



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:55 AM UTC

PDB ID : 3PWQ / pdb_00003pwq
Title : The Phenylacetyl-CoA monooxygenase PaaAC subcomplex
Authors : Cygler, M.; Grishin, A.M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2010-12-08
Resolution : 2.65 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

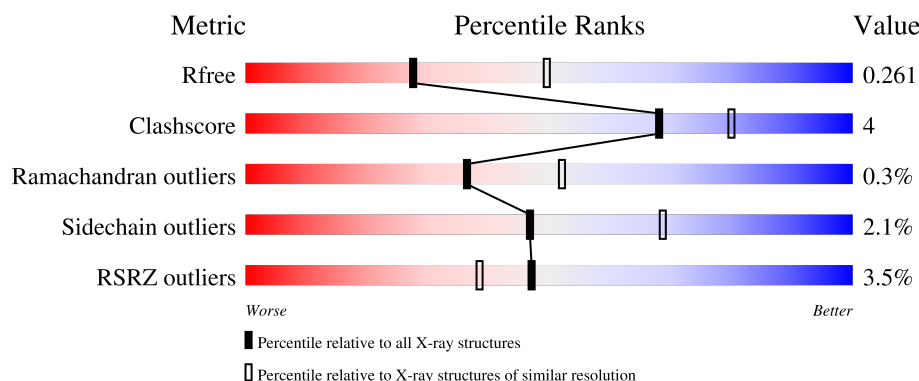
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	259	2% 91% 5% .
1	B	259	% 92% . .
1	E	259	90% 6% .
1	G	259	90% . . .
1	I	259	4% 83% 8% . 8%

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Mol	Chain	Length	Quality of chain
1	J	259	8% 84% 7% • 8%
1	K	259	5% 79% 11% • 10%
1	R	259	3% 82% 9% • 8%
2	C	311	2% 85% 9% • 5%
2	D	311	7% 88% 6% • 5%
2	F	311	5% 85% 11% • •
2	H	311	% 87% 7% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24804 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 Phenylacetic acid degradation protein paaC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1948	1229	346	367	6			
1	B	248	Total	C	N	O	S	0	0	0
			1952	1231	348	367	6			
1	E	248	Total	C	N	O	S	0	0	0
			1950	1229	344	371	6			
1	G	248	Total	C	N	O	S	0	0	0
			1935	1221	339	369	6			
1	I	238	Total	C	N	O	S	0	0	0
			1850	1165	328	351	6			
1	J	238	Total	C	N	O	S	0	0	0
			1831	1154	322	349	6			
1	K	234	Total	C	N	O	S	0	0	0
			1776	1123	315	332	6			
1	R	238	Total	C	N	O	S	0	0	0
			1850	1165	328	351	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P76079
A	-9	GLY	-	expression tag	UNP P76079
A	-8	SER	-	expression tag	UNP P76079
A	-7	SER	-	expression tag	UNP P76079
A	-6	HIS	-	expression tag	UNP P76079
A	-5	HIS	-	expression tag	UNP P76079
A	-4	HIS	-	expression tag	UNP P76079
A	-3	HIS	-	expression tag	UNP P76079
A	-2	HIS	-	expression tag	UNP P76079
A	-1	HIS	-	expression tag	UNP P76079
A	0	GLY	-	expression tag	UNP P76079
A	1	SER	-	expression tag	UNP P76079
B	-10	MET	-	expression tag	UNP P76079

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	expression tag	UNP P76079
B	-8	SER	-	expression tag	UNP P76079
B	-7	SER	-	expression tag	UNP P76079
B	-6	HIS	-	expression tag	UNP P76079
B	-5	HIS	-	expression tag	UNP P76079
B	-4	HIS	-	expression tag	UNP P76079
B	-3	HIS	-	expression tag	UNP P76079
B	-2	HIS	-	expression tag	UNP P76079
B	-1	HIS	-	expression tag	UNP P76079
B	0	GLY	-	expression tag	UNP P76079
B	1	SER	-	expression tag	UNP P76079
E	-10	MET	-	expression tag	UNP P76079
E	-9	GLY	-	expression tag	UNP P76079
E	-8	SER	-	expression tag	UNP P76079
E	-7	SER	-	expression tag	UNP P76079
E	-6	HIS	-	expression tag	UNP P76079
E	-5	HIS	-	expression tag	UNP P76079
E	-4	HIS	-	expression tag	UNP P76079
E	-3	HIS	-	expression tag	UNP P76079
E	-2	HIS	-	expression tag	UNP P76079
E	-1	HIS	-	expression tag	UNP P76079
E	0	GLY	-	expression tag	UNP P76079
E	1	SER	-	expression tag	UNP P76079
G	-10	MET	-	expression tag	UNP P76079
G	-9	GLY	-	expression tag	UNP P76079
G	-8	SER	-	expression tag	UNP P76079
G	-7	SER	-	expression tag	UNP P76079
G	-6	HIS	-	expression tag	UNP P76079
G	-5	HIS	-	expression tag	UNP P76079
G	-4	HIS	-	expression tag	UNP P76079
G	-3	HIS	-	expression tag	UNP P76079
G	-2	HIS	-	expression tag	UNP P76079
G	-1	HIS	-	expression tag	UNP P76079
G	0	GLY	-	expression tag	UNP P76079
G	1	SER	-	expression tag	UNP P76079
I	-10	MET	-	expression tag	UNP P76079
I	-9	GLY	-	expression tag	UNP P76079
I	-8	SER	-	expression tag	UNP P76079
I	-7	SER	-	expression tag	UNP P76079
I	-6	HIS	-	expression tag	UNP P76079
I	-5	HIS	-	expression tag	UNP P76079
I	-4	HIS	-	expression tag	UNP P76079

