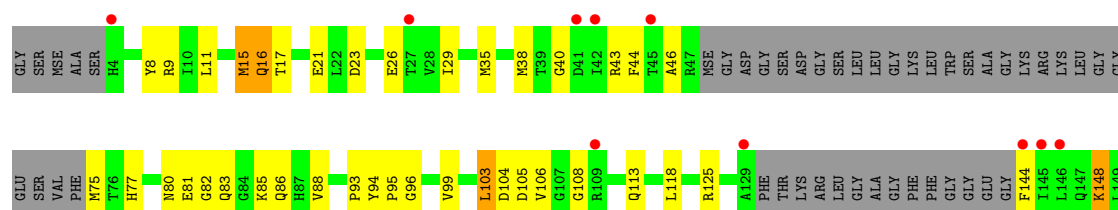
• Molecule 1: hypothetical protein PA3696

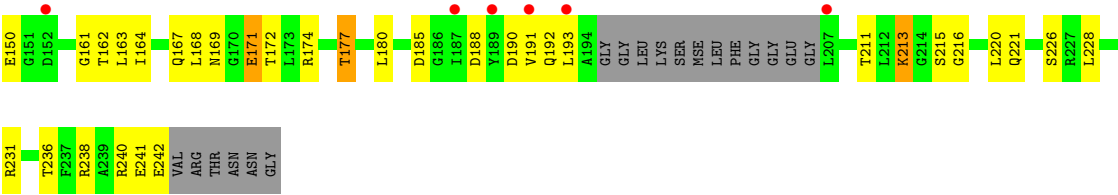


• Molecule 1: hypothetical protein PA3696



• Molecule 1: hypothetical protein PA3696





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.91Å 124.91Å 164.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.30) 99.6 (30.00-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.279 0.224 , 0.277	Depositor DCC
R_{free} test set	2952 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9193	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.48% 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

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	0.72	0/1472	0.89	0/1981
1	B	0.82	0/1494	0.97	1/2010 (0.0%)
1	C	0.82	0/1506	0.96	1/2027 (0.0%)
1	D	0.95	0/1600	1.06	6/2151 (0.3%)
1	E	0.92	0/1563	0.99	1/2100 (0.0%)
1	F	0.79	1/1448 (0.1%)	0.92	1/1950 (0.1%)
All	All	0.84	1/9083 (0.0%)	0.97	10/12219 (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
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	15	MSE	SE-CE	-9.13	1.68	1.95

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	ALA	N-CA-C	6.95	121.43	112.12
1	D	94	TYR	CA-C-N	6.87	127.25	119.83
1	D	94	TYR	C-N-CA	6.87	127.25	119.83
1	F	16	GLN	N-CA-C	6.75	119.34	109.07
1	B	88	VAL	CB-CA-C	-5.96	101.81	110.63
1	D	88	VAL	CB-CA-C	-5.59	102.36	110.63
1	D	100	ALA	CA-C-N	-5.55	115.71	123.10
1	D	100	ALA	C-N-CA	-5.55	115.71	123.10
1	C	168	LEU	N-CA-C	5.53	118.37	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	VAL	CB-CA-C	-5.20	103.08	110.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	215	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1454	0	1431	50	0
1	B	1474	0	1448	27	0
1	C	1484	0	1458	56	0
1	D	1576	0	1549	51	0
1	E	1541	0	1508	38	0
1	F	1429	0	1404	47	0
2	A	15	0	0	1	0
2	B	43	0	0	0	0
2	C	35	0	0	5	0
2	D	64	0	0	2	0
2	E	52	0	0	6	0
2	F	26	0	0	4	0
All	All	9193	0	8798	247	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 (247) 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:15:MSE:HE3	1:A:95:PRO:HB3	1.32	1.08
1:A:101:VAL:HG23	1:A:155:VAL:HG12	1.46	0.96
