



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 1RJ7 / pdb_00001rj7
Title : Crystal structure of EDA-A1
Authors : Hymowitz, S.G.; Compaaan, D.M.; Yan, M.; Ackerly, H.; Dixit, V.M.; Starovastnik, M.A.; de Vos, A.M.
Deposited on : 2003-11-18
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
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

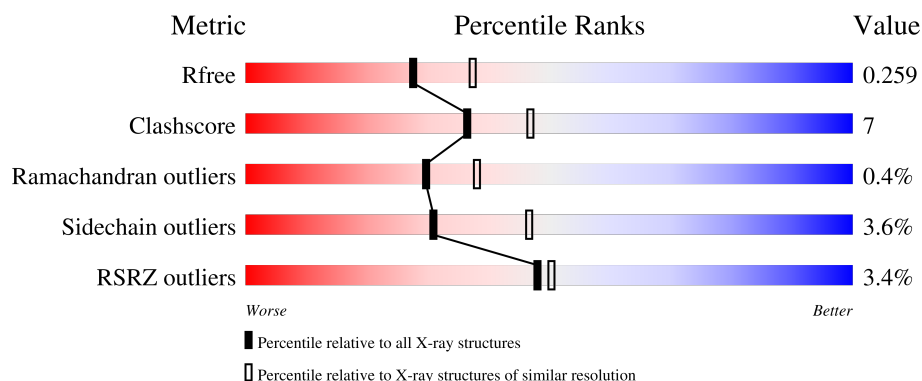
1 Overall quality at a glance

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	163	2% 72% 14% • 12%
1	B	163	4% 74% 12% • 12%
1	D	163	7% 77% 10% • 12%
1	E	163	3% 79% 10% • 9%
1	F	163	0% 75% 13% • 12%

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Mol	Chain	Length	Quality of chain
1	G	163	2% 67% 19% • 12%
1	H	163	6% 74% 12% • 13%
1	I	163	% 76% 11% • 12%
1	J	163	2% 71% 14% • 12%
1	K	163	4% 77% 10% • 11%
1	L	163	% 75% 12% •• 11%
1	M	163	% 77% 9% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13887 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 Ectodysplasin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	B	144	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	D	144	Total	C	N	O	S	0	0	0
			1125	720	190	209	6			
1	E	149	Total	C	N	O	S	0	0	0
			1168	743	200	219	6			
1	F	144	Total	C	N	O	S	0	0	0
			1129	722	191	210	6			
1	G	144	Total	C	N	O	S	0	0	0
			1125	720	190	209	6			
1	H	142	Total	C	N	O	S	0	0	0
			1113	712	188	207	6			
1	I	143	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	J	143	Total	C	N	O	S	0	0	0
			1118	715	189	208	6			
1	K	145	Total	C	N	O	S	0	0	0
			1136	725	192	213	6			
1	L	145	Total	C	N	O	S	0	0	0
			1133	724	192	211	6			
1	M	144	Total	C	N	O	S	0	0	0
			1129	722	191	210	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	GLY	-	cloning artifact	UNP Q92838
A	230	SER	-	cloning artifact	UNP Q92838
A	231	HIS	-	cloning artifact	UNP Q92838
A	232	MET	-	cloning artifact	UNP Q92838
B	229	GLY	-	cloning artifact	UNP Q92838

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Chain	Residue	Modelled	Actual	Comment	Reference
B	230	SER	-	cloning artifact	UNP Q92838
B	231	HIS	-	cloning artifact	UNP Q92838
B	232	MET	-	cloning artifact	UNP Q92838
D	229	GLY	-	cloning artifact	UNP Q92838
D	230	SER	-	cloning artifact	UNP Q92838
D	231	HIS	-	cloning artifact	UNP Q92838
D	232	MET	-	cloning artifact	UNP Q92838
E	229	GLY	-	cloning artifact	UNP Q92838
E	230	SER	-	cloning artifact	UNP Q92838
E	231	HIS	-	cloning artifact	UNP Q92838
E	232	MET	-	cloning artifact	UNP Q92838
F	229	GLY	-	cloning artifact	UNP Q92838
F	230	SER	-	cloning artifact	UNP Q92838
F	231	HIS	-	cloning artifact	UNP Q92838
F	232	MET	-	cloning artifact	UNP Q92838
G	229	GLY	-	cloning artifact	UNP Q92838
G	230	SER	-	cloning artifact	UNP Q92838
G	231	HIS	-	cloning artifact	UNP Q92838
G	232	MET	-	cloning artifact	UNP Q92838
H	229	GLY	-	cloning artifact	UNP Q92838
H	230	SER	-	cloning artifact	UNP Q92838
H	231	HIS	-	cloning artifact	UNP Q92838
H	232	MET	-	cloning artifact	UNP Q92838
I	229	GLY	-	cloning artifact	UNP Q92838
I	230	SER	-	cloning artifact	UNP Q92838
I	231	HIS	-	cloning artifact	UNP Q92838
I	232	MET	-	cloning artifact	UNP Q92838
J	229	GLY	-	cloning artifact	UNP Q92838
J	230	SER	-	cloning artifact	UNP Q92838
J	231	HIS	-	cloning artifact	UNP Q92838
J	232	MET	-	cloning artifact	UNP Q92838
K	229	GLY	-	cloning artifact	UNP Q92838
K	230	SER	-	cloning artifact	UNP Q92838
K	231	HIS	-	cloning artifact	UNP Q92838
K	232	MET	-	cloning artifact	UNP Q92838
L	229	GLY	-	cloning artifact	UNP Q92838
L	230	SER	-	cloning artifact	UNP Q92838
L	231	HIS	-	cloning artifact	UNP Q92838
L	232	MET	-	cloning artifact	UNP Q92838
M	229	GLY	-	cloning artifact	UNP Q92838
M	230	SER	-	cloning artifact	UNP Q92838
M	231	HIS	-	cloning artifact	UNP Q92838

