



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:03 am BST

PDB ID : 4IQ4
Title : Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains, triple mutant, P21212 form
Authors : Lai, Y.-T.; Sawaya, M.R.; Yeates, T.O.
Deposited on : 2013-01-10
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

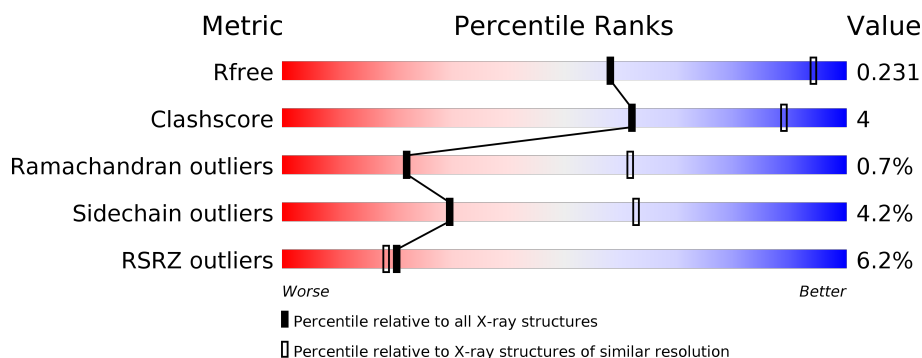
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	456	<div> <div style="width: 14%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 4%; background-color: yellow;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div> <div style="width: 14%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 4%; background-color: yellow;"></div> <div style="width: 2%; background-color: grey;"></div> </div>
1	B	456	<div> <div style="width: 9%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div> <div style="width: 9%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div>
1	C	456	<div> <div style="width: 8%; background-color: red;"></div> <div style="width: 83%; background-color: green;"></div> <div style="width: 9%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div> <div style="width: 8%; background-color: red;"></div> <div style="width: 83%; background-color: green;"></div> <div style="width: 9%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
1	D	456	<div> <div style="width: 14%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 4%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div> <div style="width: 14%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 4%; background-color: yellow;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
1	E	456	<div> <div style="width: 0%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 3%; background-color: grey;"></div> </div> <div> <div style="width: 0%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 3%; background-color: grey;"></div> </div>
1	F	456	<div> <div style="width: 4%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div> <div> <div style="width: 4%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 20388 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 Non-haem bromoperoxidase BPO-A2, Matrix protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	B	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	C	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	D	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	E	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	F	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
A	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
A	278	ALA	-	LINKER	UNP P03485
A	279	GLN	-	LINKER	UNP P03485
A	280	GLU	-	LINKER	UNP P03485
A	281	ALA	-	LINKER	UNP P03485
A	282	GLN	-	LINKER	UNP P03485
A	283	LYS	-	LINKER	UNP P03485
A	284	GLN	-	LINKER	UNP P03485
A	285	LYS	-	LINKER	UNP P03485
A	448	LEU	-	EXPRESSION TAG	UNP P03485
A	449	GLU	-	EXPRESSION TAG	UNP P03485
A	450	HIS	-	EXPRESSION TAG	UNP P03485
A	451	HIS	-	EXPRESSION TAG	UNP P03485
A	452	HIS	-	EXPRESSION TAG	UNP P03485
A	453	HIS	-	EXPRESSION TAG	UNP P03485
A	454	HIS	-	EXPRESSION TAG	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
A	455	HIS	-	EXPRESSION TAG	UNP P03485
B	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
B	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
B	278	ALA	-	LINKER	UNP P03485
B	279	GLN	-	LINKER	UNP P03485
B	280	GLU	-	LINKER	UNP P03485
B	281	ALA	-	LINKER	UNP P03485
B	282	GLN	-	LINKER	UNP P03485
B	283	LYS	-	LINKER	UNP P03485
B	284	GLN	-	LINKER	UNP P03485
B	285	LYS	-	LINKER	UNP P03485
B	448	LEU	-	EXPRESSION TAG	UNP P03485
B	449	GLU	-	EXPRESSION TAG	UNP P03485
B	450	HIS	-	EXPRESSION TAG	UNP P03485
B	451	HIS	-	EXPRESSION TAG	UNP P03485
B	452	HIS	-	EXPRESSION TAG	UNP P03485
B	453	HIS	-	EXPRESSION TAG	UNP P03485
B	454	HIS	-	EXPRESSION TAG	UNP P03485
B	455	HIS	-	EXPRESSION TAG	UNP P03485
C	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
C	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
C	278	ALA	-	LINKER	UNP P03485
C	279	GLN	-	LINKER	UNP P03485
C	280	GLU	-	LINKER	UNP P03485
C	281	ALA	-	LINKER	UNP P03485
C	282	GLN	-	LINKER	UNP P03485
C	283	LYS	-	LINKER	UNP P03485
C	284	GLN	-	LINKER	UNP P03485
C	285	LYS	-	LINKER	UNP P03485
C	448	LEU	-	EXPRESSION TAG	UNP P03485
C	449	GLU	-	EXPRESSION TAG	UNP P03485
C	450	HIS	-	EXPRESSION TAG	UNP P03485
C	451	HIS	-	EXPRESSION TAG	UNP P03485
C	452	HIS	-	EXPRESSION TAG	UNP P03485
C	453	HIS	-	EXPRESSION TAG	UNP P03485
C	454	HIS	-	EXPRESSION TAG	UNP P03485
C	455	HIS	-	EXPRESSION TAG	UNP P03485
D	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
D	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
D	278	ALA	-	LINKER	UNP P03485
D	279	GLN	-	LINKER	UNP P03485
D	280	GLU	-	LINKER	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
D	281	ALA	-	LINKER	UNP P03485
D	282	GLN	-	LINKER	UNP P03485
D	283	LYS	-	LINKER	UNP P03485
D	284	GLN	-	LINKER	UNP P03485
D	285	LYS	-	LINKER	UNP P03485
D	448	LEU	-	EXPRESSION TAG	UNP P03485
D	449	GLU	-	EXPRESSION TAG	UNP P03485
D	450	HIS	-	EXPRESSION TAG	UNP P03485
D	451	HIS	-	EXPRESSION TAG	UNP P03485
D	452	HIS	-	EXPRESSION TAG	UNP P03485
D	453	HIS	-	EXPRESSION TAG	UNP P03485
D	454	HIS	-	EXPRESSION TAG	UNP P03485
D	455	HIS	-	EXPRESSION TAG	UNP P03485
E	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
E	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
E	278	ALA	-	LINKER	UNP P03485
E	279	GLN	-	LINKER	UNP P03485
E	280	GLU	-	LINKER	UNP P03485
E	281	ALA	-	LINKER	UNP P03485
E	282	GLN	-	LINKER	UNP P03485
E	283	LYS	-	LINKER	UNP P03485
E	284	GLN	-	LINKER	UNP P03485
E	285	LYS	-	LINKER	UNP P03485
E	448	LEU	-	EXPRESSION TAG	UNP P03485
E	449	GLU	-	EXPRESSION TAG	UNP P03485
E	450	HIS	-	EXPRESSION TAG	UNP P03485
E	451	HIS	-	EXPRESSION TAG	UNP P03485
E	452	HIS	-	EXPRESSION TAG	UNP P03485
E	453	HIS	-	EXPRESSION TAG	UNP P03485
E	454	HIS	-	EXPRESSION TAG	UNP P03485
E	455	HIS	-	EXPRESSION TAG	UNP P03485
F	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
F	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
F	278	ALA	-	LINKER	UNP P03485
F	279	GLN	-	LINKER	UNP P03485
F	280	GLU	-	LINKER	UNP P03485
F	281	ALA	-	LINKER	UNP P03485
F	282	GLN	-	LINKER	UNP P03485
F	283	LYS	-	LINKER	UNP P03485
F	284	GLN	-	LINKER	UNP P03485
F	285	LYS	-	LINKER	UNP P03485
F	448	LEU	-	EXPRESSION TAG	UNP P03485