1:C:131:THR:HG22	1:C:145:ILE:HG12	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.29	0.94
1:E:150:GLU:HG2	2:E:293:HOH:O	1.66	0.94
1:F:15:MSE:HE3	1:F:95:PRO:HB3	1.50	0.93
1:D:4:HIS:HD2	1:D:27:THR:H	1.10	0.93
1:E:160:GLY:H	1:E:221:GLN:HE21	1.19	0.88
1:E:166:ARG:HG2	1:E:166:ARG:HH11	1.36	0.88
1:A:168:LEU:O	1:A:215:SER:HA	1.76	0.85
1:A:85:LYS:HD3	1:A:85:LYS:H	1.41	0.84
1:F:94:TYR:HD1	2:F:266:HOH:O	1.61	0.84
1:A:148:LYS:HB3	2:A:258:HOH:O	1.78	0.83
1:D:15:MSE:HE3	1:D:95:PRO:HB3	1.60	0.82
1:A:43:ARG:HH11	1:A:43:ARG:CG	1.92	0.82
1:C:133:ARG:O	1:C:134:LEU:HB2	1.80	0.80
1:E:219:TRP:CD1	1:E:219:TRP:N	2.52	0.78
1:A:15:MSE:HE3	1:A:95:PRO:CB	2.14	0.78
1:A:160:GLY:H	1:A:221:GLN:HE21	1.30	0.78
1:B:219:TRP:N	1:B:219:TRP:CD1	2.53	0.76
1:C:160:GLY:H	1:C:221:GLN:HE21	1.33	0.76
1:C:231:ARG:HD2	2:C:275:HOH:O	1.84	0.76
1:D:182:ALA:O	1:D:219:TRP:HD1	1.70	0.75
1:A:101:VAL:HG23	1:A:155:VAL:CG1	2.17	0.74
1:C:32:ALA:HB2	1:C:76:THR:HG21	1.71	0.73
1:D:4:HIS:CD2	1:D:27:THR:H	2.02	0.73
1:C:35:MSE:HG3	2:C:254:HOH:O	1.89	0.72
1:D:133:ARG:HH21	1:D:142:GLU:HA	1.55	0.71
1:F:171:GLU:HA	2:F:264:HOH:O	1.91	0.71
1:C:168:LEU:HD12	1:C:187:ILE:HD12	1.73	0.70
1:C:43:ARG:CG	1:C:81:GLU:HG3	2.21	0.70
1:F:15:MSE:CE	1:F:95:PRO:HB3	2.21	0.70
1:E:166:ARG:HH11	1:E:166:ARG:CG	2.05	0.70
1:E:160:GLY:H	1:E:221:GLN:NE2	1.88	0.69
1:D:38:MSE:HE1	1:D:44:PHE:HE2	1.56	0.69
1:C:215:SER:OG	1:C:216:GLY:N	2.22	0.69
1:A:43:ARG:HG2	1:A:43:ARG:NH1	1.98	0.68
1:E:182:ALA:O	1:E:219:TRP:HD1	1.77	0.68
1:C:228:LEU:HD22	1:C:232:ILE:HD12	1.75	0.67
1:A:160:GLY:H	1:A:221:GLN:NE2	1.92	0.67
1:B:165:ARG:NH2	1:B:219:TRP:HZ3	1.92	0.66
1:D:236:THR:O	1:D:237:PHE:CD1	2.49	0.66
1:C:134:LEU:HD21	1:C:191:VAL:HG11	1.77	0.66
1:E:38:MSE:HB3	1:E:88:VAL:HG13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:TRP:HZ3	2:E:278:HOH:O	1.80	0.65
1:B:80:ASN:C	1:B:80:ASN:HD22	2.03	0.64
1:C:80:ASN:ND2	1:C:82:GLY:H	1.95	0.64
1:B:165:ARG:NH2	1:B:219:TRP:CZ3	2.66	0.64
1:A:38:MSE:CE	1:A:42:ILE:HG22	2.28	0.64
1:A:12:GLY:HA2	1:C:162:THR:HG21	1.80	0.64
1:F:15:MSE:HE3	1:F:95:PRO:CB	2.24	0.64
1:A:149:LEU:HD13	1:A:155:VAL:HG21	1.79	0.64