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Chain	Residue	Modelled	Actual	Comment	Reference
M	232	MET	-	cloning artifact	UNP Q92838

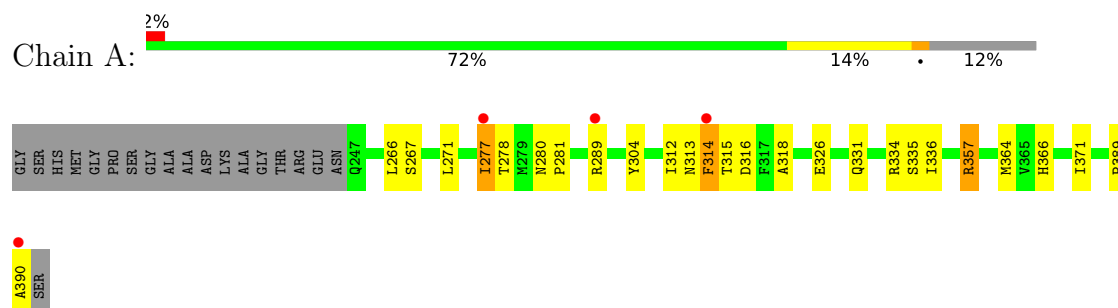
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	35	Total O 35 35	0	0
2	B	17	Total O 17 17	0	0
2	D	19	Total O 19 19	0	0
2	E	37	Total O 37 37	0	0
2	F	41	Total O 41 41	0	0
2	G	43	Total O 43 43	0	0
2	H	22	Total O 22 22	0	0
2	I	22	Total O 22 22	0	0
2	J	19	Total O 19 19	0	0
2	K	32	Total O 32 32	0	0
2	L	29	Total O 29 29	0	0
2	M	23	Total O 23 23	0	0

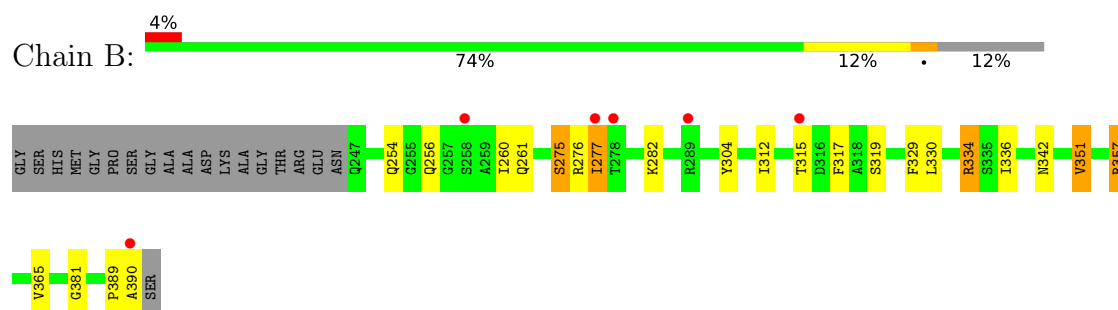
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

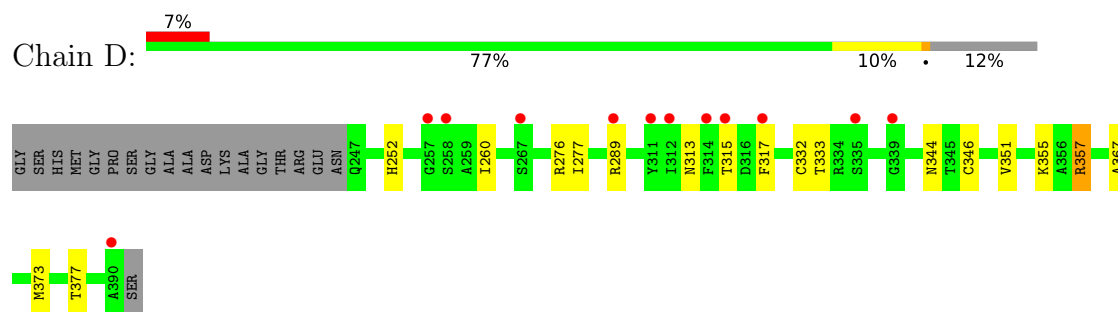
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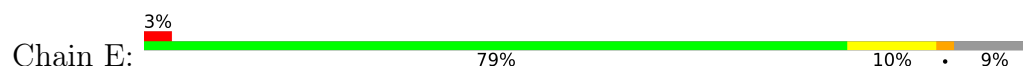
• Molecule 1: Ectodysplasins A



