



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:49 AM UTC

PDB ID : 4IQ4 / pdb_00004iq4
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 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:

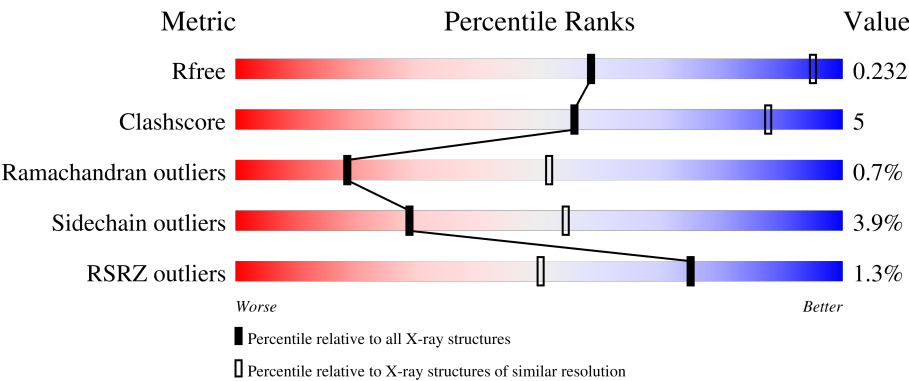
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	456	81%15%..
1	B	456	81%14%..
1	C	456	2% 83%12%..
1	D	456	4% 82%14%..
1	E	456	83%13%.

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Mol	Chain	Length	Quality of chain
1	F	456	84% 12% .

2 Entry composition

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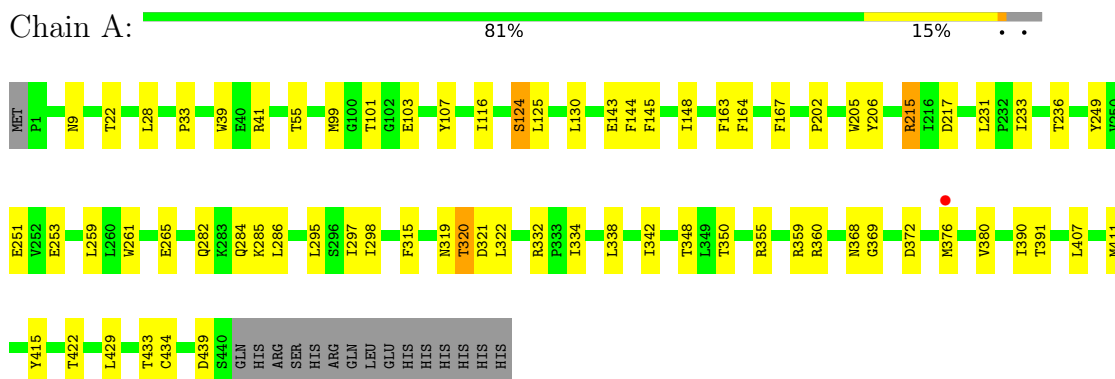
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Chain	Residue	Modelled	Actual	Comment	Reference
F	449	GLU	-	expression tag	UNP P03485
F	450	HIS	-	expression tag	UNP P03485
F	451	HIS	-	expression tag	UNP P03485
F	452	HIS	-	expression tag	UNP P03485
F	453	HIS	-	expression tag	UNP P03485
F	454	HIS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

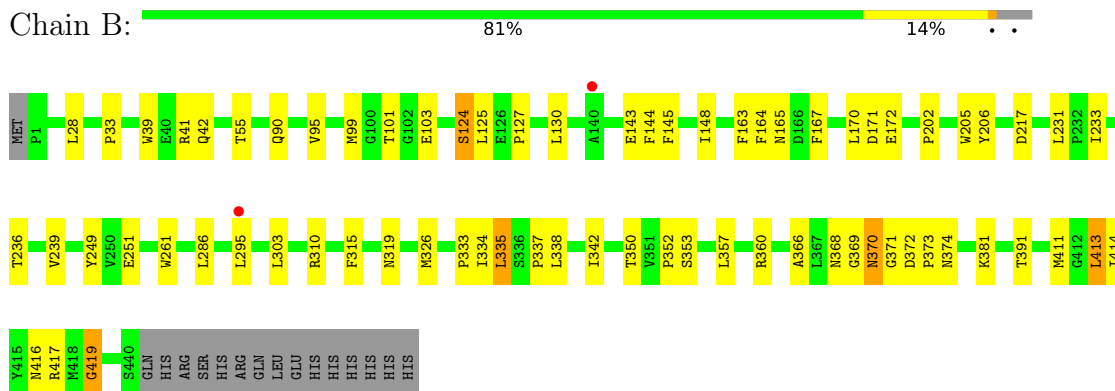
3 Residue-property plots [i](#)

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.