1:E:231:ARG:HG3	1:F:93:PRO:HB3	1.78	0.64
1:D:160:GLY:H	1:D:221:GLN:HE21	1.44	0.63
1:E:209:LEU:HD21	1:F:35:MSE:HE1	1.80	0.63
1:D:149:LEU:HD23	1:D:155:VAL:HG11	1.80	0.63
1:A:38:MSE:HE2	1:A:42:ILE:HG22	1.80	0.63
1:E:21:GLU:OE1	1:E:87:HIS:CE1	2.51	0.63
1:B:80:ASN:ND2	1:B:82:GLY:H	1.97	0.62
1:A:12:GLY:CA	1:C:162:THR:HG21	2.29	0.62
1:E:218:VAL:HG12	1:E:220:LEU:HD13	1.82	0.61
1:E:174:ARG:HG3	1:E:174:ARG:HH11	1.66	0.61
1:F:125:ARG:HB2	1:F:150:GLU:HB2	1.81	0.61
1:B:111:PHE:HE2	1:B:148:LYS:HE2	1.66	0.61
1:D:15:MSE:HE2	1:F:161:GLY:HA2	1.83	0.61
1:D:21:GLU:OE1	1:D:87:HIS:HE1	1.84	0.60
1:D:160:GLY:H	1:D:221:GLN:NE2	1.98	0.60
1:A:233:TYR:O	1:A:240:ARG:NH1	2.34	0.60
1:B:182:ALA:O	1:B:219:TRP:HD1	1.85	0.60
1:D:38:MSE:HE1	1:D:44:PHE:CE2	2.36	0.60
1:A:15:MSE:CE	1:A:95:PRO:HB3	2.21	0.60
1:A:160:GLY:N	1:A:221:GLN:HE21	2.00	0.59
1:D:15:MSE:HE3	1:D:95:PRO:CB	2.32	0.59
1:A:232:ILE:O	1:A:236:THR:HG23	2.03	0.59
1:F:231:ARG:HG2	2:F:256:HOH:O	2.03	0.59
1:A:101:VAL:CG2	1:A:155:VAL:CG1	2.80	0.58
1:A:22:LEU:HD11	1:A:28:VAL:HG12	1.84	0.58
1:F:104:ASP:C	1:F:106:VAL:H	2.10	0.58
1:D:205:GLU:OE1	1:F:238:ARG:NH2	2.36	0.58
1:B:38:MSE:HE1	1:B:44:PHE:HE2	1.69	0.57
1:B:111:PHE:CE2	1:B:148:LYS:HE2	2.38	0.57
1:C:80:ASN:HD22	1:C:80:ASN:C	2.12	0.57
1:C:130:PHE:HB3	1:C:146:LEU:HB2	1.85	0.57
1:D:4:HIS:HD2	1:D:27:THR:N	1.92	0.57
1:C:219:TRP:N	1:C:219:TRP:CD1	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:TRP:CD1	1:D:219:TRP:N	2.74	0.56
1:F:177:THR:HG21	1:F:191:VAL:HG13	1.88	0.56
1:A:238:ARG:HH22	1:B:133:ARG:HB3	1.69	0.56
1:E:231:ARG:HG3	1:F:93:PRO:CB	2.35	0.56
1:A:38:MSE:HG2	1:A:88:VAL:HG13	1.88	0.56
1:B:219:TRP:CD1	1:B:219:TRP:H	2.22	0.55
1:E:160:GLY:N	1:E:221:GLN:HE21	1.96	0.55
1:E:219:TRP:CD1	1:E:219:TRP:H	2.25	0.55
1:C:80:ASN:HD22	1:C:82:GLY:H	1.53	0.55
1:D:160:GLY:N	1:D:221:GLN:HE21	2.04	0.55
1:A:212:LEU:HD13	1:A:218:VAL:HG11	1.89	0.55
1:F:23:ASP:O	1:F:26:GLU:HG3	2.07	0.55
1:B:165:ARG:HH21	1:B:219:TRP:HZ3	1.53	0.54
1:A:42:ILE:O	1:C:174:ARG:NH2	2.34	0.54
1:F:43:ARG:HD3	1:F:81:GLU:HG3	1.88	0.54
1:F:113:GLN:HE21	1:F:144:PHE:HD1	1.55	0.54
1:D:175:VAL:HG12	1:D:176:ASP:O	2.08	0.54