• Molecule 1: Ectodysplasins A

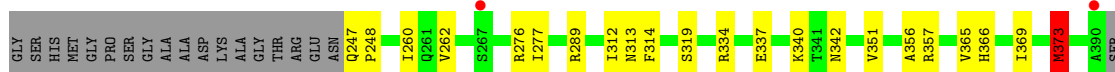
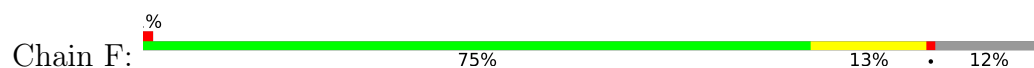


• Molecule 1: Ectodysplasins A

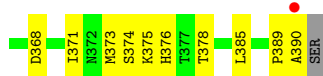




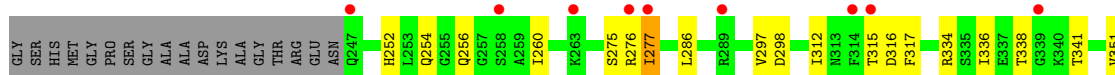
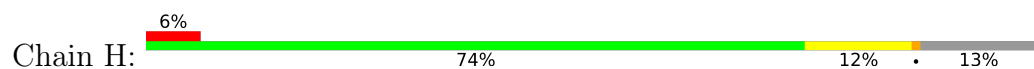
• Molecule 1: Ectodysplasin A



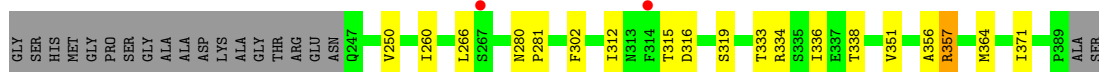
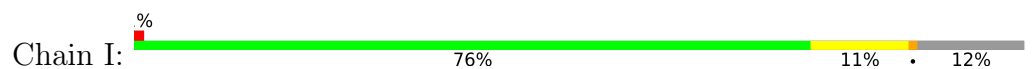
• Molecule 1: Ectodysplasin A



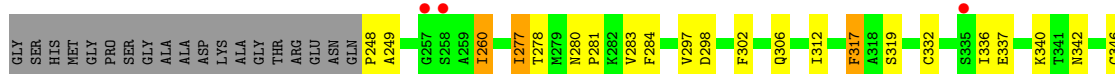
• Molecule 1: Ectodysplasin A



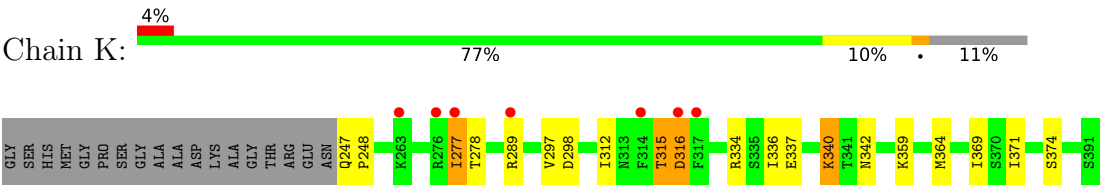
• Molecule 1: Ectodysplasin A



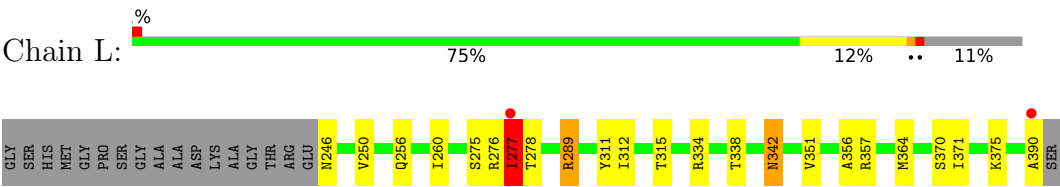
• Molecule 1: Ectodysplasin A



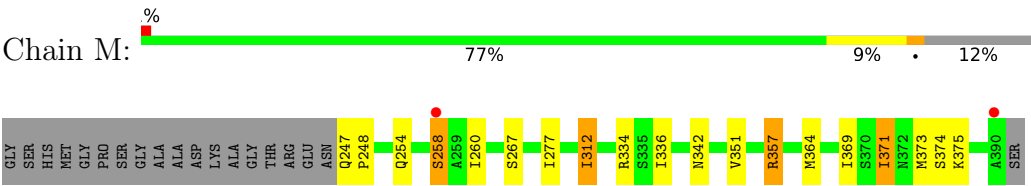
● Molecule 1: Ectodysplasin A



● Molecule 1: Ectodysplasin A



● Molecule 1: Ectodysplasin A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.66Å 279.69Å 54.17Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.30) 94.2 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.07	Depositor
R, R_{free}	0.194 , 0.260 0.197 , 0.259	Depositor DCC
R_{free} test set	7099 reflections (10.71%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.046 for h,-k,-l 0.031 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13887	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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](#)