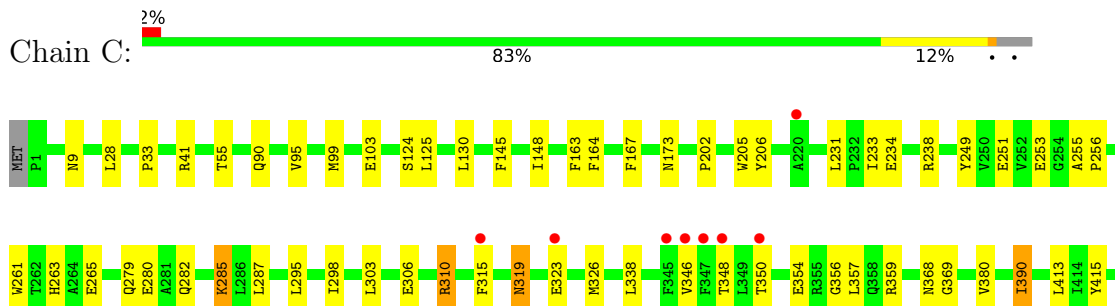
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

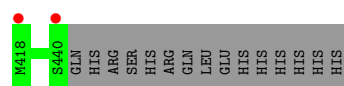


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

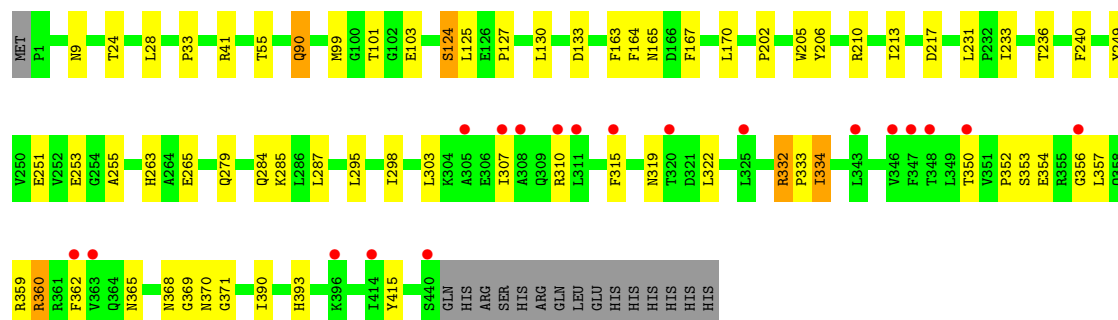
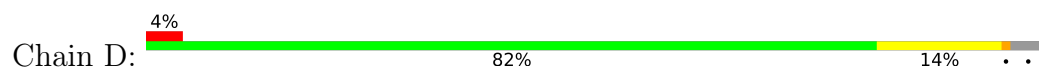


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

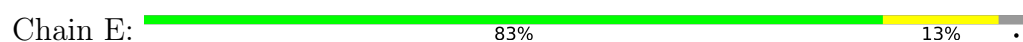




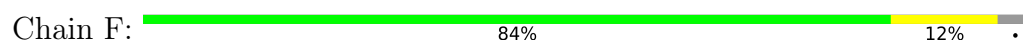
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