1:E:166:ARG:CG	1:E:166:ARG:NH1	2.69	0.54
1:C:165:ARG:HH11	1:C:167:GLN:HE22	1.54	0.54
1:B:29:ILE:HG23	1:B:75:MSE:SE	2.58	0.53
1:C:43:ARG:HG3	1:C:81:GLU:HG3	1.90	0.53
1:D:27:THR:HB	1:D:79:THR:HG22	1.91	0.53
1:A:236:THR:OG1	1:A:240:ARG:NH1	2.42	0.53
1:A:102:ASP:HA	1:A:154:LEU:HD13	1.90	0.52
1:D:137:GLY:HA3	1:D:139:PHE:CE1	2.44	0.52
1:F:38:MSE:HG2	1:F:88:VAL:HG13	1.91	0.52
1:C:133:ARG:O	1:C:134:LEU:CB	2.55	0.52
1:D:80:ASN:ND2	1:D:82:GLY:H	2.07	0.52
1:C:160:GLY:H	1:C:221:GLN:NE2	2.04	0.52
1:A:80:ASN:C	1:A:80:ASN:HD22	2.17	0.52
1:C:165:ARG:HD3	1:C:167:GLN:HE22	1.75	0.52
1:F:168:LEU:O	1:F:215:SER:HA	2.10	0.52
1:D:129:ALA:HB2	1:D:148:LYS:HB2	1.92	0.52
1:A:228:LEU:O	1:A:232:ILE:HG12	2.11	0.51
1:C:38:MSE:HE1	1:C:44:PHE:CE2	2.46	0.51
1:C:133:ARG:O	1:C:139:PHE:O	2.28	0.51
1:A:235:ALA:HB2	1:B:225:PHE:HE2	1.74	0.51
1:E:18:VAL:HG12	1:E:118:LEU:HD13	1.93	0.51
1:A:85:LYS:HD3	1:A:85:LYS:N	2.17	0.51
1:A:169:ASN:H	1:A:171:GLU:CG	2.24	0.51
1:D:130:PHE:HB3	1:D:146:LEU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:MSE:HE3	1:A:78:PHE:HD2	1.76	0.51
1:D:21:GLU:OE1	1:D:87:HIS:CE1	2.64	0.51
1:D:182:ALA:C	1:D:219:TRP:HD1	2.17	0.51
1:B:80:ASN:HD22	1:B:82:GLY:H	1.58	0.50
1:D:80:ASN:HD22	1:D:82:GLY:H	1.59	0.50
1:B:47:ARG:HE	1:B:75:MSE:HB3	1.76	0.50
1:A:9:ARG:NH2	1:F:8:TYR:O	2.44	0.50
1:B:80:ASN:C	1:B:80:ASN:ND2	2.68	0.49
1:F:113:GLN:NE2	1:F:144:PHE:HD1	2.10	0.49
1:F:236:THR:OG1	1:F:240:ARG:NH1	2.45	0.49
1:A:228:LEU:CD1	1:C:232:ILE:HD11	2.42	0.49
1:C:38:MSE:HB3	1:C:88:VAL:HG13	1.95	0.49
1:C:165:ARG:HD3	1:C:167:GLN:NE2	2.27	0.49
1:F:103:LEU:O	1:F:108:GLY:N	2.43	0.49
1:D:94:TYR:HB2	1:D:95:PRO:HD2	1.95	0.49
1:D:149:LEU:CD2	1:D:155:VAL:HG11	2.42	0.49
1:F:80:ASN:ND2	1:F:82:GLY:H	2.10	0.49
1:F:106:VAL:HG12	1:F:106:VAL:O	2.13	0.49
1:A:93:PRO:HB2	1:C:231:ARG:HG3	1.95	0.48
1:E:222:SER:CB	1:F:17:THR:OG1	2.61	0.48
1:B:165:ARG:CZ	1:B:219:TRP:CZ3	2.97	0.48
1:D:46:ALA:C	1:D:47:ARG:HG3	2.38	0.48
1:C:175:VAL:HG12	1:C:176:ASP:O	2.13	0.48
1:D:47:ARG:HE	1:D:77:HIS:CE1	2.31	0.48
1:A:193:LEU:HD12	1:A:194:ALA:H	1.78	0.48
1:C:43:ARG:HG2	1:C:81:GLU:HG3	1.95	0.48