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	0.65	0/1148	0.87	1/1556 (0.1%)
1	B	0.63	0/1148	0.88	0/1556
1	D	0.63	0/1149	0.82	0/1558
1	E	0.68	0/1192	0.87	0/1615
1	F	0.72	1/1153 (0.1%)	0.86	1/1563 (0.1%)
1	G	0.68	0/1149	0.91	2/1558 (0.1%)
1	H	0.62	0/1136	0.84	0/1539
1	I	0.59	0/1148	0.83	0/1556
1	J	0.63	0/1141	0.83	1/1546 (0.1%)
1	K	0.66	0/1160	0.85	0/1571
1	L	0.67	1/1157 (0.1%)	0.85	0/1569
1	M	0.63	0/1153	0.84	0/1563
All	All	0.65	2/13834 (0.0%)	0.85	5/18750 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	373	MET	SD-CE	-7.72	1.60	1.79
1	L	277	ILE	CA-CB	5.19	1.61	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	PHE	N-CA-C	6.95	120.75	111.30
1	J	248	PRO	N-CA-CB	6.90	110.59	103.00
1	G	317	PHE	N-CA-C	5.74	118.82	109.24
1	G	262	VAL	N-CA-C	5.47	115.67	110.42
1	F	262	VAL	N-CA-C	5.06	116.39	110.62

There are no chirality outliers.

There are no planarity outliers.

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	1124	0	1118	25	0
1	B	1124	0	1118	17	0
1	D	1125	0	1119	14	0
1	E	1168	0	1160	20	0
1	F	1129	0	1125	17	0
1	G	1125	0	1119	28	0
1	H	1113	0	1107	14	0
1	I	1124	0	1120	14	0
1	J	1118	0	1112	16	0
1	K	1136	0	1130	15	0
1	L	1133	0	1125	17	0
1	M	1129	0	1125	20	0
2	A	35	0	0	1	0
2	B	17	0	0	4	0
2	D	19	0	0	1	0
2	E	37	0	0	2	0
2	F	41	0	0	2	0
2	G	43	0	0	6	0
2	H	22	0	0	0	0
2	I	22	0	0	0	0
2	J	19	0	0	0	0
2	K	32	0	0	3	0
2	L	29	0	0	4	0
2	M	23	0	0	2	0
All	All	13887	0	13478	195	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 7.