- 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) 97.5 (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)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.200 , 0.231 0.202 , 0.232	Depositor DCC
R_{free} test set	1893 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtrriage
Anisotropy	0.260	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20388	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/3475	0.76	1/4729 (0.0%)
1	B	0.31	0/3475	0.76	2/4729 (0.0%)
1	C	0.32	0/3475	0.76	3/4729 (0.1%)
1	D	0.31	0/3475	0.76	1/4729 (0.0%)
1	E	0.30	0/3475	0.75	2/4729 (0.0%)
1	F	0.30	0/3475	0.76	1/4729 (0.0%)
All	All	0.31	0/20850	0.76	10/28374 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	371	GLY	N-CA-C	-7.48	104.72	115.64
1	B	372	ASP	CA-C-N	6.80	126.43	119.56
1	B	372	ASP	C-N-CA	6.80	126.43	119.56
1	E	9	ASN	CB-CA-C	-5.30	110.48	116.63
1	C	231	LEU	CA-C-N	5.29	125.59	119.93
1	C	231	LEU	C-N-CA	5.29	125.59	119.93
1	A	9	ASN	CB-CA-C	-5.22	110.58	116.63
1	E	233	ILE	N-CA-C	5.15	115.77	110.36
1	D	9	ASN	CB-CA-C	-5.11	110.70	116.63
1	C	9	ASN	CB-CA-C	-5.04	110.78	116.63

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	36	0
1	B	3398	0	3326	36	0
1	C	3398	0	3326	27	0
1	D	3398	0	3326	35	0
1	E	3398	0	3326	31	0
1	F	3398	0	3326	26	0
All	All	20388	0	19956	188	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 5.

All (188) 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:F:326:MET:HE3	1:F:348:THR:HG23	1.84	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:333:PRO:C	1:B:335:LEU:H	2.15	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
1:B:315:PHE:HE1	1:B:350:THR:HG21	1.75	0.51
1:B:369:GLY:C	1:B:371:GLY:H	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:417:ARG:C	1:F:419:GLY:H	2.23	0.47
1:F:415:TYR:C	1:F:417:ARG:H	2.22	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:A:143:GLU:CD	1:A:143:GLU:H	2.23	0.46
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:C:90:GLN:CD	1:C:390:ILE:HG13	2.41	0.46
1:D:249:TYR:CE2	1:D:251:GLU:HG3	2.51	0.46
1:D:369:GLY:C	1:D:371:GLY:H	2.23	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:326:MET:HE3	1:B:360:ARG:HG3	1.98	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:HA	1:A:265:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:342:ILE:HG12	1:E:411:MET:HE1	1.99	0.44
1:D:24:THR:HG21	1:D:279:GLN:CD	2.43	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:C:326:MET:HE3	1:C:348:THR:HG23	2.01	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:90:GLN:CG	1:C:390:ILE:HG13	2.48	0.43
1:C:164:PHE:HA	1:C:167:PHE:HB3	2.00	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:A:215:ARG:HD2	1:F:334:ILE:HG12	1.99	0.43
1:A:372:ASP:O	1:A:376:MET:HG2	2.18	0.43
1:E:326:MET:HE3	1:E:348:THR:HG23	2.01	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
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:C:354:GLU:C	1:C:356:GLY:H	2.28	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:HA	1:E:265:GLU:OE1	2.19	0.42
1:B:342:ILE:HG12	1:B:411:MET:HE1	2.01	0.42
1:B:357:LEU:HD22	1:B:360:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:D:265:GLU:OE1	2.20	0.42
1:E:22:THR:HG21	1:E:422:THR:HG21	2.01	0.42
1:E:202:PRO:HA	1:E:205:TRP:CD2	2.55	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:HA	1:F:265:GLU:OE1	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:B:231:LEU:HB3	1:B:236:THR:HG21	2.02	0.41
1:E:28:LEU:HB3	1:E:39:TRP:CD2	2.55	0.41
1:D:101:THR:HG21	1:D:124:SER:HA	2.03	0.41
1:F:129:LEU:HD23	1:F:129:LEU:HA	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: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:A:342:ILE:HA	1:A:411:MET:HE1	2.03	0.40
1:B:143:GLU:CD	1:B:143:GLU:H	2.29	0.40
1:B:333:PRO:C	1:B:335:LEU:N	2.80	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:D:354:GLU:C	1:D:356:GLY:H	2.29	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

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	438/456 (96%)	419 (96%)	18 (4%)	1 (0%)	43	74
1	B	438/456 (96%)	409 (93%)	23 (5%)	6 (1%)	9	38
1	C	438/456 (96%)	415 (95%)	22 (5%)	1 (0%)	43	74
1	D	438/456 (96%)	413 (94%)	20 (5%)	5 (1%)	11	43
1	E	438/456 (96%)	416 (95%)	18 (4%)	4 (1%)	14	47
1	F	438/456 (96%)	416 (95%)	20 (5%)	2 (0%)	24	57
All	All	2628/2736 (96%)	2488 (95%)	121 (5%)	19 (1%)	18	51