1:A:104:ASP:OD1	1:A:104:ASP:C	2.57	0.48
1:C:22:LEU:HB3	1:C:80:ASN:HB2	1.95	0.48
1:F:240:ARG:C	1:F:242:GLU:H	2.22	0.48
1:F:44:PHE:HA	1:F:77:HIS:O	2.14	0.48
1:E:168:LEU:HD12	1:E:187:ILE:HD12	1.97	0.47
1:C:20:ILE:HG22	1:C:22:LEU:HD13	1.96	0.47
1:F:15:MSE:HA	1:F:96:GLY:O	2.13	0.47
1:E:109:ARG:HB2	2:E:293:HOH:O	2.15	0.47
1:F:162:THR:O	1:F:221:GLN:HA	2.15	0.47
1:D:32:ALA:HA	1:D:76:THR:CG2	2.44	0.46
1:D:35:MSE:HG3	2:F:249:HOH:O	2.15	0.46
1:F:9:ARG:HD3	1:F:11:LEU:HD21	1.98	0.46
1:E:221:GLN:NE2	2:E:259:HOH:O	2.39	0.46
1:E:222:SER:HB2	1:F:17:THR:OG1	2.16	0.46
1:A:101:VAL:HG21	1:A:110:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:TYR:C	1:F:8:TYR:CD1	2.94	0.46
1:F:188:ASP:HB2	1:F:213:LYS:HD3	1.97	0.46
1:D:80:ASN:HD22	1:D:80:ASN:C	2.23	0.46
1:A:7:ASP:HB2	1:A:21:GLU:HB3	1.98	0.45
1:D:35:MSE:HE1	1:D:37:TYR:C	2.41	0.45
1:D:40:GLY:O	1:F:174:ARG:NH2	2.49	0.45
1:D:35:MSE:HB2	1:D:35:MSE:HE2	1.61	0.45
1:C:109:ARG:HD3	1:C:150:GLU:OE1	2.16	0.45
1:C:188:ASP:HB2	2:C:283:HOH:O	2.16	0.45
1:A:93:PRO:CB	1:C:231:ARG:HG3	2.46	0.45
1:C:108:GLY:HA2	2:C:253:HOH:O	2.16	0.45
1:F:174:ARG:HG2	1:F:211:THR:OG1	2.16	0.45
1:C:42:ILE:CD1	1:C:86:GLN:HB3	2.47	0.45
1:D:20:ILE:O	1:D:87:HIS:HA	2.17	0.45
1:C:75:MSE:HE2	1:C:75:MSE:HA	1.99	0.44
1:C:130:PHE:HZ	1:C:132:LYS:HD2	1.82	0.44
1:C:188:ASP:HB3	1:C:213:LYS:HG2	1.98	0.44
1:C:44:PHE:HA	1:C:77:HIS:O	2.17	0.44
1:E:44:PHE:HA	1:E:77:HIS:O	2.18	0.44
1:F:104:ASP:C	1:F:106:VAL:N	2.75	0.44
1:F:164:ILE:HB	1:F:220:LEU:HB2	2.00	0.44
1:C:42:ILE:HD11	1:C:86:GLN:HB3	1.99	0.44
1:C:80:ASN:ND2	1:C:80:ASN:C	2.76	0.44
1:D:175:VAL:HG22	1:E:37:TYR:HB3	1.99	0.44
1:A:188:ASP:HB2	1:A:213:LYS:HG2	1.99	0.44
1:B:47:ARG:NH2	1:B:77:HIS:HE1	2.16	0.44
1:E:219:TRP:HD1	1:E:219:TRP:H	1.64	0.44
1:D:148:LYS:NZ	1:D:148:LYS:HB3	2.32	0.44
1:F:40:GLY:HA3	1:F:86:GLN:NE2	2.33	0.44
1:B:219:TRP:HD1	1:B:219:TRP:H	1.64	0.43
1:C:130:PHE:CZ	1:C:132:LYS:HD2	2.53	0.43
1:C:188:ASP:O	1:C:212:LEU:HA	2.17	0.43
1:A:238:ARG:NH2	1:B:133:ARG:HB3	2.34	0.43
1:D:163:LEU:HD22	1:D:164:ILE:N	2.33	0.43
1:D:227:ARG:HD2	2:D:297:HOH:O	2.19	0.43
1:D:27:THR:HB	1:D:79:THR:CG2	2.49	0.43
