



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:32 PM UTC

PDB ID : 5OPW / pdb_00005opw
Title : Crystal structure of the GroEL mutant A109C
Authors : Yan, X.; Shi, Q.; Bracher, A.; Milicic, G.; Singh, A.K.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on : 2017-08-10
Resolution : 3.19 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

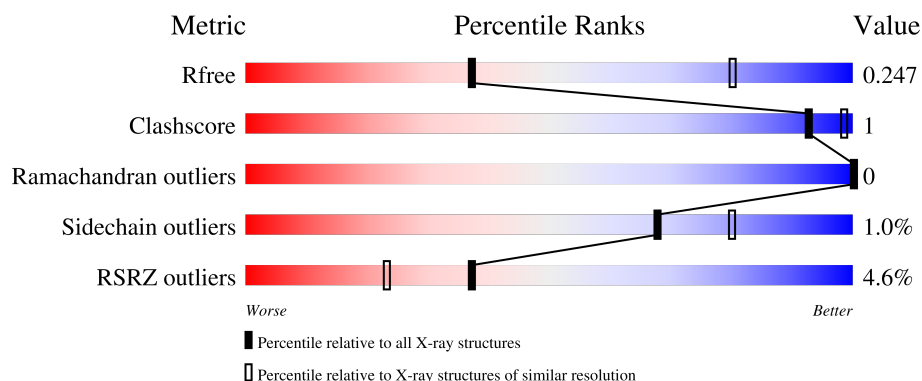
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	547	2% 91% • • •
1	B	547	% 91% • •
1	C	547	% 91% • •
1	D	547	6% 92% • •
1	E	547	8% 92% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	547	2% 91%5% .
1	G	547	6% 91%. .
1	H	547	% 92%. .
1	I	547	% 92%. .
1	J	547	2% 91%. . .
1	K	547	11% 92%. .
1	L	547	3% 91%. . .
1	M	547	5% 90%5% . .
1	N	547	12% 91%5% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53984 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	B	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	C	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	D	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	E	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	F	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	G	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	CYS	ALA	engineered mutation	UNP P0A6F5

Continued on next page...

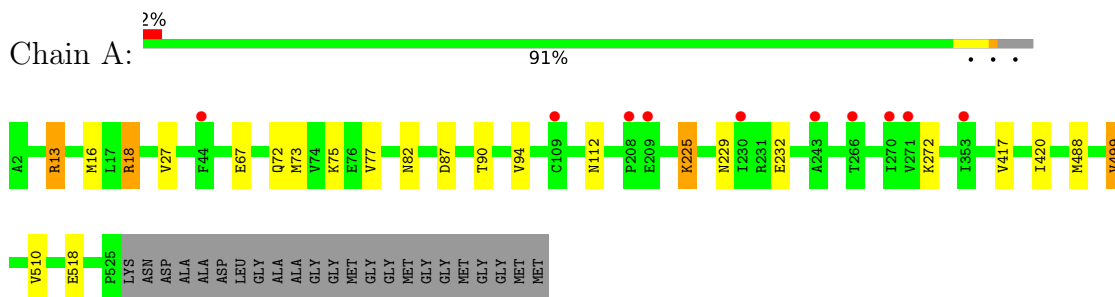
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	CYS	ALA	engineered mutation	UNP P0A6F5
C	109	CYS	ALA	engineered mutation	UNP P0A6F5
D	109	CYS	ALA	engineered mutation	UNP P0A6F5
E	109	CYS	ALA	engineered mutation	UNP P0A6F5
F	109	CYS	ALA	engineered mutation	UNP P0A6F5
G	109	CYS	ALA	engineered mutation	UNP P0A6F5
H	109	CYS	ALA	engineered mutation	UNP P0A6F5
I	109	CYS	ALA	engineered mutation	UNP P0A6F5
J	109	CYS	ALA	engineered mutation	UNP P0A6F5
K	109	CYS	ALA	engineered mutation	UNP P0A6F5
L	109	CYS	ALA	engineered mutation	UNP P0A6F5
M	109	CYS	ALA	engineered mutation	UNP P0A6F5
N	109	CYS	ALA	engineered mutation	UNP P0A6F5