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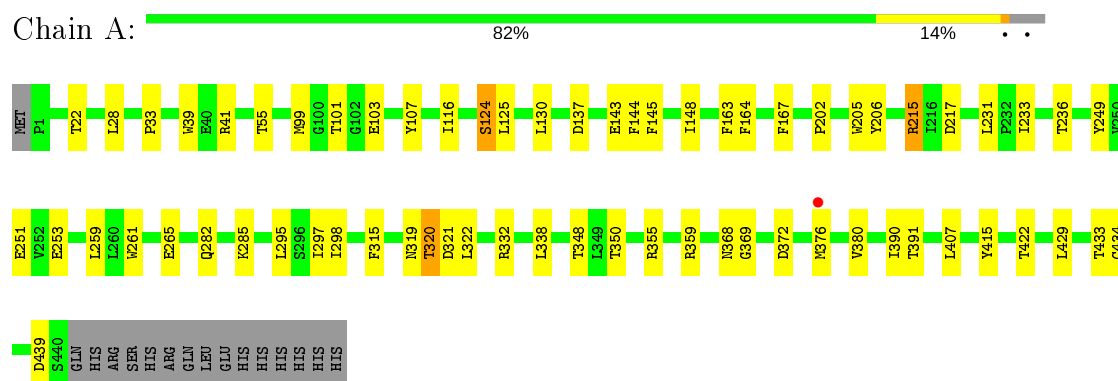
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Chain	Residue	Modelled	Actual	Comment	Reference
F	449	GLU	-	EXPRESSION TAG	UNP P03485
F	450	HIS	-	EXPRESSION TAG	UNP P03485
F	451	HIS	-	EXPRESSION TAG	UNP P03485
F	452	HIS	-	EXPRESSION TAG	UNP P03485
F	453	HIS	-	EXPRESSION TAG	UNP P03485
F	454	HIS	-	EXPRESSION TAG	UNP P03485
F	455	HIS	-	EXPRESSION TAG	UNP P03485

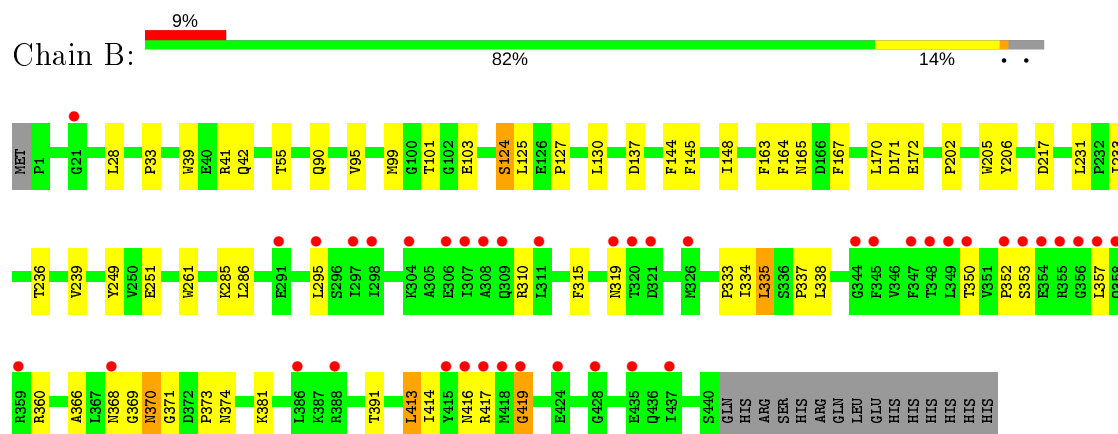
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