1:E:111:PHE:HA	1:E:147:GLN:O	2.19	0.43
1:E:189:TYR:HB3	1:E:212:LEU:HD23	2.01	0.43
1:F:83:GLN:CD	1:F:83:GLN:H	2.26	0.43
1:F:191:VAL:O	1:F:192:GLN:HG2	2.19	0.43
1:D:142:GLU:HB2	1:D:145:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLU:CD	1:C:33:GLY:H	2.27	0.42
1:D:15:MSE:CE	1:F:161:GLY:HA2	2.49	0.42
1:C:95:PRO:HA	2:C:262:HOH:O	2.19	0.42
1:B:38:MSE:HB3	1:B:88:VAL:HG13	2.01	0.42
1:B:169:ASN:H	1:B:171:GLU:CD	2.26	0.42
1:D:174:ARG:NH2	1:E:39:THR:O	2.49	0.42
1:E:174:ARG:HG3	1:E:174:ARG:NH1	2.33	0.42
1:C:35:MSE:HB2	1:C:35:MSE:HE2	1.64	0.42
1:C:236:THR:O	1:C:237:PHE:HD1	2.02	0.42
1:E:95:PRO:HA	2:E:273:HOH:O	2.20	0.42
1:C:42:ILE:HG12	1:C:88:VAL:HG22	2.02	0.42
1:F:21:GLU:CD	1:F:85:LYS:HD2	2.45	0.42
1:D:189:TYR:HA	1:D:211:THR:O	2.20	0.41
1:E:109:ARG:CB	2:E:293:HOH:O	2.67	0.41
1:F:83:GLN:CD	1:F:83:GLN:N	2.78	0.41
1:B:23:ASP:O	1:B:24:PRO:C	2.63	0.41
1:C:42:ILE:HD13	1:C:87:HIS:O	2.21	0.41
1:E:218:VAL:CG1	1:E:220:LEU:HD13	2.49	0.41
1:E:132:LYS:HA	1:E:132:LYS:HD3	1.63	0.41
1:A:182:ALA:O	1:A:219:TRP:HD1	2.04	0.41
1:D:227:ARG:NH1	2:D:297:HOH:O	2.41	0.41
1:F:103:LEU:HB3	1:F:108:GLY:HA2	2.03	0.41
1:A:126:VAL:HG23	1:A:127:GLY:H	1.85	0.41
1:B:16:GLN:OE1	1:B:97:SER:HB2	2.20	0.41
1:B:130:PHE:HB3	1:B:146:LEU:HB2	2.02	0.41
1:B:189:TYR:HB3	1:B:212:LEU:HD23	2.02	0.41
1:F:148:LYS:NZ	1:F:148:LYS:HB2	2.35	0.41
1:E:96:GLY:HA3	1:E:159:ALA:O	2.20	0.41
1:C:181:VAL:CG2	1:C:221:GLN:HB3	2.51	0.40
1:D:16:GLN:OE1	1:D:97:SER:HB2	2.21	0.40
1:D:196:GLY:O	1:E:44:PHE:HE1	2.04	0.40
1:A:41:ASP:CG	1:A:82:GLY:HA3	2.46	0.40
1:D:46:ALA:O	1:D:47:ARG:HG3	2.21	0.40
1:F:167:GLN:HA	1:F:216:GLY:O	2.21	0.40
1:A:16:GLN:OE1	1:A:97:SER:HB2	2.21	0.40
1:C:35:MSE:HG3	1:C:35:MSE:O	2.20	0.40
1:C:168:LEU:HD23	1:C:168:LEU:HA	1.92	0.40
1:E:103:LEU:HA	1:E:106:VAL:HG22	2.03	0.40
1:A:109:ARG:HD2	1:A:185:ASP:OD2	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	182/250 (73%)	167 (92%)	11 (6%)	4 (2%)	5	4
1	B	187/250 (75%)	179 (96%)	7 (4%)	1 (0%)	24	31
1	C	190/250 (76%)	174 (92%)	13 (7%)	3 (2%)	7	7
1	D	205/250 (82%)	197 (96%)	7 (3%)	1 (0%)	24	31
1	E	197/250 (79%)	186 (94%)	10 (5%)	1 (0%)	24	31