All (195) 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:G:334:ARG:NH2	2:G:392:HOH:O	2.00	0.94
1:G:297:VAL:HB	2:G:426:HOH:O	1.69	0.92
1:F:260:ILE:HD12	1:F:373:MET:HG3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:GLN:N	2:F:426:HOH:O	2.15	0.80
1:E:242:GLY:HA2	2:E:422:HOH:O	1.84	0.76
1:H:256:GLN:HG3	1:H:275:SER:HB2	1.67	0.75
1:E:314:PHE:O	1:E:315:THR:OG1	2.05	0.74
1:A:314:PHE:HB2	1:E:314:PHE:CD1	2.23	0.73
1:F:312:ILE:HG13	1:F:369:ILE:HG22	1.72	0.72
1:A:334:ARG:HH12	1:B:334:ARG:HE	1.38	0.70
1:H:312:ILE:HD12	1:H:336:ILE:HB	1.75	0.68
1:K:337:GLU:HB3	1:K:340:LYS:HE3	1.76	0.68
1:F:247:GLN:N	2:F:427:HOH:O	2.26	0.68
1:G:254:GLN:NE2	1:G:375:LYS:HG2	2.09	0.67
1:M:364:MET:HE2	1:M:371:ILE:HD11	1.76	0.66
1:G:364:MET:SD	1:G:371:ILE:HD11	2.37	0.66
1:L:276:ARG:HD2	2:L:405:HOH:O	1.97	0.65
1:A:277:ILE:HG13	1:A:278:THR:H	1.62	0.65
1:B:365:VAL:HG13	2:B:7:HOH:O	1.97	0.65
1:A:312:ILE:HD12	1:A:336:ILE:HB	1.78	0.65
1:D:260:ILE:HD12	1:D:373:MET:HG3	1.78	0.64
1:L:277:ILE:HG23	1:L:278:THR:H	1.63	0.63
1:E:389:PRO:O	1:E:390:ALA:CB	2.46	0.62
1:L:256:GLN:NE2	2:L:407:HOH:O	2.33	0.62
1:K:247:GLN:HB3	1:K:248:PRO:HD3	1.82	0.61
1:H:315:THR:HG22	1:H:317:PHE:HB3	1.83	0.61
1:D:355:LYS:HE2	2:D:120:HOH:O	2.02	0.60
1:A:314:PHE:CD1	1:E:314:PHE:HB3	2.36	0.59
1:F:337:GLU:HB2	1:F:340:LYS:HE2	1.84	0.59
1:K:312:ILE:CG2	1:K:315:THR:HG23	2.33	0.59
1:L:312:ILE:O	1:L:338:THR:O	2.21	0.59
1:M:254:GLN:NE2	1:M:277:ILE:HD11	2.19	0.58
1:B:256:GLN:HG3	1:B:275:SER:HB2	1.86	0.57
1:F:312:ILE:CG1	1:F:369:ILE:HG22	2.34	0.57
1:J:340:LYS:HE3	1:J:342:ASN:HD21	1.68	0.57
1:E:312:ILE:HD12	1:E:336:ILE:HB	1.87	0.57
1:M:312:ILE:HD11	1:M:336:ILE:HB	1.86	0.57
1:A:334:ARG:NH1	1:B:334:ARG:HE	2.03	0.57
1:E:266:LEU:HD11	1:E:271:LEU:HD23	1.86	0.56
1:M:260:ILE:HD12	1:M:373:MET:HG3	1.88	0.55
1:M:260:ILE:HD12	1:M:373:MET:CG	2.37	0.55
1:H:252:HIS:HD2	1:H:277:ILE:HD11	1.71	0.55
1:B:312:ILE:HD12	1:B:336:ILE:HB	1.89	0.55
1:D:315:THR:HG21	1:D:367:ALA:HB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:ILE:O	1:G:312:ILE:HG13	2.07	0.54
1:M:312:ILE:HG23	1:M:369:ILE:HG12	1.89	0.54
1:H:254:GLN:HG3	1:H:277:ILE:HD11	1.90	0.54
1:I:302:PHE:HD1	1:I:351:VAL:HG22	1.73	0.54
1:M:312:ILE:CD1	1:M:336:ILE:HB	2.37	0.54
1:D:357:ARG:CG	1:D:357:ARG:HH11	2.21	0.53
1:B:365:VAL:CG1	2:B:7:HOH:O	2.54	0.53
1:A:314:PHE:CB	1:E:314:PHE:CD1	2.90	0.53
1:I:260:ILE:HD13	1:I:266:LEU:HD21	1.90	0.53
1:G:254:GLN:NE2	1:G:277:ILE:CD1	2.72	0.53
1:A:366:HIS:ND1	1:A:366:HIS:C	2.67	0.53
1:B:282:LYS:HA	2:B:125:HOH:O	2.08	0.53
1:K:312:ILE:CD1	1:K:336:ILE:HB	2.39	0.53
1:A:335:SER:HB2	1:D:344:ASN:HD21	1.73	0.53
1:K:312:ILE:HD12	1:K:336:ILE:HB	1.90	0.53
1:H:276:ARG:HH11	1:H:286:LEU:HD23	1.74	0.52
1:J:317:PHE:CE1	1:J:319:SER:HB2	2.43	0.52
1:K:364:MET:HE2	1:K:371:ILE:HD11	1.91	0.52
1:D:357:ARG:NH1	1:D:357:ARG:HG3	2.23	0.52
1:G:389:PRO:O	1:G:390:ALA:CB	2.58	0.52
1:E:389:PRO:O	1:E:390:ALA:HB2	2.11	0.51
1:A:304:TYR:OH	1:B:351:VAL:HG23	2.11	0.51
1:B:389:PRO:O	1:B:390:ALA:HB3	2.10	0.51
1:K:337:GLU:HB3	1:K:340:LYS:CE	2.41	0.51
1:A:313:ASN:O	1:A:314:PHE:CD1	2.63	0.51
1:L:364:MET:HE2	1:L:371:ILE:HD11	1.92	0.51
1:G:247:GLN:N	2:G:422:HOH:O	2.44	0.51
1:A:331:GLN:HB3	1:D:377:THR:HG22	1.93	0.50
1:G:251:VAL:HG11	1:G:293:LEU:HD21	1.93	0.50
1:I:364:MET:SD	1:I:371:ILE:HD11	2.52	0.50
1:M:248:PRO:HD2	2:M:169:HOH:O	2.09	0.50
1:M:254:GLN:NE2	1:M:375:LYS:O	2.44	0.50
1:A:314:PHE:CE1	1:E:314:PHE:O	2.65	0.50
1:E:334:ARG:HH12	1:F:334:ARG:NH1	2.09	0.50
1:L:356:ALA:O	1:L:357:ARG:HB2	2.12	0.50
1:I:312:ILE:HD12	1:I:336:ILE:HB	1.94	0.49
1:M:364:MET:CE	1:M:371:ILE:HD11	2.42	0.49
1:I:250:VAL:HG11	1:J:351:VAL:HG11	1.95	0.49
1:J:249:ALA:CB	1:J:283:VAL:HG21	2.42	0.49
1:A:357:ARG:CG	1:A:357:ARG:HH11	2.24	0.49
1:D:357:ARG:HH11	1:D:357:ARG:HG3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:GLN:N	1:G:248:PRO:CD	2.76	0.49
1:K:316:ASP:OD1	1:K:316:ASP:C	2.55	0.49
1:L:390:ALA:HA	2:L:403:HOH:O	2.13	0.49
1:J:260:ILE:HD12	1:J:373:MET:HG3	1.95	0.48
1:M:357:ARG:HG3	1:M:357:ARG:HH11	1.78	0.48
1:M:357:ARG:HG3	1:M:357:ARG:NH1	2.28	0.48
1:L:250:VAL:HG11	1:M:351:VAL:HG21	1.96	0.48
1:A:314:PHE:HB2	1:E:314:PHE:CG	2.49	0.48
1:J:302:PHE:HD1	1:J:351:VAL:HG22	1.79	0.48
1:F:313:ASN:HB3	1:F:314:PHE:CD2	2.48	0.48
1:H:312:ILE:CD1	1:H:336:ILE:HB	2.44	0.47
1:B:317:PHE:CE1	1:B:319:SER:HB2	2.49	0.47
1:A:267:SER:HA	2:A:60:HOH:O	2.14	0.47
1:G:334:ARG:HG3	1:G:334:ARG:HH11	1.79	0.47
1:L:375:LYS:HG2	2:L:408:HOH:O	2.14	0.47
1:D:317:PHE:HE1	1:D:333:THR:HB	1.80	0.47
1:H:356:ALA:O	1:H:357:ARG:HB2	2.14	0.47
1:E:356:ALA:O	1:E:357:ARG:HB2	2.15	0.47
1:K:315:THR:HB	2:K:410:HOH:O	2.15	0.47
1:L:289:ARG:HH11	1:L:289:ARG:HB3	1.80	0.47
1:J:337:GLU:HB3	1:J:340:LYS:HE2	1.97	0.47
1:D:276:ARG:O	1:D:276:ARG:HG3	2.15	0.47
1:J:332:CYS:SG	1:J:346:CYS:HB3	2.54	0.47
1:M:357:ARG:HH11	1:M:357:ARG:CG	2.28	0.47
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.28	0.47
1:L:256:GLN:HG2	1:L:275:SER:HB2	1.96	0.47
1:H:315:THR:O	1:H:316:ASP:HB2	2.15	0.46
1:I:315:THR:O	1:I:338:THR:HG22	2.15	0.46