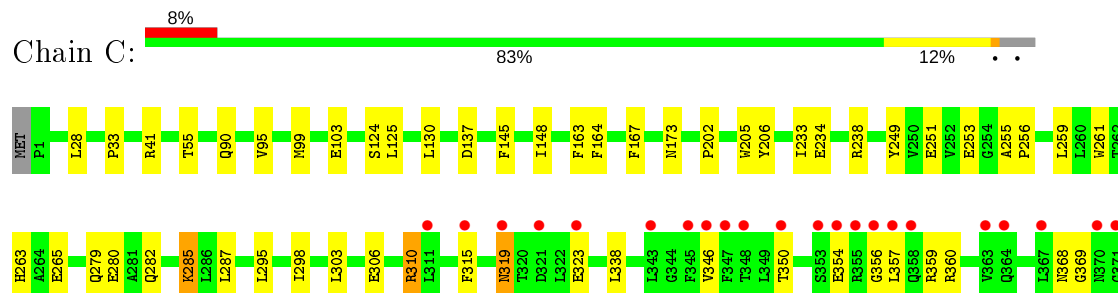
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

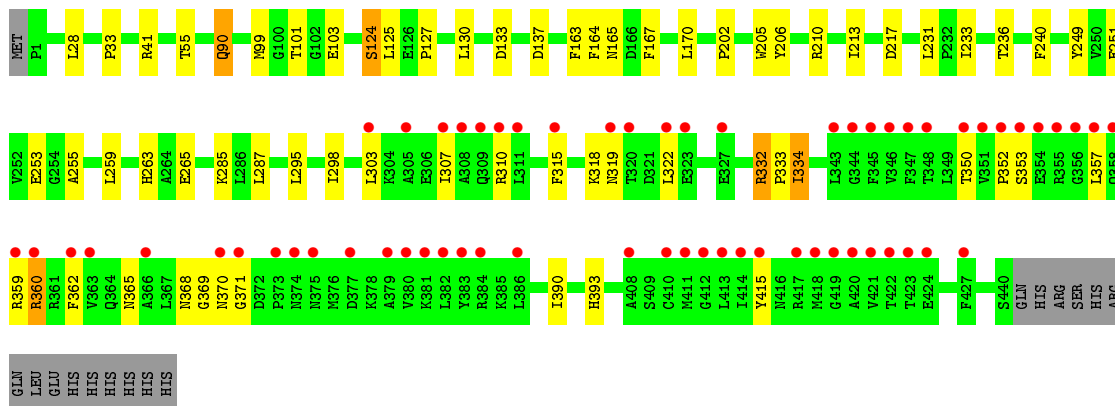
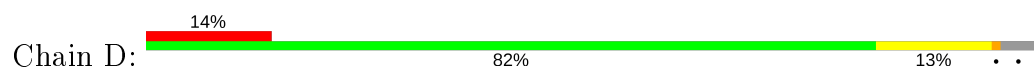


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

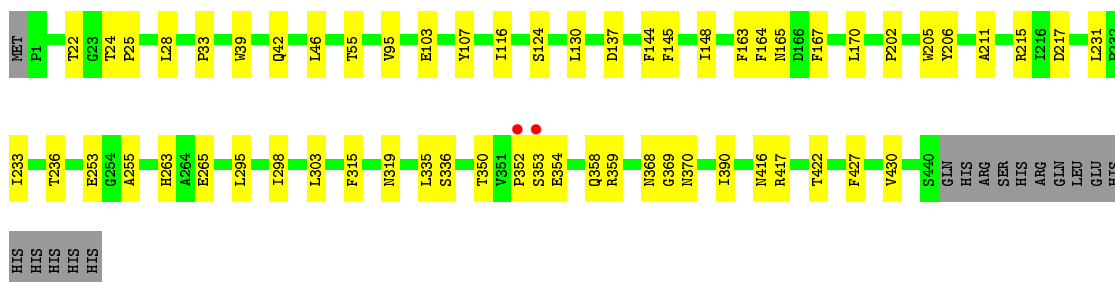
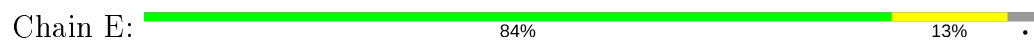