1	F	178/250 (71%)	165 (93%)	11 (6%)	2 (1%)	11	13
All	All	1139/1500 (76%)	1068 (94%)	59 (5%)	12 (1%)	11	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	194	ALA
1	F	105	ASP
1	A	40	GLY
1	A	126	VAL
1	C	133	ARG
1	E	83	GLN
1	A	242	GLU
1	C	134	LEU
1	F	46	ALA
1	A	194	ALA
1	B	205	GLU
1	D	32	ALA

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	150/183 (82%)	126 (84%)	24 (16%)	2	2
1	B	151/183 (82%)	134 (89%)	17 (11%)	5	7
1	C	151/183 (82%)	132 (87%)	19 (13%)	4	5
1	D	160/183 (87%)	145 (91%)	15 (9%)	8	11
1	E	158/183 (86%)	140 (89%)	18 (11%)	5	6
1	F	148/183 (81%)	128 (86%)	20 (14%)	4	4
All	All	918/1098 (84%)	805 (88%)	113 (12%)	4	5

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	31	GLU
1	A	41	ASP
1	A	43	ARG
1	A	45	THR
1	A	81	GLU
1	A	83	GLN
1	A	85	LYS
1	A	88	VAL
1	A	99	VAL
1	A	103	LEU
1	A	104	ASP
1	A	118	LEU
1	A	124	THR
1	A	128	ILE
1	A	148	LYS
1	A	150	GLU
1	A	154	LEU
1	A	165	ARG
1	A	168	LEU
1	A	171	GLU
1	A	213	LYS
1	A	228	LEU
1	A	241	GLU
1	B	29	ILE
1	B	35	MSE
1	B	76	THR
1	B	80	ASN

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Mol	Chain	Res	Type
1	B	88	VAL
1	B	103	LEU
1	B	118	LEU
1	B	149	LEU
1	B	162	THR
1	B	163	LEU
1	B	171	GLU
1	B	175	VAL
1	B	205	GLU
1	B	207	LEU
1	B	209	LEU
1	B	219	TRP
1	B	228	LEU
1	C	14	SER
1	C	22	LEU
1	C	35	MSE
1	C	42	ILE
1	C	47	ARG
1	C	99	VAL
1	C	103	LEU
1	C	131	THR
1	C	133	ARG
1	C	134	LEU
1	C	155	VAL
1	C	162	THR
1	C	163	LEU
1	C	164	ILE
1	C	165	ARG
1	C	172	THR
1	C	193	LEU
1	C	219	TRP
1	C	228	LEU
1	D	27	THR
1	D	35	MSE
1	D	75	MSE
1	D	76	THR
1	D	79	THR
1	D	88	VAL
1	D	99	VAL
1	D	103	LEU
1	D	118	LEU
1	D	148	LYS

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Mol	Chain	Res	Type
1	D	149	LEU
1	D	163	LEU
1	D	168	LEU
1	D	172	THR
1	D	219	TRP
1	E	11	LEU
1	E	14	SER
1	E	48	MSE
1	E	88	VAL
1	E	99	VAL
1	E	103	LEU
1	E	118	LEU
1	E	125	ARG
1	E	155	VAL
1	E	162	THR
1	E	163	LEU
1	E	166	ARG
1	E	169	ASN
1	E	175	VAL
1	E	219	TRP
1	E	220	LEU
1	E	223	LEU
1	E	227	ARG
1	F	16	GLN
1	F	29	ILE
1	F	75	MSE
1	F	99	VAL
1	F	103	LEU
1	F	118	LEU
1	F	148	LYS
1	F	163	LEU
1	F	169	ASN
1	F	171	GLU
1	F	172	THR
1	F	177	THR
1	F	180	LEU
1	F	185	ASP
1	F	190	ASP
1	F	193	LEU