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	HIS	-	expression tag	UNP P76079
I	-2	HIS	-	expression tag	UNP P76079
I	-1	HIS	-	expression tag	UNP P76079
I	0	GLY	-	expression tag	UNP P76079
I	1	SER	-	expression tag	UNP P76079
J	-10	MET	-	expression tag	UNP P76079
J	-9	GLY	-	expression tag	UNP P76079
J	-8	SER	-	expression tag	UNP P76079
J	-7	SER	-	expression tag	UNP P76079
J	-6	HIS	-	expression tag	UNP P76079
J	-5	HIS	-	expression tag	UNP P76079
J	-4	HIS	-	expression tag	UNP P76079
J	-3	HIS	-	expression tag	UNP P76079
J	-2	HIS	-	expression tag	UNP P76079
J	-1	HIS	-	expression tag	UNP P76079
J	0	GLY	-	expression tag	UNP P76079
J	1	SER	-	expression tag	UNP P76079
K	-10	MET	-	expression tag	UNP P76079
K	-9	GLY	-	expression tag	UNP P76079
K	-8	SER	-	expression tag	UNP P76079
K	-7	SER	-	expression tag	UNP P76079
K	-6	HIS	-	expression tag	UNP P76079
K	-5	HIS	-	expression tag	UNP P76079
K	-4	HIS	-	expression tag	UNP P76079
K	-3	HIS	-	expression tag	UNP P76079
K	-2	HIS	-	expression tag	UNP P76079
K	-1	HIS	-	expression tag	UNP P76079
K	0	GLY	-	expression tag	UNP P76079
K	1	SER	-	expression tag	UNP P76079
R	-10	MET	-	expression tag	UNP P76079
R	-9	GLY	-	expression tag	UNP P76079
R	-8	SER	-	expression tag	UNP P76079
R	-7	SER	-	expression tag	UNP P76079
R	-6	HIS	-	expression tag	UNP P76079
R	-5	HIS	-	expression tag	UNP P76079
R	-4	HIS	-	expression tag	UNP P76079
R	-3	HIS	-	expression tag	UNP P76079
R	-2	HIS	-	expression tag	UNP P76079
R	-1	HIS	-	expression tag	UNP P76079
R	0	GLY	-	expression tag	UNP P76079
R	1	SER	-	expression tag	UNP P76079

- Molecule 2 is a protein called Phenylacetic acid degradation protein paaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	296	Total	C	N	O	S	0	0	0
			2359	1490	423	430	16			
2	D	297	Total	C	N	O	S	0	0	0
			2379	1499	427	437	16			
2	F	301	Total	C	N	O	S	0	0	0
			2385	1504	423	442	16			
2	H	295	Total	C	N	O	S	0	0	0
			2372	1498	424	434	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP P76077
C	0	ARG	-	expression tag	UNP P76077
C	1	SER	-	expression tag	UNP P76077
D	-1	MET	-	expression tag	UNP P76077
D	0	ARG	-	expression tag	UNP P76077
D	1	SER	-	expression tag	UNP P76077
F	-1	MET	-	expression tag	UNP P76077
F	0	ARG	-	expression tag	UNP P76077
F	1	SER	-	expression tag	UNP P76077
H	-1	MET	-	expression tag	UNP P76077
H	0	ARG	-	expression tag	UNP P76077
H	1	SER	-	expression tag	UNP P76077

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	C	29	Total	O	0	0
			29	29		
3	B	21	Total	O	0	0
			21	21		
3	D	15	Total	O	0	0
			15	15		
3	E	16	Total	O	0	0
			16	16		
3	F	19	Total	O	0	0
			19	19		
3	G	31	Total	O	0	0
			31	31		
3	H	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	11	Total 11	O 11	0	0
3	J	12	Total 12	O 12	0	0
3	K	9	Total 9	O 9	0	0
3	R	8	Total 8	O 8	0	0

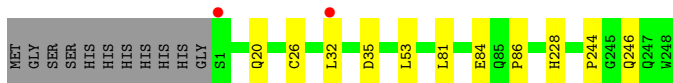
3 Residue-property plots [i](#)

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.

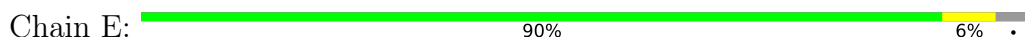
- Molecule 1: Phenylacetic acid degradation protein paaC



- Molecule 1: Phenylacetic acid degradation protein paaC



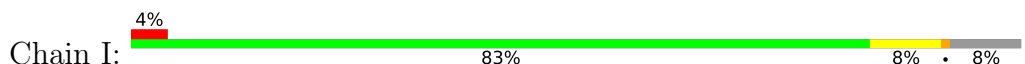
- Molecule 1: Phenylacetic acid degradation protein paaC



- Molecule 1: Phenylacetic acid degradation protein paaC

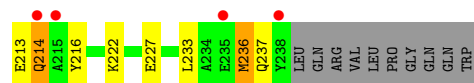
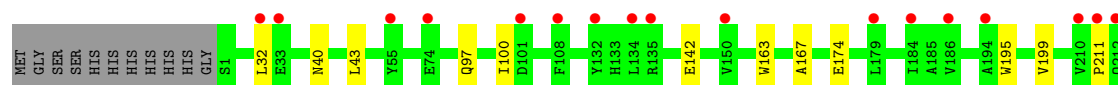
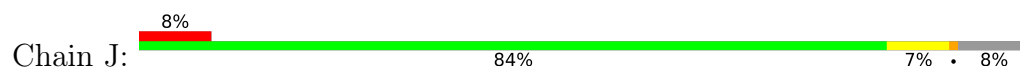