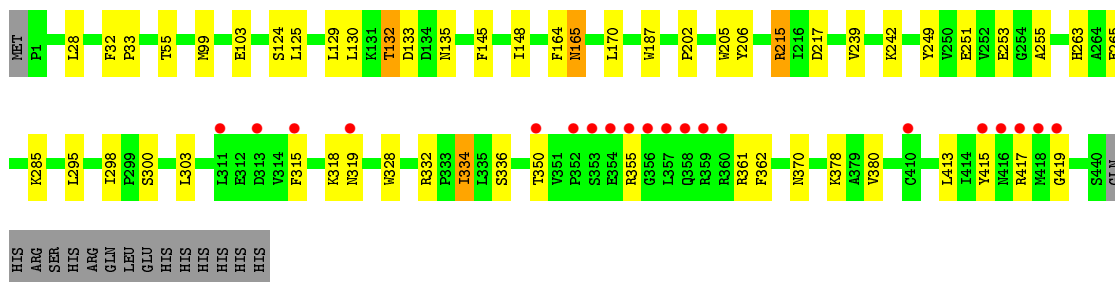
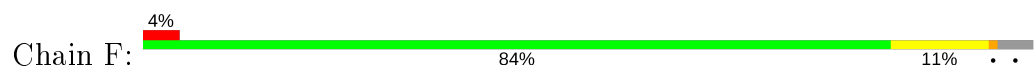
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.71Å 137.87Å 171.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.29 – 3.50 93.29 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (93.29-3.50) 97.6 (93.29-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.200 , 0.231 0.201 , 0.231	Depositor DCC
R_{free} test set	1893 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20388	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0815e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.23	0/3475	0.42	0/4729
1	B	0.22	0/3475	0.42	0/4729
1	C	0.24	0/3475	0.42	0/4729
1	D	0.22	0/3475	0.42	0/4729
1	E	0.22	0/3475	0.41	0/4729
1	F	0.22	0/3475	0.42	0/4729
All	All	0.23	0/20850	0.42	0/28374

There are no bond length outliers.

There are no bond angle outliers.