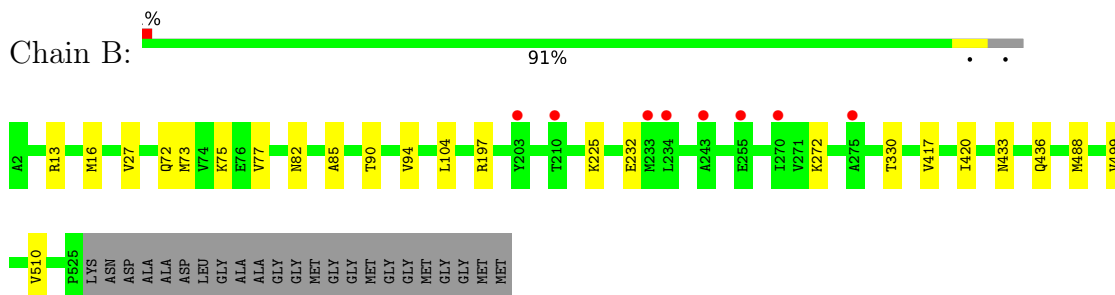
3 Residue-property plots [i](#)

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.

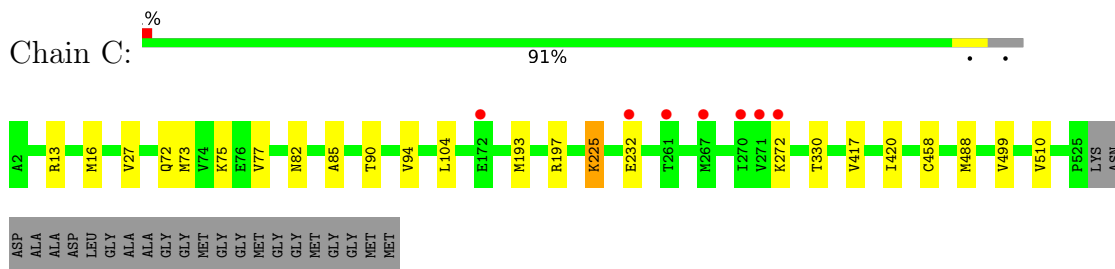
- Molecule 1: 60 kDa chaperonin



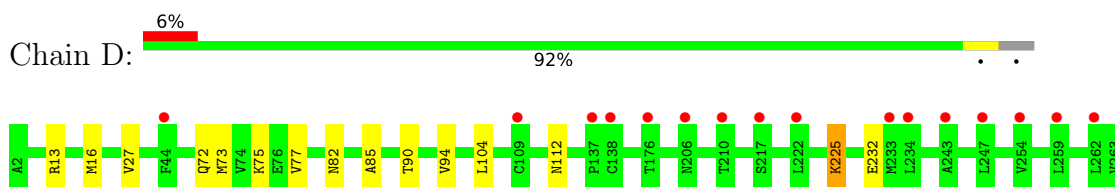
- Molecule 1: 60 kDa chaperonin

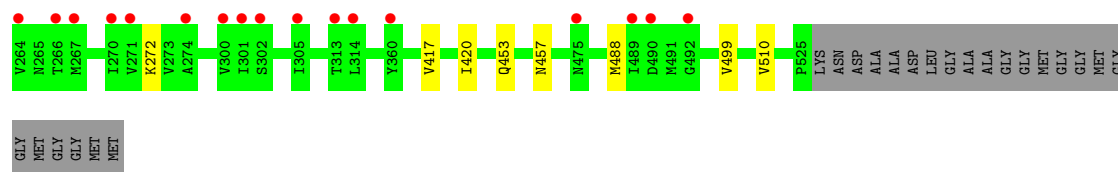


- Molecule 1: 60 kDa chaperonin