- Molecule 1: Phenylacetic acid degradation protein paaC

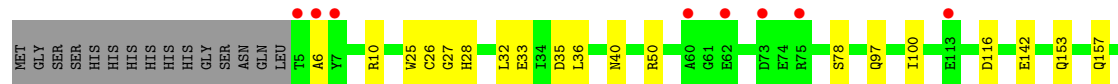
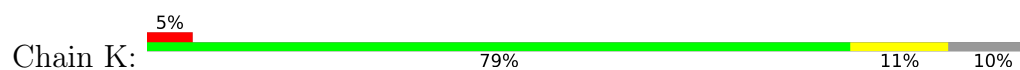




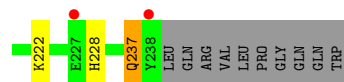
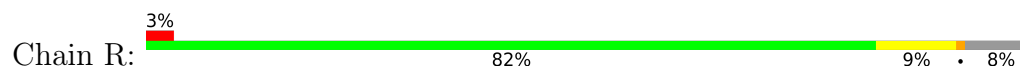
- Molecule 1: Phenylacetic acid degradation protein paaC



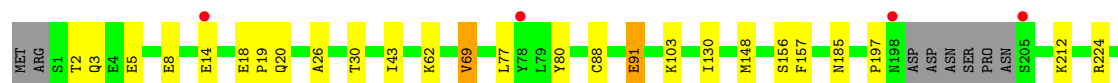
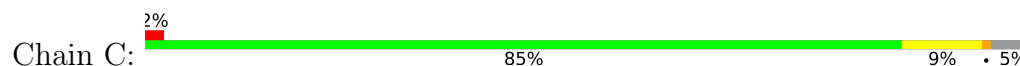
- Molecule 1: Phenylacetic acid degradation protein paaC



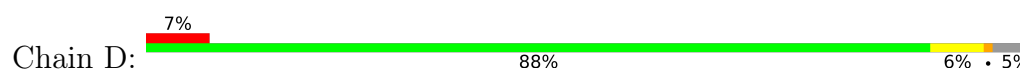
- Molecule 1: Phenylacetic acid degradation protein paaC

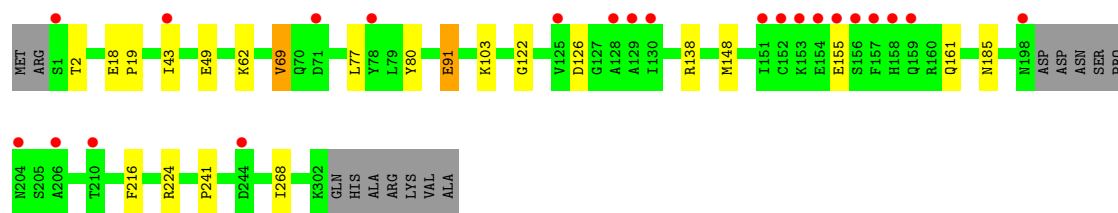


- Molecule 2: Phenylacetic acid degradation protein paaA

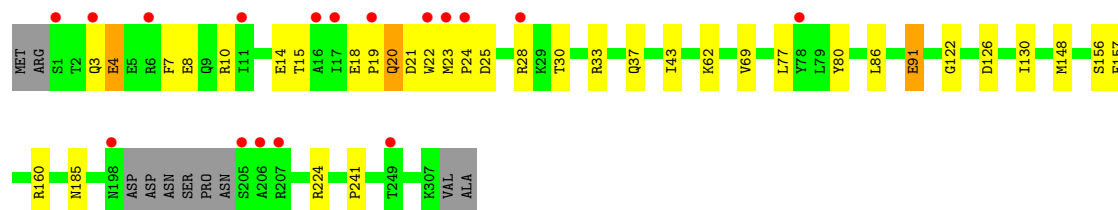
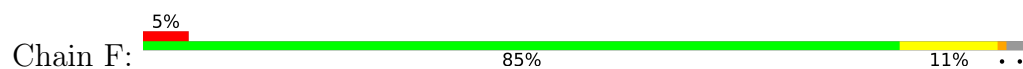


- Molecule 2: Phenylacetic acid degradation protein paaA

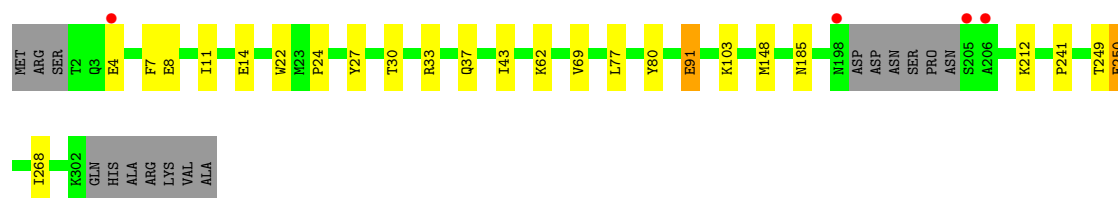
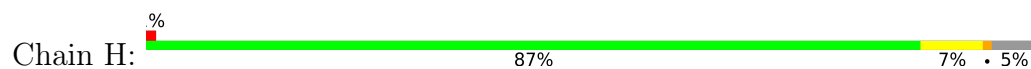