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	3398	0	3326	35	0
1	B	3398	0	3326	32	0
1	C	3398	0	3326	25	0
1	D	3398	0	3326	33	0
1	E	3398	0	3326	29	0
1	F	3398	0	3326	25	0
All	All	20388	0	19956	176	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 (176) 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:B:357:LEU:HB3	1:B:360:ARG:HH12	1.37	0.85
1:B:370:ASN:HB2	1:E:211:ALA:HB3	1.58	0.85
1:A:107:TYR:HE2	1:A:116:ILE:HD11	1.45	0.81
1:A:407:LEU:HB3	1:A:433:THR:HG22	1.63	0.81
1:E:107:TYR:HE2	1:E:116:ILE:HD11	1.51	0.76
1:B:414:ILE:HG23	1:B:419:GLY:HA3	1.68	0.74
1:D:357:LEU:HD22	1:D:360:ARG:HH12	1.56	0.70
1:B:373:PRO:HB2	1:B:413:LEU:HD12	1.79	0.63
1:F:132:THR:OG1	1:F:133:ASP:N	2.29	0.63
1:B:369:GLY:O	1:B:371:GLY:N	2.31	0.63
1:D:28:LEU:HB2	1:D:55:THR:HG22	1.83	0.61
1:E:354:GLU:OE1	1:E:359:ARG:NH1	2.35	0.60
1:A:22:THR:HG21	1:A:422:THR:HG21	1.85	0.59
1:A:107:TYR:CE2	1:A:116:ILE:HD11	2.34	0.59
1:C:130:LEU:HB2	1:C:206:TYR:HB2	1.84	0.59
1:E:107:TYR:CE2	1:E:116:ILE:HD11	2.36	0.58
1:F:145:PHE:HA	1:F:148:ILE:HD12	1.85	0.58
1:C:315:PHE:HE1	1:C:350:THR:HG21	1.70	0.57
1:E:130:LEU:HB2	1:E:206:TYR:HB2	1.87	0.57
1:A:359:ARG:NH1	1:A:415:TYR:O	2.38	0.56
1:C:368:ASN:OD1	1:C:369:GLY:N	2.38	0.56
1:B:28:LEU:HB2	1:B:55:THR:HG22	1.88	0.56
1:B:90:GLN:HB2	1:B:391:THR:HG21	1.88	0.56
1:B:337:PRO:O	1:B:366:ALA:HB1	2.06	0.55
1:C:28:LEU:HB2	1:C:55:THR:HG22	1.86	0.55
1:E:28:LEU:HB2	1:E:55:THR:HG22	1.88	0.55
1:E:315:PHE:HE1	1:E:350:THR:HG21	1.72	0.55
1:A:231:LEU:HB3	1:A:236:THR:HG21	1.88	0.55
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.87	0.55
1:E:22:THR:HG22	1:E:390:ILE:HD11	1.89	0.55
1:F:28:LEU:HB2	1:F:55:THR:HG22	1.89	0.55
1:D:90:GLN:HB3	1:D:390:ILE:HG23	1.88	0.54
1:C:145:PHE:HA	1:C:148:ILE:HD12	1.90	0.54
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.90	0.54
1:F:130:LEU:HB2	1:F:206:TYR:HB2	1.90	0.54
1:F:328:TRP:O	1:F:332:ARG:HG2	2.08	0.54
1:A:215:ARG:NH2	1:F:300:SER:O	2.41	0.53
1:D:369:GLY:O	1:D:371:GLY:N	2.41	0.53
1:C:323:GLU:HG3	1:C:357:LEU:HD11	1.92	0.52
1:E:303:LEU:HD21	1:E:335:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:PHE:HE1	1:B:350:THR:HG21	1.75	0.51
1:B:145:PHE:HA	1:B:148:ILE:HD12	1.93	0.51
1:D:315:PHE:HE1	1:D:350:THR:HG21	1.76	0.50
1:A:101:THR:HG21	1:A:124:SER:HA	1.92	0.50
1:A:33:PRO:HD3	1:A:163:PHE:CE2	2.46	0.50
1:B:368:ASN:ND2	1:B:416:ASN:HD21	2.09	0.50
1:F:328:TRP:CE2	1:F:332:ARG:HD2	2.47	0.49
1:C:99:MET:HA	1:C:125:LEU:HD11	1.95	0.49
1:B:333:PRO:O	1:B:335:LEU:N	2.45	0.49
1:E:145:PHE:HA	1:E:148:ILE:HD12	1.94	0.49
1:F:315:PHE:HE1	1:F:350:THR:HG21	1.77	0.49
1:A:297:ILE:HD11	1:A:434:CYS:O	2.13	0.49
1:B:333:PRO:C	1:B:335:LEU:H	2.15	0.49
1:E:368:ASN:OD1	1:E:369:GLY:N	2.45	0.49
1:D:360:ARG:HG2	1:D:362:PHE:CE2	2.47	0.49
1:A:295:LEU:HA	1:A:298:ILE:HD12	1.95	0.49
1:A:164:PHE:HA	1:A:167:PHE:HB3	1.94	0.49
1:D:33:PRO:HD3	1:D:163:PHE:CE2	2.48	0.49
1:D:90:GLN:HG2	1:D:390:ILE:HD12	1.95	0.49
1:A:99:MET:HA	1:A:125:LEU:HD11	1.95	0.48
1:E:165:ASN:HA	1:E:170:LEU:HD12	1.94	0.48
1:C:295:LEU:HA	1:C:298:ILE:HD12	1.95	0.48
1:F:380:VAL:HG22	1:F:413:LEU:HD21	1.95	0.48
1:E:164:PHE:HA	1:E:167:PHE:HB3	1.95	0.48
1:B:101:THR:HG21	1:B:124:SER:HA	1.95	0.48
1:A:28:LEU:HB2	1:A:55:THR:HG22	1.96	0.48
1:E:144:PHE:CE2	1:E:148:ILE:HD11	2.49	0.48
1:A:368:ASN:OD1	1:A:369:GLY:N	2.46	0.48
1:A:429:LEU:O	1:A:433:THR:HG23	2.14	0.48
1:D:127:PRO:HB2	1:D:210:ARG:HG2	1.96	0.47
1:D:231:LEU:HB3	1:D:236:THR:HG21	1.95	0.47
1:D:165:ASN:HA	1:D:170:LEU:HD12	1.97	0.47
1:C:359:ARG:HD2	1:C:415:TYR:CZ	2.50	0.47
1:B:144:PHE:CE2	1:B:148:ILE:HD11	2.51	0.46
1:C:282:GLN:HA	1:C:285:LYS:HG2	1.97	0.46
1:E:33:PRO:HD3	1:E:163:PHE:CE2	2.50	0.46
1:A:202:PRO:HA	1:A:205:TRP:CD2	2.51	0.46
1:A:28:LEU:HB3	1:A:39:TRP:CE2	2.51	0.46
1:C:33:PRO:HD3	1:C:163:PHE:CE2	2.49	0.46
1:D:360:ARG:HG2	1:D:362:PHE:CD2	2.50	0.46
1:B:369:GLY:C	1:B:371:GLY:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:PHE:HA	1:B:167:PHE:HB3	1.96	0.46
1:B:165:ASN:HA	1:B:170:LEU:HD12	1.97	0.46
1:D:249:TYR:CE2	1:D:251:GLU:HG3	2.51	0.46
1:D:287:LEU:HD22	1:D:315:PHE:CE1	2.52	0.45
1:D:359:ARG:HB3	1:D:415:TYR:CE2	2.51	0.45
1:B:33:PRO:HD3	1:B:163:PHE:CE2	2.51	0.45
1:B:41:ARG:NH1	1:B:261:TRP:O	2.50	0.45