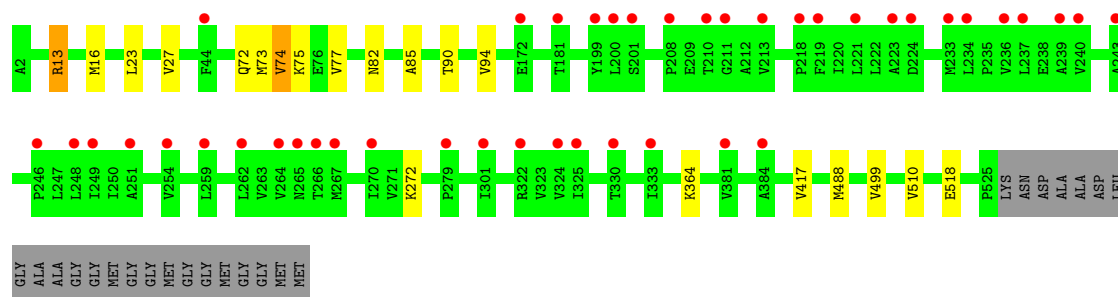


- Molecule 1: 60 kDa chaperonin

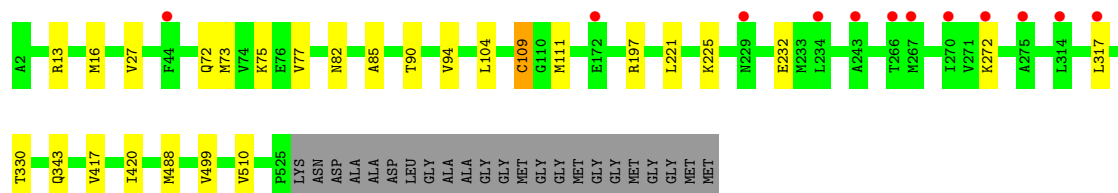




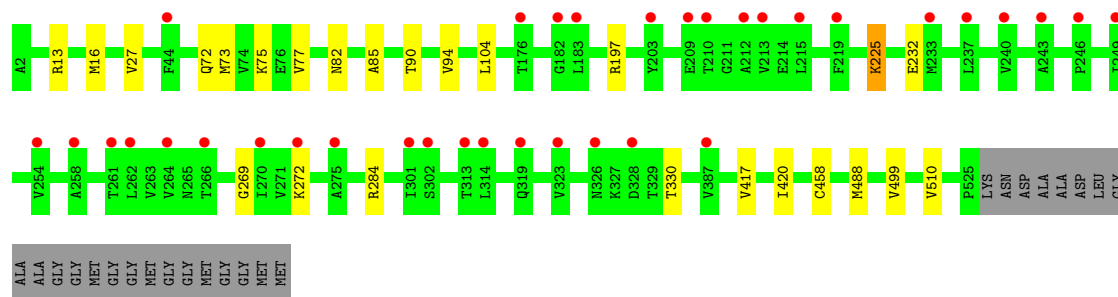
- Molecule 1: 60 kDa chaperonin



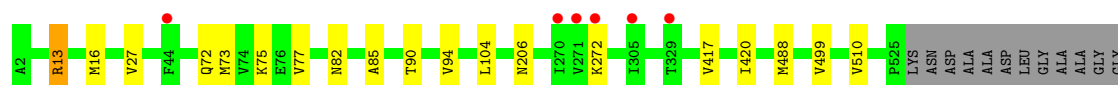
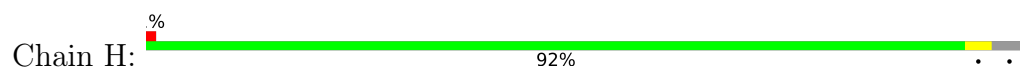
- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin

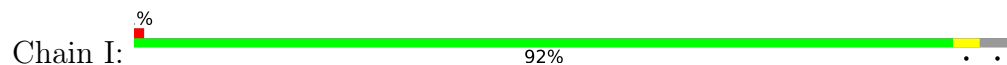


- Molecule 1: 60 kDa chaperonin



MET
GLY
GLY
MET
GLY
GLY
MET
GLY
GLY
MET

- Molecule 1: 60 kDa chaperonin



A2 M16 V27 F44 Q72 M73 V74 K75 E76 V77 N82 A85 T90 V94 M166 D167 T176 K225 E232 P246 V264 M267 K272 V417 I420 M488 V499 V510 P525 LYS ASN ASP ALA ASP LEU GLY MET

ALA
GLY
GLY
MET
GLY
GLY
MET
GLY
MET
MET

- Molecule 1: 60 kDa chaperonin



A2 M16 V27 F44 Q72 M73 V74 K75 E76 V77 N82 A85 T90 V94 M166 D167 T176 K225 E232 P246 V264 M267 K272 V417 I420 M488 V499 V510 P525 LYS ASN ASP ALA ASP LEU GLY MET

I420 M488 V499 V510 P525 LYS ASN ASP ALA ASP LEU GLY MET

- Molecule 1: 60 kDa chaperonin



A2 M16 V27 F44 Q72 M73 V74 K75 E76 V77 N82 A85 T90 V94 M166 D167 T176 K225 E232 P246 V264 M267 K272 V417 I420 M488 V499 V510 P525 LYS ASN ASP ALA ASP LEU GLY MET

E232 M233 V236 L237 V240 P246 L247 L248 I249 D253 V254 L259 L262 V263 M266 M267 I270 V271 K272 V273 A274 A275 P279 G280 F281 M288 T299 V300 I301 I305 L309 T313 L314 E315 D316 L317 G318 D328 T329 T330 T331 I332 V417