● Molecule 2: Phenylacetic acid degradation protein paaA



● Molecule 2: Phenylacetic acid degradation protein paaA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.26Å 109.06Å 305.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.65 49.20 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.20-2.65) 99.9 (49.20-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.234 , 0.267 0.229 , 0.261	Depositor DCC
R_{free} test set	5363 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24804	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.63% 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	0.59	0/1987	0.83	0/2693
1	B	0.52	0/1991	0.82	0/2698
1	E	0.51	0/1989	0.80	0/2697
1	G	0.69	2/1974 (0.1%)	0.82	0/2679
1	I	0.54	0/1885	0.91	1/2555 (0.0%)
1	J	0.57	0/1866	0.90	1/2532 (0.0%)
1	K	0.53	0/1811	0.87	0/2461
1	R	0.54	0/1885	0.87	0/2555
2	C	0.57	0/2415	0.85	0/3269
2	D	0.56	0/2435	0.85	1/3294 (0.0%)
2	F	0.60	0/2441	0.89	4/3307 (0.1%)
2	H	0.56	0/2428	0.83	1/3283 (0.0%)
All	All	0.57	2/25107 (0.0%)	0.85	8/34023 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	64	ASP	C-O	-7.22	1.18	1.24
1	G	66	ASP	C-O	-5.11	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	20	GLN	CB-CA-C	-9.10	95.38	110.85
2	F	20	GLN	N-CA-C	8.95	121.11	111.36
1	I	236	MET	N-CA-C	-6.61	103.69	111.03
1	J	236	MET	N-CA-C	-6.45	105.23	113.23
2	F	3	GLN	N-CA-C	-5.73	106.42	113.41
2	H	250	GLU	N-CA-C	-5.29	99.54	110.80
2	D	155	GLU	N-CA-C	5.27	117.03	111.28
2	F	24	PRO	CB-CA-C	-5.06	103.21	111.56

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	1948	0	1894	14	0
1	B	1952	0	1902	13	0
1	E	1950	0	1888	14	0
1	G	1935	0	1859	12	0
1	I	1850	0	1793	10	0
1	J	1831	0	1758	12	0
1	K	1776	0	1694	21	0
1	R	1850	0	1793	17	0
2	C	2359	0	2271	31	0
2	D	2379	0	2291	31	0
2	F	2385	0	2270	35	0
2	H	2372	0	2295	20	0
3	A	30	0	0	1	0
3	B	21	0	0	0	0
3	C	29	0	0	2	0
3	D	15	0	0	0	0
3	E	16	0	0	0	0
3	F	19	0	0	1	0
3	G	31	0	0	2	0
3	H	16	0	0	0	0
3	I	11	0	0	0	0
3	J	12	0	0	0	0
3	K	9	0	0	0	0
3	R	8	0	0	0	0
All	All	24804	0	23708	175	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 4.