1:E:295:LEU:HA	1:E:298:ILE:HD12	1.99	0.45
1:A:202:PRO:HA	1:A:205:TRP:CE2	2.52	0.45
1:F:164:PHE:HE2	1:F:187:TRP:HA	1.82	0.45
1:B:374:ASN:OD1	1:B:417:ARG:NH1	2.49	0.44
1:C:323:GLU:HB2	1:C:357:LEU:HD21	1.99	0.44
1:B:249:TYR:CE2	1:B:251:GLU:HG3	2.51	0.44
1:D:164:PHE:HA	1:D:167:PHE:HB3	2.00	0.44
1:D:287:LEU:HB3	1:D:315:PHE:CD2	2.53	0.44
1:F:239:VAL:HA	1:F:242:LYS:HE3	2.00	0.44
1:B:99:MET:HA	1:B:125:LEU:HD11	1.99	0.44
1:A:145:PHE:HA	1:A:148:ILE:HD12	2.00	0.44
1:A:265:GLU:OE1	1:A:265:GLU:HA	2.17	0.44
1:D:287:LEU:HD13	1:D:315:PHE:CG	2.52	0.44
1:A:144:PHE:CE2	1:A:148:ILE:HD11	2.52	0.44
1:C:202:PRO:HA	1:C:205:TRP:CD2	2.53	0.44
1:C:265:GLU:OE1	1:C:265:GLU:HA	2.18	0.44
1:C:306:GLU:O	1:C:310:ARG:HD2	2.18	0.44
1:A:322:LEU:HD21	1:A:348:THR:HG22	2.00	0.43
1:B:28:LEU:HD23	1:B:95:VAL:HB	1.99	0.43
1:E:202:PRO:HA	1:E:205:TRP:CE2	2.52	0.43
1:D:332:ARG:NE	1:D:333:PRO:HD2	2.33	0.43
1:E:231:LEU:HB3	1:E:236:THR:HG21	1.99	0.43
1:B:171:ASP:OD1	1:B:172:GLU:HG3	2.19	0.43
1:C:164:PHE:HA	1:C:167:PHE:HB3	2.00	0.43
1:C:90:GLN:CG	1:C:390:ILE:HG13	2.48	0.43
1:D:295:LEU:HA	1:D:298:ILE:HD12	2.01	0.43
1:F:215:ARG:HA	1:F:215:ARG:HD3	1.81	0.43
1:D:33:PRO:HD3	1:D:163:PHE:HE2	1.82	0.43
1:F:415:TYR:C	1:F:417:ARG:H	2.22	0.43
1:A:372:ASP:O	1:A:376:MET:HG2	2.18	0.43
1:A:215:ARG:HD2	1:F:334:ILE:HG12	1.99	0.43
1:F:165:ASN:HA	1:F:170:LEU:HD12	2.01	0.43
1:D:202:PRO:HA	1:D:205:TRP:CD2	2.54	0.43
1:D:365:ASN:HA	1:D:368:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:MET:HA	1:D:125:LEU:HD11	2.01	0.43
1:A:321:ASP:HA	1:A:355:ARG:NH2	2.34	0.42
1:D:255:ALA:HA	1:D:263:HIS:CE1	2.54	0.42
1:A:249:TYR:CE2	1:A:251:GLU:HG3	2.53	0.42
1:C:249:TYR:CE2	1:C:251:GLU:HG3	2.53	0.42
1:E:39:TRP:O	1:E:42:GLN:N	2.52	0.42
1:F:132:THR:HG23	1:F:135:ASN:HB3	2.01	0.42
1:F:202:PRO:HA	1:F:205:TRP:CD2	2.54	0.42
1:A:319:ASN:O	1:A:321:ASP:N	2.45	0.42
1:B:202:PRO:HA	1:B:205:TRP:CD2	2.54	0.42
1:B:39:TRP:O	1:B:42:GLN:N	2.53	0.42
1:C:173:ASN:ND2	1:C:256:PRO:HG3	2.35	0.42
1:D:322:LEU:HD23	1:D:357:LEU:HD12	2.00	0.42
1:E:416:ASN:O	1:E:417:ARG:HB2	2.19	0.42
1:A:315:PHE:HE1	1:A:350:THR:HG21	1.85	0.42
1:E:265:GLU:OE1	1:E:265:GLU:HA	2.19	0.42
1:B:357:LEU:HD22	1:B:360:ARG:HH22	1.85	0.42
1:C:41:ARG:NH1	1:C:261:TRP:O	2.52	0.42
1:E:427:PHE:HA	1:E:430:VAL:HG12	2.01	0.42
1:F:417:ARG:C	1:F:419:GLY:H	2.23	0.42
1:A:41:ARG:NH1	1:A:261:TRP:O	2.52	0.42
1:C:255:ALA:HA	1:C:263:HIS:CE1	2.55	0.42
1:D:130:LEU:HB2	1:D:206:TYR:HB2	2.01	0.42
1:D:202:PRO:HA	1:D:205:TRP:CE2	2.55	0.42
1:D:265:GLU:OE1	1:D:265:GLU:HA	2.20	0.42
1:E:202:PRO:HA	1:E:205:TRP:CD2	2.55	0.42
1:E:22:THR:HG21	1:E:422:THR:HG21	2.01	0.42
1:F:99:MET:HA	1:F:125:LEU:HD11	2.01	0.42
1:F:249:TYR:CE2	1:F:251:GLU:HG3	2.55	0.42
1:A:28:LEU:HB3	1:A:39:TRP:CD2	2.55	0.42
1:E:28:LEU:HB3	1:E:39:TRP:CE2	2.55	0.42
1:F:265:GLU:OE1	1:F:265:GLU:HA	2.20	0.42
1:E:28:LEU:HD23	1:E:95:VAL:HB	2.02	0.42
1:E:24:THR:HA	1:E:25:PRO:HD3	1.88	0.41
1:F:255:ALA:HA	1:F:263:HIS:CE1	2.55	0.41
1:C:28:LEU:HD23	1:C:95:VAL:HB	2.02	0.41
1:F:295:LEU:HA	1:F:298:ILE:HD12	2.01	0.41
1:A:143:GLU:CD	1:A:143:GLU:H	2.23	0.41
1:B:231:LEU:HB3	1:B:236:THR:HG21	2.02	0.41
1:C:90:GLN:CD	1:C:390:ILE:HG13	2.41	0.41
1:E:28:LEU:HB3	1:E:39:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:THR:HG21	1:D:124:SER:HA	2.03	0.41
1:F:129:LEU:HA	1:F:129:LEU:HD23	1.95	0.41
1:A:332:ARG:NE	1:A:332:ARG:HA	2.35	0.41
1:C:234:GLU:HA	1:C:238:ARG:HG3	2.03	0.41
1:F:32:PHE:HA	1:F:33:PRO:HA	1.85	0.41
1:D:369:GLY:C	1:D:371:GLY:H	2.23	0.41
1:B:28:LEU:HB3	1:B:39:TRP:CE2	2.56	0.41
1:D:213:ILE:HD12	1:D:240:PHE:CE1	2.56	0.40
1:B:127:PRO:HD3	1:B:239:VAL:HG13	2.04	0.40
1:C:354:GLU:O	1:C:356:GLY:N	2.52	0.40
1:D:307:ILE:HA	1:D:310:ARG:HH21	1.87	0.40
1:A:376:MET:O	1:A:380:VAL:HG23	2.22	0.40
1:E:255:ALA:HA	1:E:263:HIS:CE1	2.56	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	438/456 (96%)	419 (96%)	18 (4%)	1 (0%)	47	81
1	B	438/456 (96%)	409 (93%)	23 (5%)	6 (1%)	11	46
1	C	438/456 (96%)	415 (95%)	22 (5%)	1 (0%)	47	81
1	D	438/456 (96%)	413 (94%)	20 (5%)	5 (1%)	14	52
1	E	438/456 (96%)	416 (95%)	18 (4%)	4 (1%)	17	56
1	F	438/456 (96%)	416 (95%)	20 (5%)	2 (0%)	29	68
All	All	2628/2736 (96%)	2488 (95%)	121 (5%)	19 (1%)	22	61