1:B:254:GLN:HG3	1:B:277:ILE:HD11	1.98	0.46
1:F:356:ALA:O	1:F:357:ARG:HB2	2.15	0.46
1:G:254:GLN:NE2	1:G:277:ILE:HD11	2.30	0.46
1:I:312:ILE:CD1	1:I:336:ILE:HB	2.46	0.46
1:A:364:MET:HE2	1:A:371:ILE:HD11	1.98	0.46
1:E:334:ARG:HH12	1:F:334:ARG:CZ	2.28	0.46
1:D:332:CYS:SG	1:D:346:CYS:HB3	2.56	0.46
1:I:319:SER:OG	1:I:333:THR:HG22	2.14	0.46
1:A:326:GLU:OE1	1:G:376:HIS:NE2	2.47	0.46
1:D:317:PHE:CE1	1:D:333:THR:HB	2.51	0.46
1:H:256:GLN:CG	1:H:275:SER:HB2	2.42	0.46
1:J:297:VAL:HG12	1:J:298:ASP:O	2.16	0.46
1:M:258:SER:HB2	2:M:141:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:HIS:O	1:D:277:ILE:HG22	2.16	0.45
1:K:369:ILE:HD12	2:K:411:HOH:O	2.17	0.45
1:G:254:GLN:CD	1:G:277:ILE:HD12	2.40	0.45
1:G:368:ASP:HB2	2:G:413:HOH:O	2.16	0.45
1:J:283:VAL:HG23	1:J:284:PHE:CD2	2.52	0.45
1:L:334:ARG:HH12	1:M:334:ARG:CZ	2.30	0.45
1:G:260:ILE:HD12	1:G:373:MET:HG3	1.98	0.45
1:L:342:ASN:HD22	1:L:342:ASN:HA	1.59	0.45
1:E:340:LYS:HG3	2:E:392:HOH:O	2.17	0.44
1:H:334:ARG:HH12	1:I:334:ARG:CZ	2.30	0.44
1:J:280:ASN:HB3	1:J:283:VAL:HG22	1.98	0.44
1:B:261:GLN:HB3	2:B:3:HOH:O	2.16	0.44
1:G:247:GLN:N	1:G:248:PRO:HD2	2.33	0.44
1:H:357:ARG:HH11	1:H:357:ARG:HG3	1.82	0.44
1:J:280:ASN:HA	1:J:281:PRO:HD3	1.85	0.44
1:L:250:VAL:HB	1:M:351:VAL:HG11	1.99	0.44
1:D:252:HIS:O	1:D:277:ILE:CG2	2.66	0.44
1:G:276:ARG:HG2	2:G:408:HOH:O	2.18	0.44
1:J:312:ILE:HD11	1:J:336:ILE:O	2.18	0.44
1:G:315:THR:HG23	1:G:315:THR:O	2.17	0.43
1:K:334:ARG:HH12	1:L:334:ARG:CZ	2.32	0.43
1:A:312:ILE:HD11	1:A:318:ALA:HB2	2.00	0.43
1:B:312:ILE:HG22	1:B:315:THR:O	2.18	0.43
1:B:389:PRO:O	1:B:390:ALA:CB	2.66	0.43
1:A:315:THR:O	1:A:316:ASP:OD1	2.37	0.43
1:E:319:SER:O	1:E:365:VAL:HG22	2.19	0.43
1:G:319:SER:O	1:G:365:VAL:HG22	2.19	0.43
1:I:280:ASN:HA	1:I:281:PRO:HD3	1.88	0.43
1:G:313:ASN:HB3	1:G:368:ASP:HB3	2.01	0.42
1:F:366:HIS:O	1:F:366:HIS:CD2	2.72	0.42
1:J:306:GLN:O	1:J:378:THR:HA	2.19	0.42
1:G:306:GLN:O	1:G:378:THR:HA	2.20	0.42
1:K:337:GLU:HB2	1:K:342:ASN:ND2	2.34	0.42
1:M:254:GLN:CD	1:M:277:ILE:HD11	2.45	0.42
1:A:389:PRO:O	1:A:390:ALA:HB3	2.19	0.42
1:E:250:VAL:HG11	1:F:351:VAL:HG21	2.02	0.42
1:J:389:PRO:O	1:J:390:ALA:CB	2.67	0.42
1:B:329:PHE:CD2	1:B:330:LEU:HG	2.55	0.42
1:I:316:ASP:HB2	1:I:336:ILE:O	2.20	0.42
1:K:297:VAL:HG12	1:K:298:ASP:O	2.19	0.42
1:L:315:THR:O	1:L:338:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:247:GLN:HA	1:M:247:GLN:OE1	2.19	0.42
1:A:357:ARG:CG	1:A:357:ARG:NH1	2.83	0.41
1:E:312:ILE:HD11	1:E:336:ILE:HD12	2.02	0.41
1:M:254:GLN:HB2	1:M:375:LYS:O	2.20	0.41
1:G:312:ILE:O	1:G:338:THR:O	2.38	0.41
1:G:256:GLN:O	1:G:257:GLY:C	2.62	0.41
1:F:312:ILE:HG13	1:F:369:ILE:CG2	2.47	0.41
1:I:356:ALA:O	1:I:357:ARG:HB2	2.21	0.41
1:K:277:ILE:HG13	1:K:278:THR:N	2.34	0.41
1:F:319:SER:O	1:F:365:VAL:HG22	2.21	0.41
1:B:304:TYR:CZ	1:B:381:GLY:HA3	2.55	0.41
1:G:368:ASP:CB	2:G:413:HOH:O	2.68	0.41
1:L:311:TYR:HB3	1:L:370:SER:HB2	2.02	0.41
1:J:277:ILE:HG23	1:J:278:THR:O	2.20	0.41
1:F:276:ARG:H	1:F:276:ARG:HG2	1.76	0.41
1:A:280:ASN:HA	1:A:281:PRO:HD3	1.90	0.41
1:G:364:MET:HE2	1:G:371:ILE:HD11	2.02	0.41
1:I:315:THR:C	1:I:338:THR:HG22	2.46	0.41
1:E:314:PHE:C	1:E:315:THR:HG1	2.15	0.40
1:K:359:LYS:HE3	2:K:414:HOH:O	2.21	0.40
1:A:366:HIS:C	1:A:366:HIS:HD1	2.29	0.40
1:E:335:SER:OG	1:G:342:ASN:HB2	2.21	0.40
1:F:373:MET:HE3	1:F:373:MET:HB3	2.00	0.40
1:H:297:VAL:HG12	1:H:298:ASP:O	2.21	0.40
1:H:357:ARG:HG3	1:H:357:ARG:NH1	2.37	0.40
1:A:266:LEU:HD11	1:A:271:LEU:HD23	2.04	0.40
1:F:248:PRO:HG2	1:G:385:LEU:HB3	2.02	0.40
1:I:357:ARG:CG	1:I:357:ARG:HH11	2.35	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	142/163 (87%)	132 (93%)	9 (6%)	1 (1%)	18	23
1	B	142/163 (87%)	132 (93%)	10 (7%)	0	100	100
1	D	142/163 (87%)	137 (96%)	5 (4%)	0	100	100
1	E	147/163 (90%)	138 (94%)	6 (4%)	3 (2%)	6	5
1	F	142/163 (87%)	132 (93%)	10 (7%)	0	100	100
1	G	142/163 (87%)	134 (94%)	7 (5%)	1 (1%)	18	23
1	H	140/163 (86%)	133 (95%)	7 (5%)	0	100	100
1	I	141/163 (86%)	136 (96%)	5 (4%)	0	100	100
1	J	141/163 (86%)	133 (94%)	8 (6%)	0	100	100
1	K	143/163 (88%)	137 (96%)	6 (4%)	0	100	100
1	L	143/163 (88%)	132 (92%)	10 (7%)	1 (1%)	18	23
1	M	142/163 (87%)	137 (96%)	5 (4%)	0	100	100
All	All	1707/1956 (87%)	1613 (94%)	88 (5%)	6 (0%)	30	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	257	GLY
1	E	262	VAL
1	E	315	THR
1	G	257	GLY
1	A	277	ILE
1	L	277	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	123/136 (90%)	121 (98%)	2 (2%)	55	73
1	B	123/136 (90%)	115 (94%)	8 (6%)	15	22
1	D	123/136 (90%)	119 (97%)	4 (3%)	33	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	128/136 (94%)	125 (98%)	3 (2%)	44	63
1	F	124/136 (91%)	120 (97%)	4 (3%)	34	51
1	G	123/136 (90%)	119 (97%)	4 (3%)	33	50
1	H	122/136 (90%)	117 (96%)	5 (4%)	27	41
1	I	124/136 (91%)	123 (99%)	1 (1%)	73	86
1	J	122/136 (90%)	118 (97%)	4 (3%)	33	50
1	K	125/136 (92%)	119 (95%)	6 (5%)	23	35
1	L	124/136 (91%)	119 (96%)	5 (4%)	28	42
1	M	124/136 (91%)	117 (94%)	7 (6%)	19	28
All	All	1485/1632 (91%)	1432 (96%)	53 (4%)	31	47