All (175) 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:E:32:LEU:HD23	2:F:77:LEU:CD2	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD23	2:D:77:LEU:CD2	1.94	0.98
2:D:138:ARG:HH11	1:K:28:HIS:HA	1.32	0.95
1:R:212:GLN:HA	1:R:213:GLU:CB	2.01	0.90
1:A:32:LEU:HD23	2:C:77:LEU:CD2	2.06	0.86
1:G:32:LEU:HD23	2:H:77:LEU:CD2	2.09	0.83
2:C:224:ARG:HG2	1:J:32:LEU:CD2	2.09	0.82
2:D:138:ARG:NH1	1:K:28:HIS:HA	1.94	0.81
2:H:249:THR:HG23	2:H:249:THR:O	1.79	0.78
1:E:32:LEU:HD23	2:F:77:LEU:HD23	1.64	0.78
1:E:32:LEU:HD23	2:F:77:LEU:HD21	1.67	0.77
1:E:32:LEU:HD21	2:F:77:LEU:HG	1.66	0.77
1:E:32:LEU:CD2	2:F:77:LEU:HG	2.15	0.77
1:A:20:GLN:OE1	2:C:62:LYS:HE2	1.85	0.77
1:B:32:LEU:HD23	2:D:77:LEU:HD23	1.65	0.77
2:D:216:PHE:CZ	1:K:32:LEU:HB2	2.20	0.76
1:B:32:LEU:CD2	2:D:77:LEU:HG	2.16	0.76
1:G:20:GLN:OE1	2:H:62:LYS:HE2	1.86	0.75
1:G:32:LEU:HD23	2:H:77:LEU:HD23	1.68	0.75
1:A:32:LEU:HD23	2:C:77:LEU:HD23	1.68	0.74
2:C:224:ARG:HG2	1:J:32:LEU:HD21	1.68	0.73
1:I:237:GLN:O	1:I:238:TYR:C	2.30	0.72
2:D:224:ARG:HG2	1:K:36:LEU:CD1	2.21	0.71
1:E:20:GLN:OE1	2:F:62:LYS:HE2	1.91	0.70
1:B:32:LEU:HD21	2:D:77:LEU:HG	1.75	0.69
1:R:206:ALA:O	1:R:207:THR:HG22	1.94	0.68
2:F:4:GLU:O	2:F:8:GLU:HG2	1.93	0.68
2:D:224:ARG:NH1	1:K:33:GLU:OE1	2.27	0.68
2:H:249:THR:O	2:H:249:THR:CG2	2.43	0.66
1:R:212:GLN:CA	1:R:213:GLU:CB	2.75	0.65
1:B:20:GLN:OE1	2:D:62:LYS:HE2	1.97	0.65
1:G:64:ASP:OD1	1:G:66:ASP:N	2.30	0.64
2:F:22:TRP:HA	3:F:311:HOH:O	1.97	0.63
1:R:70:PHE:O	1:R:237:GLN:HG2	1.98	0.62
1:B:244:PRO:O	1:B:246:GLN:HG2	1.99	0.62
1:E:86:PRO:HG3	1:E:228:HIS:CD2	2.35	0.62
2:F:28:ARG:HG3	2:F:86:LEU:HD22	1.82	0.61
2:C:224:ARG:HG2	1:J:32:LEU:HD23	1.81	0.61
1:J:163:TRP:CG	1:J:211:PRO:HG2	2.36	0.61
1:A:244:PRO:O	1:A:246:GLN:HG2	2.00	0.61
1:E:244:PRO:O	1:E:246:GLN:HG2	1.99	0.61
1:K:212:GLN:HA	1:K:213:GLU:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:GLN:HG2	2:F:21:ASP:H	1.67	0.59
1:K:187:ASP:OD1	1:K:189:ARG:HG2	2.02	0.59
1:G:64:ASP:OD1	1:G:64:ASP:C	2.46	0.59
1:B:86:PRO:HG3	1:B:228:HIS:CD2	2.38	0.58
1:A:149:ASP:HB3	3:A:259:HOH:O	2.02	0.58
2:H:4:GLU:O	2:H:8:GLU:HG3	2.03	0.58
1:I:153:GLN:HG2	1:I:157:GLN:HE21	1.68	0.58
1:B:32:LEU:HD23	2:D:77:LEU:HD21	1.83	0.58
2:C:254:TYR:OH	1:I:75:ARG:HB3	2.04	0.58
1:G:86:PRO:HG3	1:G:228:HIS:CD2	2.39	0.56
2:C:3:GLN:C	2:C:5:GLU:H	2.13	0.56
1:E:32:LEU:HD23	2:F:77:LEU:CG	2.36	0.56
1:J:163:TRP:CD2	1:J:211:PRO:HG2	2.41	0.56
1:I:212:GLN:HA	1:I:213:GLU:CB	2.36	0.56
1:A:32:LEU:CD2	2:C:77:LEU:HG	2.37	0.54
1:A:32:LEU:HD21	2:C:77:LEU:HG	1.89	0.54
2:F:23:MET:HE3	2:F:28:ARG:HH21	1.72	0.54
1:E:32:LEU:CD2	2:F:77:LEU:CG	2.85	0.54
2:F:160:ARG:HB2	1:R:43:LEU:CD2	2.38	0.54
1:K:97:GLN:O	1:K:100:ILE:HG22	2.07	0.54
1:B:32:LEU:HD23	2:D:77:LEU:CG	2.38	0.54
2:D:224:ARG:HG2	1:K:36:LEU:HD11	1.89	0.54
1:R:195:TRP:CE2	1:R:199:VAL:HG21	2.44	0.54
1:G:32:LEU:CD2	2:H:77:LEU:HG	2.38	0.53
2:F:18:GLU:HB3	2:F:19:PRO:CD	2.38	0.53
1:J:195:TRP:CE2	1:J:199:VAL:HG21	2.44	0.53
2:D:18:GLU:HB3	2:D:19:PRO:CD	2.40	0.52
2:D:224:ARG:CG	1:K:36:LEU:CD1	2.86	0.52
2:F:224:ARG:O	2:F:224:ARG:HD3	2.10	0.52
2:C:88:CYS:HB2	3:C:319:HOH:O	2.10	0.52
1:I:195:TRP:CE2	1:I:199:VAL:HG21	2.45	0.52
1:J:233:LEU:O	1:J:237:GLN:HG3	2.11	0.51
2:F:28:ARG:HD3	2:F:86:LEU:O	2.11	0.51
1:K:195:TRP:CE2	1:K:199:VAL:HG21	2.46	0.51
1:J:97:GLN:O	1:J:100:ILE:HG22	2.11	0.51
2:F:43:ILE:CD1	2:F:80:TYR:HE2	2.24	0.50
2:C:197:PRO:HA	2:C:261:TRP:CH2	2.46	0.50
1:B:32:LEU:CD2	2:D:77:LEU:CG	2.89	0.50
2:D:43:ILE:HD11	2:D:80:TYR:HE2	1.76	0.50
1:J:213:GLU:O	1:J:214:GLN:O	2.30	0.50
2:D:148:MET:HA	2:D:148:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:ASP:OD2	2:F:25:ASP:O	2.30	0.50
1:A:32:LEU:HD23	2:C:77:LEU:HD21	1.93	0.49
1:G:32:LEU:HD21	2:H:77:LEU:HG	1.94	0.49
2:D:185:ASN:HA	2:D:241:PRO:HG3	1.95	0.49
1:R:97:GLN:O	1:R:100:ILE:HG22	2.13	0.49
2:D:138:ARG:NH1	1:K:27:GLY:O	2.45	0.49
2:F:130:ILE:HD11	2:F:156:SER:HA	1.95	0.48
2:H:7:PHE:CZ	2:H:11:ILE:HD11	2.48	0.48
2:D:43:ILE:CD1	2:D:80:TYR:HE2	2.26	0.48
2:F:148:MET:HA	2:F:148:MET:HE2	1.95	0.48
1:R:206:ALA:O	1:R:207:THR:CG2	2.61	0.48
2:C:148:MET:HA	2:C:148:MET:HE2	1.95	0.48
2:F:43:ILE:HD11	2:F:80:TYR:HE2	1.78	0.47