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	334	ILE
1	B	370	ASN
1	D	334	ILE
1	D	370	ASN
1	E	319	ASN
1	B	319	ASN
1	B	352	PRO
1	B	419	GLY
1	C	319	ASN
1	D	319	ASN
1	D	352	PRO
1	D	353	SER
1	E	352	PRO
1	E	353	SER
1	E	370	ASN
1	F	319	ASN
1	A	320	THR
1	B	353	SER
1	F	334	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	354/370 (96%)	339 (96%)	15 (4%)	30	63
1	B	354/370 (96%)	341 (96%)	13 (4%)	34	65
1	C	354/370 (96%)	335 (95%)	19 (5%)	22	55
1	D	354/370 (96%)	337 (95%)	17 (5%)	25	60
1	E	354/370 (96%)	344 (97%)	10 (3%)	43	72
1	F	354/370 (96%)	338 (96%)	16 (4%)	27	61
All	All	2124/2220 (96%)	2034 (96%)	90 (4%)	30	63

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	124	SER
1	A	137	ASP
1	A	215	ARG
1	A	217	ASP
1	A	233	ILE
1	A	253	GLU
1	A	259	LEU
1	A	282	GLN
1	A	285	LYS
1	A	320	THR
1	A	338	LEU
1	A	390	ILE
1	A	391	THR
1	A	439	ASP
1	B	103	GLU
1	B	124	SER
1	B	137	ASP
1	B	217	ASP
1	B	233	ILE
1	B	285	LYS
1	B	286	LEU
1	B	295	LEU
1	B	310	ARG
1	B	335	LEU
1	B	338	LEU
1	B	381	LYS
1	B	413	LEU
1	C	103	GLU
1	C	124	SER
1	C	137	ASP
1	C	233	ILE
1	C	253	GLU
1	C	259	LEU
1	C	279	GLN
1	C	280	GLU
1	C	285	LYS
1	C	287	LEU
1	C	303	LEU
1	C	310	ARG
1	C	319	ASN
1	C	338	LEU
1	C	346	VAL

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Mol	Chain	Res	Type
1	C	360	ARG
1	C	380	VAL
1	C	390	ILE
1	C	413	LEU
1	D	41	ARG
1	D	90	GLN
1	D	103	GLU
1	D	124	SER
1	D	133	ASP
1	D	137	ASP
1	D	217	ASP
1	D	233	ILE
1	D	253	GLU
1	D	259	LEU
1	D	285	LYS
1	D	303	LEU
1	D	318	LYS
1	D	332	ARG
1	D	334	ILE
1	D	360	ARG
1	D	393	HIS
1	E	46	LEU
1	E	103	GLU
1	E	124	SER
1	E	137	ASP
1	E	215	ARG
1	E	217	ASP
1	E	233	ILE
1	E	253	GLU
1	E	336	SER
1	E	358	GLN
1	F	103	GLU
1	F	124	SER
1	F	132	THR
1	F	165	ASN
1	F	215	ARG
1	F	217	ASP
1	F	253	GLU
1	F	285	LYS
1	F	303	LEU
1	F	318	LYS
1	F	336	SER