I420 M488 V499 V510 P525 LYS ASN ASP ALA ASP LEU GLY MET

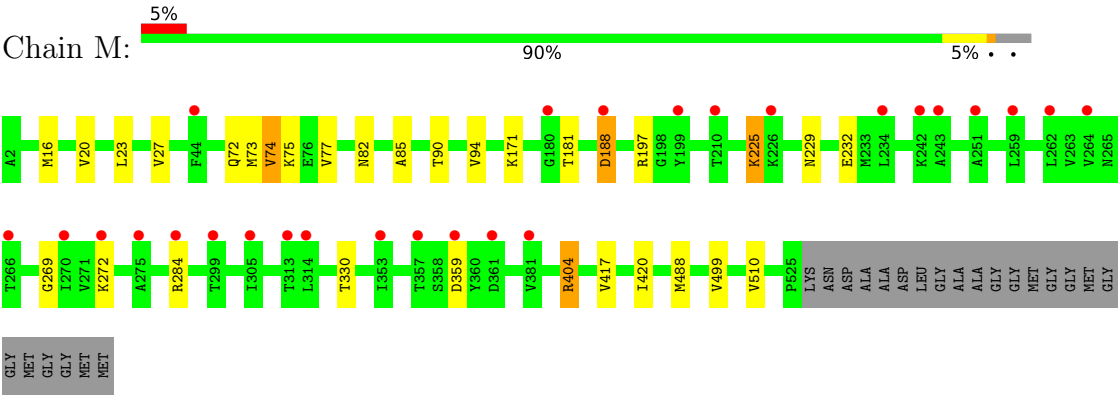
- Molecule 1: 60 kDa chaperonin



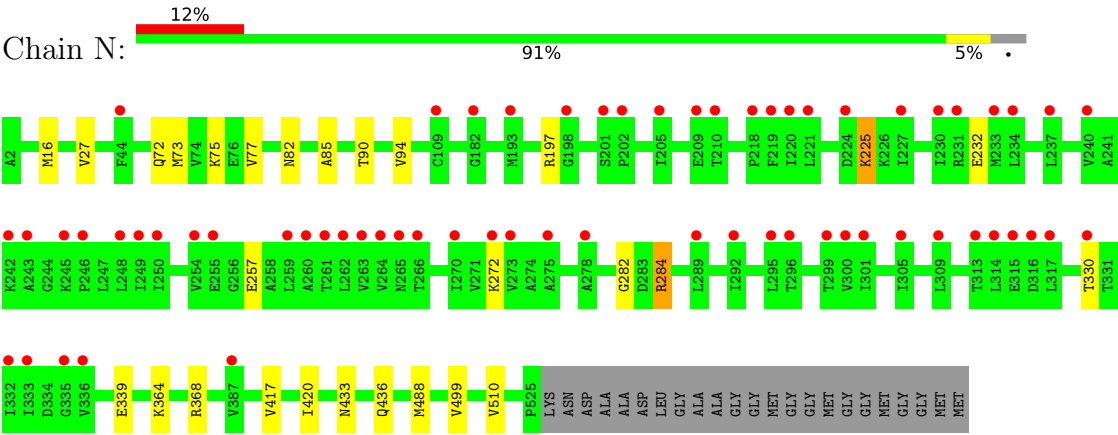
A2 M10 R13 M16 V27 F44 Q72 M73 V74 K75 E76 V77 N82 A85 T90 V94 L104 C109 G110 M111 K171 M193 P218 K225 K226 I227 V233 L234 L237 A243 G244 I250 L259 L262 T266 G269

I270 V271 K272 S302 I305 Y360 Q366 R404 V417 I420 M488 V499 V510 L524 P525 LYS ASN ASP ALA ASP LEU GLY MET

- Molecule 1: 60 kDa chaperonin



● Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.69Å 262.05Å 149.21Å 90.00° 100.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.19 50.00 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-3.19) 99.5 (50.00-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.245 , 0.252 0.240 , 0.247	Depositor DCC
R_{free} test set	8289 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	63.9	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	53984	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/3884	0.74	3/5244 (0.1%)
1	B	0.41	0/3884	0.71	0/5244
1	C	0.41	0/3884	0.71	1/5244 (0.0%)
1	D	0.42	0/3884	0.72	0/5244
1	E	0.41	0/3884	0.72	2/5244 (0.0%)
1	F	0.43	0/3884	0.73	2/5244 (0.0%)
1	G	0.41	0/3884	0.72	1/5244 (0.0%)
1	H	0.41	0/3884	0.72	1/5244 (0.0%)
1	I	0.40	0/3884	0.71	1/5244 (0.0%)
1	J	0.42	1/3884 (0.0%)	0.72	1/5244 (0.0%)
1	K	0.42	0/3884	0.72	1/5244 (0.0%)
1	L	0.44	0/3884	0.75	4/5244 (0.1%)
1	M	0.42	0/3884	0.74	3/5244 (0.1%)
1	N	0.46	3/3884 (0.1%)	0.82	3/5244 (0.1%)
All	All	0.42	4/54376 (0.0%)	0.73	23/73416 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	368	ARG	CD-NE	-7.92	1.35	1.46