2:D:224:ARG:HG2	1:K:36:LEU:HD12	1.95	0.47
1:A:135:ARG:NE	1:R:204:ASN:ND2	2.62	0.47
2:C:26:ALA:O	2:C:30:THR:HG23	2.14	0.47
2:H:148:MET:HA	2:H:148:MET:HE2	1.95	0.47
1:K:25:TRP:O	1:K:26:CYS:C	2.56	0.47
2:C:185:ASN:HA	2:C:241:PRO:HG3	1.96	0.47
2:D:224:ARG:CG	1:K:36:LEU:HD12	2.44	0.47
2:H:185:ASN:HA	2:H:241:PRO:HG3	1.97	0.47
1:I:236:MET:O	1:I:237:GLN:C	2.56	0.47
2:C:43:ILE:HD11	2:C:80:TYR:HE2	1.80	0.46
2:F:185:ASN:HA	2:F:241:PRO:HG3	1.97	0.46
2:F:18:GLU:HA	2:F:18:GLU:OE1	2.15	0.46
1:G:221:LYS:NZ	3:G:273:HOH:O	2.49	0.46
2:C:157:PHE:HA	1:J:43:LEU:HD21	1.97	0.46
1:I:97:GLN:O	1:I:100:ILE:HG22	2.15	0.46
2:F:157:PHE:HA	1:R:43:LEU:HD21	1.96	0.46
1:A:135:ARG:CZ	1:R:204:ASN:ND2	2.79	0.46
2:C:43:ILE:CD1	2:C:80:TYR:HE2	2.29	0.45
2:D:91:GLU:H	2:D:91:GLU:CD	2.23	0.45
2:H:91:GLU:H	2:H:91:GLU:CD	2.24	0.45
2:D:103:LYS:HE2	2:D:268:ILE:O	2.17	0.45
2:H:4:GLU:OE1	2:H:22:TRP:CH2	2.69	0.45
1:J:233:LEU:O	1:J:237:GLN:HB2	2.16	0.45
2:F:91:GLU:H	2:F:91:GLU:CD	2.24	0.45
2:C:14:GLU:OE2	2:C:212:LYS:NZ	2.50	0.45
1:B:32:LEU:HD23	2:D:77:LEU:HG	1.94	0.45
2:F:224:ARG:HA	2:F:224:ARG:HE	1.82	0.45
2:C:91:GLU:CD	2:C:91:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:GLU:HB3	2:D:19:PRO:HD2	2.00	0.44
2:F:4:GLU:O	2:F:7:PHE:HB3	2.17	0.44
1:I:209:ASN:O	1:I:211:PRO:HD3	2.18	0.44
1:G:145:GLY:HA2	1:G:152:GLY:HA2	2.00	0.44
2:F:160:ARG:HB2	1:R:43:LEU:HD22	1.99	0.44
1:B:81:LEU:O	1:B:84:GLU:HG2	2.17	0.43
2:F:224:ARG:HA	2:F:224:ARG:NE	2.33	0.43
2:H:4:GLU:OE1	2:H:24:PRO:HG3	2.17	0.43
2:C:3:GLN:C	2:C:5:GLU:N	2.74	0.43
2:C:130:ILE:HD11	2:C:156:SER:HA	2.00	0.43
1:E:32:LEU:CD2	2:F:77:LEU:CD2	2.75	0.43
2:H:43:ILE:CD1	2:H:80:TYR:HE2	2.31	0.43
2:H:43:ILE:HD11	2:H:80:TYR:HE2	1.83	0.43
1:A:20:GLN:OE1	2:C:62:LYS:CE	2.61	0.43
2:C:18:GLU:HB3	2:C:19:PRO:HD2	1.99	0.43
2:F:122:GLY:O	2:F:126:ASP:HB2	2.18	0.43
2:C:103:LYS:HE2	2:C:268:ILE:O	2.18	0.43
1:K:153:GLN:HG2	1:K:157:GLN:HE21	1.84	0.43
2:D:161:GLN:OE1	1:K:50:ARG:NH1	2.49	0.43
1:J:167:ALA:HB2	1:J:216:TYR:CD2	2.53	0.43
2:H:33:ARG:O	2:H:37:GLN:HG3	2.19	0.42
1:E:81:LEU:O	1:E:84:GLU:HG2	2.20	0.42
2:F:33:ARG:O	2:F:37:GLN:HG3	2.19	0.42
2:H:14:GLU:OE2	2:H:212:LYS:NZ	2.51	0.42
1:A:26:CYS:SG	2:C:69:VAL:HG11	2.59	0.42
1:I:236:MET:O	1:I:238:TYR:N	2.52	0.42
1:E:145:GLY:HA2	1:E:152:GLY:HA2	2.02	0.42
2:D:216:PHE:CE1	1:K:32:LEU:HB2	2.55	0.42
1:I:10:ARG:NH2	1:I:173:ASP:OD2	2.52	0.42
1:G:246:GLN:HG3	3:G:277:HOH:O	2.19	0.42
2:C:18:GLU:HB3	2:C:19:PRO:CD	2.49	0.41
2:F:160:ARG:CB	1:R:43:LEU:HD23	2.50	0.41
2:H:103:LYS:HE2	2:H:268:ILE:O	2.19	0.41
1:A:81:LEU:O	1:A:84:GLU:HG2	2.21	0.41
1:B:26:CYS:SG	2:D:69:VAL:HG11	2.61	0.41
2:C:20:GLN:CD	2:C:20:GLN:H	2.28	0.41
2:C:62:LYS:NZ	3:C:338:HOH:O	2.54	0.41
1:K:116:ASP:HB2	1:K:184:ILE:HG23	2.03	0.41
1:A:73:ASP:OD1	1:A:73:ASP:C	2.64	0.41
2:D:122:GLY:O	2:D:126:ASP:HB2	2.20	0.41
2:H:27:TYR:HA	2:H:30:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:ARG:NH2	1:K:173:ASP:OD2	2.54	0.41
1:R:80:LEU:O	1:R:83:VAL:HG22	2.21	0.41
1:R:86:PRO:HG3	1:R:228:HIS:CD2	2.55	0.41
1:E:85:GLN:HE22	1:E:226:THR:HG21	1.85	0.40
2:F:10:ARG:HB3	2:F:15:THR:HB	2.03	0.40
2:C:235:MET:HE2	2:C:235:MET:HB3	1.95	0.40
1:R:31:GLU:HB2	1:R:34:ILE:HD12	2.03	0.40
1:K:6:ALA:O	1:K:10:ARG:HG3	2.20	0.40
1:R:127:ILE:O	1:R:131:ARG:HG3	2.22	0.40
1:G:73:ASP:OD1	1:G:73:ASP:C	2.64	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	246/259 (95%)	240 (98%)	6 (2%)	0	100	100
1	B	246/259 (95%)	243 (99%)	3 (1%)	0	100	100
1	E	246/259 (95%)	242 (98%)	4 (2%)	0	100	100
1	G	246/259 (95%)	242 (98%)	4 (2%)	0	100	100
1	I	236/259 (91%)	227 (96%)	6 (2%)	3 (1%)	9	16
1	J	236/259 (91%)	231 (98%)	4 (2%)	1 (0%)	30	45
1	K	232/259 (90%)	225 (97%)	5 (2%)	2 (1%)	14	24
1	R	236/259 (91%)	230 (98%)	4 (2%)	2 (1%)	16	27
2	C	292/311 (94%)	289 (99%)	3 (1%)	0	100	100
2	D	293/311 (94%)	293 (100%)	0	0	100	100
2	F	297/311 (96%)	286 (96%)	11 (4%)	0	100	100
2	H	291/311 (94%)	288 (99%)	2 (1%)	1 (0%)	36	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3097/3316 (93%)	3036 (98%)	52 (2%)	9 (0%)	36	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	250	GLU
1	I	214	GLN
1	J	214	GLN
1	R	213	GLU
1	R	214	GLN
1	I	213	GLU
1	K	213	GLU
1	K	214	GLN
1	I	237	GLN