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Mol	Chain	Res	Type
1	F	355	ARG
1	F	361	ARG
1	F	362	PHE
1	F	370	ASN
1	F	378	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	368	ASN
1	C	257	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/456 (96%)	-0.02	1 (0%) 95 93	57, 80, 118, 154	0
1	B	440/456 (96%)	0.41	41 (9%) 8 9	55, 97, 188, 208	0
1	C	440/456 (96%)	0.33	37 (8%) 11 11	51, 81, 254, 279	0
1	D	440/456 (96%)	0.62	62 (14%) 2 3	54, 82, 285, 309	0
1	E	440/456 (96%)	-0.05	2 (0%) 91 88	63, 88, 119, 161	0
1	F	440/456 (96%)	0.18	20 (4%) 33 29	60, 92, 132, 181	0
All	All	2640/2736 (96%)	0.24	163 (6%) 20 18	51, 87, 212, 309	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	356	GLY	15.1
1	D	370	ASN	9.6
1	C	419	GLY	8.5
1	D	355	ARG	8.5
1	F	353	SER	8.4
1	D	419	GLY	8.0
1	D	350	THR	8.0
1	B	319	ASN	7.8
1	D	379	ALA	7.5
1	C	418	MET	7.5
1	B	353	SER	7.1
1	D	418	MET	7.0
1	D	354	GLU	6.7
1	B	358	GLN	6.6
1	F	357	LEU	6.5
1	F	359	ARG	6.4
1	D	377	ASP	6.4
1	B	352	PRO	6.2
1	C	353	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	414	ILE	6.1
1	D	352	PRO	6.1
1	B	321	ASP	5.9
1	D	380	VAL	5.7
1	D	410	CYS	5.4
1	C	357	LEU	5.3
1	D	319	ASN	5.3
1	C	410	CYS	5.2
1	B	357	LEU	5.1
1	F	352	PRO	5.0
1	D	359	ARG	5.0
1	D	357	LEU	5.0
1	D	411	MET	4.9
1	F	354	GLU	4.9
1	C	355	ARG	4.8
1	D	323	GLU	4.8
1	B	320	THR	4.8
1	D	346	VAL	4.8
1	D	320	THR	4.8
1	D	374	ASN	4.7
1	D	347	PHE	4.7
1	F	419	GLY	4.7
1	B	354	GLU	4.6
1	C	411	MET	4.6
1	D	308	ALA	4.6
1	B	355	ARG	4.4
1	D	381	LYS	4.4
1	F	418	MET	4.3
1	B	416	ASN	4.3
1	F	358	GLN	4.2
1	D	371	GLY	4.2
1	F	355	ARG	4.2
1	B	308	ALA	4.1
1	C	414	ILE	4.1
1	C	370	ASN	4.0
1	C	350	THR	4.0
1	D	417	ARG	4.0
1	D	423	THR	4.0
1	B	417	ARG	3.9
1	D	315	PHE	3.9
1	C	354	GLU	3.8
1	B	418	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	310	ARG	3.8
1	D	383	TYR	3.8
1	D	413	LEU	3.7
1	C	371	GLY	3.7
1	B	349	LEU	3.6
1	C	373	PRO	3.6
1	D	408	ALA	3.5
1	C	323	GLU	3.5
1	D	307	ILE	3.4
1	F	415	TYR	3.4
1	B	415	TYR	3.4
1	D	415	TYR	3.4
1	D	345	PHE	3.4
1	F	319	ASN	3.4
1	C	358	GLN	3.4
1	C	347	PHE	3.4
1	B	386	LEU	3.3
1	F	360	ARG	3.3
1	C	348	THR	3.3
1	D	348	THR	3.3
1	F	356	GLY	3.3
1	D	353	SER	3.2
1	C	363	VAL	3.2
1	D	351	VAL	3.2
1	B	419	GLY	3.2
1	D	375	ASN	3.2
1	C	377	ASP	3.2
1	C	382	LEU	3.1
1	D	373	PRO	3.1
1	D	360	ARG	3.0
1	F	417	ARG	3.0
1	B	311	LEU	3.0
1	D	327	GLU	3.0
1	C	315	PHE	3.0
1	D	309	GLN	3.0
1	C	375	ASN	3.0
1	E	352	PRO	3.0
1	E	353	SER	2.9
1	C	346	VAL	2.9
1	D	382	LEU	2.9
1	D	420	ALA	2.9
1	B	350	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	428	GLY	2.8
1	C	343	LEU	2.8
1	B	345	PHE	2.8
1	C	384	ARG	2.8
1	D	363	VAL	2.8
1	C	364	GLN	2.8
1	F	350	THR	2.7
1	F	311	LEU	2.7
1	C	356	GLY	2.7
1	B	291	GLU	2.7
1	D	366	ALA	2.7
1	B	348	THR	2.6
1	D	362	PHE	2.6
1	B	326	MET	2.6
1	B	368	ASN	2.6
1	A	376	MET	2.6
1	F	416	ASN	2.6
1	C	374	ASN	2.6
1	C	319	ASN	2.5
1	B	356	GLY	2.5
1	B	295	LEU	2.5
1	D	322	LEU	2.5
1	D	358	GLN	2.5
1	B	359	ARG	2.5
1	D	305	ALA	2.4
1	F	410	CYS	2.4
1	B	435	GLU	2.4
1	D	386	LEU	2.4
1	D	422	THR	2.4
1	F	315	PHE	2.4
1	B	437	ILE	2.4
1	C	386	LEU	2.4
1	F	313	ASP	2.3
1	D	427	PHE	2.3
1	B	347	PHE	2.3
1	B	21	GLY	2.3
1	B	309	GLN	2.2
1	D	344	GLY	2.2
1	D	421	VAL	2.2
1	D	384	ARG	2.2
1	C	311	LEU	2.2
1	C	379	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	343	LEU	2.2
1	D	303	LEU	2.2
1	B	298	ILE	2.2
1	C	345	PHE	2.1
1	D	424	GLU	2.1
1	C	413	LEU	2.1
1	B	344	GLY	2.1
1	B	297	ILE	2.1
1	B	307	ILE	2.1
1	B	306	GLU	2.1
1	D	412	GLY	2.1
1	C	423	THR	2.1
1	B	304	LYS	2.1
1	B	388	ARG	2.1
1	C	367	LEU	2.1
1	B	424	GLU	2.1
1	D	311	LEU	2.0
1	C	321	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.