1	F	213	LYS
1	F	226	SER
1	F	228	LEU

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Mol	Chain	Res	Type
1	F	241	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	80	ASN
1	A	86	GLN
1	A	221	GLN
1	B	77	HIS
1	B	80	ASN
1	B	83	GLN
1	B	113	GLN
1	B	167	GLN
1	C	80	ASN
1	C	83	GLN
1	C	113	GLN
1	C	147	GLN
1	C	167	GLN
1	C	221	GLN
1	D	4	HIS
1	D	77	HIS
1	D	80	ASN
1	D	87	HIS
1	D	221	GLN
1	E	80	ASN
1	E	83	GLN
1	E	87	HIS
1	E	192	GLN
1	E	221	GLN
1	F	80	ASN
1	F	86	GLN
1	F	87	HIS
1	F	113	GLN
1	F	167	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	186/250 (74%)	1.12	29 (15%) 5 6	33, 61, 82, 90	0
1	B	191/250 (76%)	0.27	7 (3%) 45 48	28, 38, 54, 69	0
1	C	192/250 (76%)	0.45	3 (1%) 70 72	30, 45, 63, 69	0
1	D	204/250 (81%)	0.12	4 (1%) 65 66	25, 35, 51, 70	0
1	E	198/250 (79%)	0.15	3 (1%) 72 73	23, 37, 52, 65	0
1	F	182/250 (72%)	0.94	16 (8%) 15 17	31, 58, 76, 83	0
All	All	1153/1500 (76%)	0.50	62 (5%) 31 33	23, 43, 71, 90	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	243	VAL	6.1
1	D	237	PHE	4.9
1	B	204	GLY	4.5
1	F	193	LEU	4.3
1	C	133	ARG	4.2
1	A	83	GLN	4.1
1	D	47	ARG	3.9
1	A	194	ALA	3.8
1	A	239	ALA	3.8
1	B	47	ARG	3.8
1	A	195	GLY	3.8
1	D	2	ALA	3.7
1	F	207	LEU	3.5
1	A	191	VAL	3.5
1	B	237	PHE	3.5
1	A	187	ILE	3.4
1	F	109	ARG	3.3
1	E	237	PHE	3.1
1	F	144	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	3.0
1	A	186	GLY	3.0
1	A	142	GLU	2.9
1	A	241	GLU	2.9
1	A	129	ALA	2.7
1	F	129	ALA	2.7
1	B	46	ALA	2.7
1	A	209	LEU	2.7
1	D	219	TRP	2.6
1	A	238	ARG	2.6
1	A	193	LEU	2.5
1	B	203	GLY	2.5
1	C	237	PHE	2.4
1	A	144	PHE	2.4
1	F	42	ILE	2.4
1	B	32	ALA	2.4
1	E	206	GLY	2.3
1	A	47	ARG	2.3
1	A	146	LEU	2.3
1	E	135	GLY	2.3
1	A	42	ILE	2.3
1	C	47	ARG	2.3
1	F	45	THR	2.3
1	F	145	ILE	2.3
1	A	207	LEU	2.2
1	A	154	LEU	2.2
1	F	41	ASP	2.2
1	A	76	THR	2.2
1	A	189	TYR	2.2
1	F	189	TYR	2.2
1	A	244	ARG	2.2
1	A	111	PHE	2.1
1	A	128	ILE	2.1
1	A	29	ILE	2.1
1	F	4	HIS	2.1
1	A	168	LEU	2.1
1	F	191	VAL	2.1
1	F	27	THR	2.0
1	F	146	LEU	2.0
1	F	152	ASP	2.0
1	A	208	LEU	2.0
1	A	109	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	187	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.