1	N	368	ARG	CZ-NH1	-7.04	1.22	1.32
1	J	404	ARG	CA-CB	5.36	1.61	1.53
1	N	368	ARG	CZ-NH2	5.28	1.40	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	368	ARG	NE-CZ-NH2	20.33	137.50	119.20
1	N	368	ARG	NE-CZ-NH1	-19.70	101.80	121.50
1	A	499	VAL	CB-CA-C	-9.85	99.04	112.24
1	M	404	ARG	CG-CD-NE	-7.85	94.73	112.00
1	A	499	VAL	CA-CB-CG2	6.87	122.08	110.40
1	L	193	MET	N-CA-CB	6.80	122.09	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	225	LYS	CB-CA-C	-6.78	99.04	110.43
1	F	232	GLU	CG-CD-OE2	-6.65	103.11	118.40
1	C	193	MET	CG-SD-CE	-6.61	86.36	100.90
1	J	272	LYS	CB-CG-CD	6.59	126.45	111.30
1	L	404	ARG	CG-CD-NE	-6.55	97.59	112.00
1	E	364	LYS	N-CA-CB	6.31	120.06	110.28
1	G	284	ARG	CD-NE-CZ	6.15	133.01	124.40
1	F	232	GLU	CG-CD-OE1	6.05	132.32	118.40
1	E	13	ARG	NE-CZ-NH2	-5.88	113.90	119.20
1	H	13	ARG	NE-CZ-NH2	-5.83	113.95	119.20
1	L	13	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	M	284	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	13	ARG	NE-CZ-NH2	-5.75	114.03	119.20
1	N	284	ARG	CD-NE-CZ	5.52	132.13	124.40
1	K	524	LEU	CB-CA-C	5.51	118.14	109.27
1	M	225	LYS	CG-CD-CE	-5.47	98.71	111.30
1	I	225	LYS	CG-CD-CE	-5.45	98.77	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3975	14	0
1	B	3856	0	3975	11	0
1	C	3856	0	3975	12	0
1	D	3856	0	3975	12	0
1	E	3856	0	3975	8	0
1	F	3856	0	3975	11	0
1	G	3856	0	3975	12	0
1	H	3856	0	3975	9	0
1	I	3856	0	3975	8	1
1	J	3856	0	3975	12	0
1	K	3856	0	3975	12	0
1	L	3856	0	3975	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3856	0	3975	20	1
1	N	3856	0	3975	16	0
All	All	53984	0	55650	160	1