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	195/208 (94%)	192 (98%)	3 (2%)	57	75
1	B	196/208 (94%)	194 (99%)	2 (1%)	68	81
1	E	196/208 (94%)	192 (98%)	4 (2%)	48	69
1	G	192/208 (92%)	188 (98%)	4 (2%)	47	69
1	I	184/208 (88%)	177 (96%)	7 (4%)	29	49
1	J	180/208 (86%)	174 (97%)	6 (3%)	33	55
1	K	170/208 (82%)	165 (97%)	5 (3%)	37	58
1	R	184/208 (88%)	179 (97%)	5 (3%)	39	61
2	C	238/259 (92%)	234 (98%)	4 (2%)	53	73
2	D	242/259 (93%)	238 (98%)	4 (2%)	53	73
2	F	239/259 (92%)	234 (98%)	5 (2%)	47	69
2	H	242/259 (93%)	240 (99%)	2 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2458/2700 (91%)	2407 (98%)	51 (2%)	47 69

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	53	LEU
1	A	150	VAL
2	C	2	THR
2	C	8	GLU
2	C	69	VAL
2	C	91	GLU
1	B	35	ASP
1	B	53	LEU
2	D	2	THR
2	D	49	GLU
2	D	69	VAL
2	D	91	GLU
1	E	8	THR
1	E	35	ASP
1	E	53	LEU
1	E	222	LYS
2	F	4	GLU
2	F	14	GLU
2	F	30	THR
2	F	69	VAL
2	F	91	GLU
1	G	35	ASP
1	G	53	LEU
1	G	150	VAL
1	G	246	GLN
2	H	69	VAL
2	H	91	GLU
1	I	35	ASP
1	I	62	GLU
1	I	78	SER
1	I	142	GLU
1	I	154	LYS
1	I	222	LYS
1	I	227	GLU
1	J	40	ASN
1	J	142	GLU

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Mol	Chain	Res	Type
1	J	174	GLU
1	J	222	LYS
1	J	227	GLU
1	J	236	MET
1	K	35	ASP
1	K	40	ASN
1	K	78	SER
1	K	142	GLU
1	K	222	LYS
1	R	40	ASN
1	R	78	SER
1	R	142	GLU
1	R	222	LYS
1	R	237	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	85	GLN
1	A	157	GLN
2	C	3	GLN
2	C	70	GLN
2	C	133	GLN
1	B	51	ASN
1	B	85	GLN
1	B	157	GLN
2	D	70	GLN
2	D	133	GLN
2	D	265	ASN
1	E	3	GLN
1	E	48	GLN
1	E	51	ASN
1	E	85	GLN
1	E	97	GLN
1	E	157	GLN
2	F	51	ASN
2	F	70	GLN
2	F	133	GLN
1	G	51	ASN
1	G	85	GLN
1	G	97	GLN