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	A	357	ARG
1	B	260	ILE
1	B	275	SER
1	B	276	ARG
1	B	277	ILE
1	B	334	ARG
1	B	342	ASN
1	B	351	VAL
1	B	357	ARG
1	D	289	ARG
1	D	313	ASN
1	D	351	VAL
1	D	357	ARG
1	E	289	ARG
1	E	335	SER
1	E	340	LYS
1	F	277	ILE
1	F	289	ARG
1	F	342	ASN
1	F	373	MET
1	G	260	ILE
1	G	334	ARG
1	G	351	VAL
1	G	374	SER

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Mol	Chain	Res	Type
1	H	260	ILE
1	H	277	ILE
1	H	338	THR
1	H	341	THR
1	H	351	VAL
1	I	357	ARG
1	J	260	ILE
1	J	277	ILE
1	J	317	PHE
1	J	351	VAL
1	K	277	ILE
1	K	289	ARG
1	K	315	THR
1	K	316	ASP
1	K	340	LYS
1	K	374	SER
1	L	246	ASN
1	L	260	ILE
1	L	289	ARG
1	L	342	ASN
1	L	351	VAL
1	M	258	SER
1	M	267	SER
1	M	312	ILE
1	M	342	ASN
1	M	357	ARG
1	M	371	ILE
1	M	374	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	ASN
1	B	254	GLN
1	B	264	ASN
1	B	342	ASN
1	D	344	ASN
1	F	366	HIS
1	G	254	GLN
1	G	256	GLN
1	G	342	ASN
1	G	366	HIS