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 1.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:OD1	1:G:269:GLY:O	1.83	0.95
1:L:171:LYS:O	1:L:404:ARG:NH1	2.02	0.93
1:M:171:LYS:O	1:M:404:ARG:NH2	2.07	0.86
1:J:225:LYS:HG2	1:J:226:LYS:N	1.92	0.85
1:M:20:VAL:HG13	1:M:74:VAL:HG21	1.67	0.74
1:A:18:ARG:HH11	1:A:18:ARG:HB2	1.53	0.74
1:E:13:ARG:NH2	1:E:518:GLU:OE2	2.21	0.73
1:A:13:ARG:NH2	1:A:518:GLU:OE2	2.21	0.72
1:M:188:ASP:N	1:M:188:ASP:OD1	2.25	0.70
1:N:284:ARG:HE	1:N:364:LYS:HB3	1.58	0.69
1:K:524:LEU:HG	1:K:525:PRO:HD2	1.81	0.62
1:J:400:LEU:O	1:J:404:ARG:HG2	2.00	0.61
1:M:269:GLY:O	1:N:257:GLU:HG3	2.00	0.60
1:L:269:GLY:O	1:M:229:ASN:OD1	2.18	0.60
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.86	0.58
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.86	0.58
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.86	0.58
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.86	0.58
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.58
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.86	0.58
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.86	0.58
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.58
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.58
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.58
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.86	0.58
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.86	0.57
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.57
1:D:453:GLN:O	1:D:457:ASN:OD1	2.25	0.54
1:J:225:LYS:NZ	1:J:232:GLU:OE1	2.40	0.54
1:N:225:LYS:NZ	1:N:232:GLU:OE1	2.41	0.53
1:C:225:LYS:NZ	1:C:232:GLU:OE1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:LYS:NZ	1:D:232:GLU:OE1	2.41	0.53
1:N:284:ARG:CZ	1:N:364:LYS:HD2	2.39	0.52
1:E:72:GLN:OE1	1:E:75:LYS:HE2	2.10	0.52
1:I:72:GLN:OE1	1:I:75:LYS:HE2	2.10	0.52
1:I:225:LYS:NZ	1:I:232:GLU:OE1	2.39	0.52
1:A:225:LYS:NZ	1:A:232:GLU:OE1	2.41	0.52
1:F:72:GLN:OE1	1:F:75:LYS:HE2	2.10	0.52
1:G:72:GLN:OE1	1:G:75:LYS:HE2	2.10	0.52
1:H:72:GLN:OE1	1:H:75:LYS:HE2	2.10	0.52
1:M:225:LYS:NZ	1:M:232:GLU:OE1	2.39	0.51
1:J:72:GLN:OE1	1:J:75:LYS:HE2	2.10	0.51
1:N:72:GLN:OE1	1:N:75:LYS:HE2	2.10	0.51
1:B:433:ASN:ND2	1:B:436:GLN:OE1	2.44	0.51
1:L:72:GLN:OE1	1:L:75:LYS:HE2	2.10	0.51
1:M:72:GLN:OE1	1:M:75:LYS:HE2	2.10	0.51
1:F:221:LEU:HA	1:F:317:LEU:HD23	1.93	0.51
1:E:23:LEU:HD23	1:E:74:VAL:CG2	2.41	0.51
1:A:72:GLN:OE1	1:A:75:LYS:HE2	2.10	0.51
1:H:206:ASN:HD22	1:H:272:LYS:NZ	2.09	0.51
1:K:72:GLN:OE1	1:K:75:LYS:HE2	2.10	0.51
1:N:433:ASN:ND2	1:N:436:GLN:OE1	2.44	0.51
1:B:72:GLN:OE1	1:B:75:LYS:HE2	2.10	0.50
1:D:72:GLN:OE1	1:D:75:LYS:HE2	2.12	0.50
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.94	0.49
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.94	0.49
1:F:77:VAL:HG21	1:F:510:VAL:HB	1.94	0.49
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.94	0.49
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.94	0.49
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.95	0.49
1:G:77:VAL:HG21	1:G:510:VAL:HB	1.95	0.49
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.95	0.49
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.95	0.49
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.94	0.49
1:B:77:VAL:HG21	1:B:510:VAL:HB	1.94	0.49
1:C:72:GLN:OE1	1:C:75:LYS:HE2	2.12	0.49
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.94	0.49
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.95	0.49
1:C:72:GLN:OE1	1:C:72:GLN:HA	2.13	0.49
1:G:225:LYS:NZ	1:G:232:GLU:OE1	2.41	0.49
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.95	0.49
1:M:23:LEU:HD23	1:M:74:VAL:CG2	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:GLN:OE1	1:D:72:GLN:HA	2.13	0.48