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Mol	Chain	Res	Type
1	G	157	GLN
2	H	9	GLN
2	H	70	GLN
2	H	133	GLN
1	I	3	GLN
1	I	51	ASN
1	I	157	GLN
1	I	228	HIS
1	J	51	ASN
1	J	118	GLN
1	K	28	HIS
1	K	51	ASN
1	K	118	GLN
1	K	157	GLN
1	R	51	ASN
1	R	204	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 ⓘ

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	248/259 (95%)	0.06	4 (1%) 70 66	32, 46, 61, 67	0
1	B	248/259 (95%)	-0.10	2 (0%) 82 79	32, 46, 61, 68	0
1	E	248/259 (95%)	-0.05	1 (0%) 88 87	32, 46, 61, 66	0
1	G	248/259 (95%)	-0.14	1 (0%) 88 87	32, 46, 61, 66	0
1	I	238/259 (91%)	0.57	11 (4%) 37 29	44, 68, 85, 94	0
1	J	238/259 (91%)	0.89	21 (8%) 15 12	37, 68, 85, 94	0
1	K	234/259 (90%)	0.63	13 (5%) 30 24	44, 68, 85, 94	0
1	R	238/259 (91%)	0.66	7 (2%) 53 46	44, 68, 85, 94	0
2	C	296/311 (95%)	0.22	5 (1%) 69 64	33, 51, 72, 93	0
2	D	297/311 (95%)	0.43	22 (7%) 20 15	33, 52, 68, 94	0
2	F	301/311 (96%)	0.33	17 (5%) 30 24	33, 52, 81, 95	0
2	H	295/311 (94%)	0.11	4 (1%) 73 69	33, 51, 72, 93	0
All	All	3129/3316 (94%)	0.29	108 (3%) 47 38	32, 54, 82, 95	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	238	TYR	7.2
1	R	238	TYR	6.9
1	I	238	TYR	6.0
1	K	238	TYR	5.4
2	D	129	ALA	5.4
1	A	1	SER	5.2
2	D	153	LYS	4.8
2	D	155	GLU	4.5
2	D	156	SER	4.3
2	D	152	CYS	4.2
2	C	198	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	158	HIS	4.1
2	H	205	SER	4.0
2	F	23	MET	3.9
1	J	215	ALA	3.9
2	H	198	ASN	3.7
2	F	205	SER	3.6
2	H	206	ALA	3.3
2	D	244	ASP	3.3
1	J	101	ASP	3.3
1	I	32	LEU	3.3
2	D	154	GLU	3.3
2	D	198	ASN	3.2
1	J	210	VAL	3.2
1	A	32	LEU	3.1
1	K	212	GLN	3.1
2	F	16	ALA	3.1
2	F	1	SER	3.1
2	F	28	ARG	3.0
2	F	198	ASN	3.0
2	D	157	PHE	3.0
1	K	7	TYR	2.9
1	J	150	VAL	2.9
1	J	235	GLU	2.9
1	B	32	LEU	2.8
1	J	212	GLN	2.8
2	C	205	SER	2.8
2	F	78	TYR	2.8
1	J	214	GLN	2.7
2	D	151	ILE	2.7
1	J	132	TYR	2.7
2	D	125	VAL	2.7
1	J	33	GLU	2.6
1	K	60	ALA	2.6
1	K	62	GLU	2.6
2	D	128	ALA	2.6
2	D	206	ALA	2.6
1	K	73	ASP	2.6
2	D	130	ILE	2.6
1	J	108	PHE	2.6
1	K	237	GLN	2.6
2	C	78	TYR	2.5
2	F	22	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	215	ALA	2.5
2	F	24	PRO	2.5
1	I	210	VAL	2.5
1	R	126	ALA	2.5
2	F	206	ALA	2.5
2	D	71	ASP	2.5
1	I	132	TYR	2.5
1	R	210	VAL	2.5
1	J	32	LEU	2.4
2	D	210	THR	2.4
2	C	14	GLU	2.4
1	J	74	GLU	2.4
2	F	207	ARG	2.4
1	A	2	ASN	2.4
1	R	101	ASP	2.4
1	J	211	PRO	2.4
1	K	5	THR	2.3
2	D	1	SER	2.3
1	J	134	LEU	2.3
2	H	4	GLU	2.3
2	D	78	TYR	2.3
2	D	204	ASN	2.3
2	F	3	GLN	2.3
1	J	184	ILE	2.2
1	J	194	ALA	2.2
1	R	227	GLU	2.2
1	I	204	ASN	2.2
1	K	214	GLN	2.2
1	J	179	LEU	2.2
1	J	135	ARG	2.2
1	B	1	SER	2.2
1	I	149	ASP	2.2
2	F	19	PRO	2.2
2	D	43	ILE	2.2
1	I	69	ALA	2.1
2	F	249	THR	2.1
2	D	159	GLN	2.1
1	K	6	ALA	2.1
1	I	33	GLU	2.1
1	K	113	GLU	2.1
2	F	6	ARG	2.1
1	K	216	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	1	SER	2.1
1	I	200	PHE	2.1
1	I	237	GLN	2.1
1	J	55	TYR	2.1
2	C	261	TRP	2.1
1	A	3	GLN	2.1
2	F	11	ILE	2.1
1	K	75	ARG	2.0
1	I	233	LEU	2.0
1	R	113	GLU	2.0
1	G	3	GLN	2.0
2	F	17	ILE	2.0
1	J	186	VAL	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.