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%)	336 (95%)	18 (5%)	21	48
1	B	354/370 (96%)	342 (97%)	12 (3%)	32	57
1	C	354/370 (96%)	338 (96%)	16 (4%)	24	50
1	D	354/370 (96%)	339 (96%)	15 (4%)	26	52
1	E	354/370 (96%)	346 (98%)	8 (2%)	44	64
1	F	354/370 (96%)	340 (96%)	14 (4%)	28	54
All	All	2124/2220 (96%)	2041 (96%)	83 (4%)	28	54

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	124	SER
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	284	GLN
1	A	285	LYS
1	A	286	LEU
1	A	320	THR
1	A	334	ILE
1	A	338	LEU
1	A	360	ARG
1	A	390	ILE
1	A	391	THR
1	A	439	ASP
1	B	103	GLU
1	B	124	SER
1	B	217	ASP
1	B	233	ILE

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Mol	Chain	Res	Type
1	B	286	LEU
1	B	295	LEU
1	B	303	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	233	ILE
1	C	253	GLU
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
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	217	ASP
1	D	233	ILE
1	D	253	GLU
1	D	284	GLN
1	D	285	LYS
1	D	303	LEU
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

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Mol	Chain	Res	Type
1	E	217	ASP
1	E	233	ILE
1	E	253	GLU
1	E	284	GLN
1	E	358	GLN
1	F	103	GLU
1	F	124	SER
1	F	132	THR
1	F	217	ASP
1	F	233	ILE
1	F	253	GLU
1	F	284	GLN
1	F	303	LEU
1	F	318	LYS
1	F	336	SER
1	F	355	ARG
1	F	360	ARG
1	F	361	ARG
1	F	378	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	165	ASN
1	A	365	ASN
1	B	42	GLN
1	B	63	GLN
1	B	165	ASN
1	B	364	GLN
1	B	368	ASN
1	C	42	GLN
1	C	63	GLN
1	C	173	ASN
1	C	257	HIS
1	C	319	ASN
1	D	90	GLN
1	D	165	ASN
1	D	319	ASN
1	E	37	HIS
1	E	63	GLN
1	E	165	ASN

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Mol	Chain	Res	Type
1	E	263	HIS
1	F	42	GLN
1	F	63	GLN
1	F	90	GLN
1	F	165	ASN
1	F	241	HIS

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	440/456 (96%)	-0.36	1 (0%) 91 82	57, 80, 118, 154	0
1	B	440/456 (96%)	-0.12	2 (0%) 87 68	55, 97, 188, 208	0
1	C	440/456 (96%)	-0.03	10 (2%) 61 37	51, 81, 254, 279	0
1	D	440/456 (96%)	0.08	19 (4%) 40 21	54, 82, 285, 309	0
1	E	440/456 (96%)	-0.35	1 (0%) 91 82	63, 88, 119, 161	0
1	F	440/456 (96%)	-0.26	2 (0%) 87 68	60, 92, 132, 181	0
All	All	2640/2736 (96%)	-0.17	35 (1%) 75 50	51, 87, 212, 309	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	347	PHE	4.6
1	D	350	THR	4.5
1	C	346	VAL	4.4
1	C	440	SER	3.6
1	D	346	VAL	3.4
1	D	315	PHE	3.3
1	D	308	ALA	3.3
1	D	325	LEU	3.1
1	A	376	MET	3.1
1	D	440	SER	3.0
1	D	310	ARG	2.9
1	C	315	PHE	2.8
1	B	140	ALA	2.8
1	C	323	GLU	2.7
1	F	440	SER	2.7
1	C	418	MET	2.7
1	D	311	LEU	2.7
1	D	343	LEU	2.6
1	C	345	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	320	THR	2.5
1	D	362	PHE	2.4
1	D	363	VAL	2.4
1	D	348	THR	2.4
1	D	356	GLY	2.3
1	D	396	LYS	2.3
1	D	307	ILE	2.3
1	C	348	THR	2.3
1	D	414	ILE	2.2
1	C	220	ALA	2.2
1	B	295	LEU	2.2
1	C	347	PHE	2.2
1	E	376	MET	2.1
1	D	305	ALA	2.1
1	F	419	GLY	2.1
1	C	350	THR	2.1

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.