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Mol	Chain	Res	Type
1	H	256	GLN
1	H	366	HIS
1	H	376	HIS
1	I	254	GLN
1	J	331	GLN
1	J	342	ASN
1	K	254	GLN
1	K	344	ASN
1	K	366	HIS
1	K	376	HIS
1	L	342	ASN
1	M	254	GLN
1	M	342	ASN

5.3.3 RNA [i](#)

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	144/163 (88%)	-0.05	4 (2%)	55	57	2, 5, 15, 21	0
1	B	144/163 (88%)	0.43	6 (4%)	40	42	2, 5, 14, 19	0
1	D	144/163 (88%)	0.52	12 (8%)	17	19	2, 5, 12, 16	0
1	E	149/163 (91%)	0.18	5 (3%)	48	50	2, 5, 16, 27	0
1	F	144/163 (88%)	-0.19	2 (1%)	73	75	2, 5, 13, 24	0
1	G	144/163 (88%)	-0.09	4 (2%)	55	57	2, 5, 15, 23	0
1	H	142/163 (87%)	0.48	10 (7%)	22	24	2, 5, 13, 18	0
1	I	143/163 (87%)	-0.05	2 (1%)	73	75	2, 5, 14, 20	0
1	J	143/163 (87%)	0.40	3 (2%)	63	65	2, 5, 11, 16	0
1	K	145/163 (88%)	0.27	7 (4%)	35	37	2, 5, 14, 24	0
1	L	145/163 (88%)	0.01	2 (1%)	73	75	2, 5, 14, 22	0
1	M	144/163 (88%)	0.00	2 (1%)	73	75	2, 5, 14, 21	0
All	All	1731/1956 (88%)	0.16	59 (3%)	48	50	2, 5, 14, 27	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	390	ALA	6.1
1	D	315	THR	5.9
1	E	390	ALA	5.3
1	H	258	SER	4.9
1	B	277	ILE	4.3
1	H	315	THR	4.1
1	L	390	ALA	4.1
1	B	258	SER	4.0
1	M	258	SER	3.9
1	B	390	ALA	3.9
1	G	390	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	L	277	ILE	3.8
1	E	314	PHE	3.6
1	D	390	ALA	3.5
1	J	258	SER	3.5
1	H	314	PHE	3.5
1	I	314	PHE	3.4
1	A	390	ALA	3.4
1	D	314	PHE	3.3
1	K	317	PHE	3.3
1	B	278	THR	3.3
1	H	339	GLY	3.2
1	K	314	PHE	3.1
1	E	264	ASN	3.1
1	H	388	ALA	3.0
1	D	289	ARG	3.0
1	G	316	ASP	2.8
1	D	317	PHE	2.8
1	H	247	GLN	2.7
1	D	257	GLY	2.7
1	M	390	ALA	2.7
1	K	316	ASP	2.7
1	E	258	SER	2.7
1	G	315	THR	2.6
1	I	267	SER	2.5
1	H	276	ARG	2.4
1	K	277	ILE	2.4
1	H	289	ARG	2.3
1	D	312	ILE	2.3
1	H	277	ILE	2.3
1	B	289	ARG	2.3
1	K	276	ARG	2.3
1	A	277	ILE	2.3
1	D	339	GLY	2.2
1	K	263	LYS	2.2
1	A	314	PHE	2.2
1	K	289	ARG	2.2
1	D	258	SER	2.2
1	G	317	PHE	2.2
1	B	315	THR	2.2
1	H	263	LYS	2.1
1	D	267	SER	2.1
1	J	257	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	335	SER	2.1
1	E	312	ILE	2.1
1	A	289	ARG	2.1
1	J	335	SER	2.0
1	D	311	TYR	2.0
1	F	267	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 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.