1:M:16:MET:O	1:M:20:VAL:HG23	2.14	0.48
1:C:458:CYS:O	1:D:112:ASN:ND2	2.44	0.48
1:H:13:ARG:HD2	1:H:104:LEU:HD22	1.95	0.48
1:F:109:CYS:SG	1:F:111:MET:HE3	2.54	0.47
1:B:225:LYS:NZ	1:B:232:GLU:OE1	2.44	0.47
1:K:225:LYS:NZ	1:K:232:GLU:OE1	2.44	0.47
1:L:13:ARG:HD2	1:L:104:LEU:HD22	1.95	0.47
1:L:109:CYS:SG	1:L:111:MET:HE3	2.56	0.46
1:A:87:ASP:O	1:A:499:VAL:HG13	2.16	0.45
1:M:20:VAL:CG1	1:M:74:VAL:HG11	2.47	0.45
1:L:16:MET:SD	1:L:73:MET:HE1	2.57	0.45
1:B:16:MET:SD	1:B:73:MET:HE1	2.57	0.45
1:D:16:MET:SD	1:D:73:MET:HE1	2.57	0.45
1:G:16:MET:SD	1:G:73:MET:HE1	2.57	0.45
1:E:16:MET:SD	1:E:73:MET:HE1	2.57	0.45
1:F:16:MET:SD	1:F:73:MET:HE1	2.57	0.45
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.99	0.45
1:K:16:MET:SD	1:K:73:MET:HE1	2.57	0.45
1:J:109:CYS:SG	1:J:111:MET:HE3	2.57	0.45
1:A:16:MET:SD	1:A:73:MET:HE1	2.57	0.45
1:C:16:MET:SD	1:C:73:MET:HE1	2.57	0.45
1:J:16:MET:SD	1:J:73:MET:HE1	2.57	0.44
1:M:16:MET:SD	1:M:73:MET:HE1	2.57	0.44
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.99	0.44
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.99	0.44
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.99	0.44
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.99	0.44
1:N:16:MET:SD	1:N:73:MET:HE1	2.57	0.44
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.99	0.44
1:H:16:MET:SD	1:H:73:MET:HE1	2.57	0.44
1:I:16:MET:SD	1:I:73:MET:HE1	2.57	0.44
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.99	0.44
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.99	0.44
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.99	0.44
1:A:417:VAL:HG21	1:A:488:MET:HG3	1.99	0.44
1:M:20:VAL:HG11	1:M:74:VAL:HG11	2.00	0.44
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.99	0.44
1:D:417:VAL:HG21	1:D:488:MET:HG3	1.99	0.44
1:N:197:ARG:O	1:N:330:THR:OG1	2.34	0.44
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:417:VAL:HG21	1:M:488:MET:HG3	1.99	0.43
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.99	0.43
1:E:417:VAL:HG21	1:E:488:MET:HG3	2.00	0.43
1:F:417:VAL:HG21	1:F:488:MET:HG3	1.99	0.43
1:I:417:VAL:HG21	1:I:488:MET:HG3	1.99	0.43
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.99	0.43
1:B:417:VAL:HG21	1:B:488:MET:HG3	2.00	0.43
1:H:417:VAL:HG21	1:H:488:MET:HG3	1.99	0.43
1:L:417:VAL:HG21	1:L:488:MET:HG3	1.99	0.43
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.99	0.43
1:G:417:VAL:HG21	1:G:488:MET:HG3	1.99	0.43
1:J:417:VAL:HG21	1:J:488:MET:HG3	1.99	0.43
1:K:524:LEU:CG	1:K:525:PRO:HD2	2.48	0.43
1:C:417:VAL:HG21	1:C:488:MET:HG3	1.99	0.43
1:K:197:ARG:O	1:K:330:THR:OG1	2.34	0.42
1:K:417:VAL:HG21	1:K:488:MET:HG3	2.00	0.42
1:C:197:ARG:O	1:C:330:THR:OG1	2.34	0.42
1:N:417:VAL:HG21	1:N:488:MET:HG3	2.00	0.42
1:G:197:ARG:O	1:G:330:THR:OG1	2.34	0.42
1:M:181:THR:HA	1:N:282:GLY:CA	2.49	0.42
1:F:197:ARG:O	1:F:330:THR:OG1	2.34	0.42
1:J:383:ALA:O	1:K:281:PHE:HZ	2.02	0.42
1:B:13:ARG:HD2	1:B:104:LEU:HD22	2.02	0.42
1:B:197:ARG:O	1:B:330:THR:OG1	2.34	0.42
1:G:13:ARG:HD2	1:G:104:LEU:HD22	2.02	0.42
1:A:112:ASN:ND2	1:G:458:CYS:O	2.49	0.41
1:C:13:ARG:HD2	1:C:104:LEU:HD22	2.02	0.41
1:D:13:ARG:HD2	1:D:104:LEU:HD22	2.02	0.41
1:C:417:VAL:HA	1:C:420:ILE:HG22	2.03	0.41
1:D:417:VAL:HA	1:D:420:ILE:HG22	2.03	0.41
1:F:417:VAL:HA	1:F:420:ILE:HG22	2.03	0.41
1:B:417:VAL:HA	1:B:420:ILE:HG22	2.03	0.41
1:G:417:VAL:HA	1:G:420:ILE:HG22	2.03	0.41
1:J:417:VAL:HA	1:J:420:ILE:HG22	2.03	0.41
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.03	0.41
1:M:417:VAL:HA	1:M:420:ILE:HG22	2.03	0.41
1:N:417:VAL:HA	1:N:420:ILE:HG22	2.03	0.41
1:F:13:ARG:HD2	1:F:104:LEU:HD22	2.02	0.41
1:L:417:VAL:HA	1:L:420:ILE:HG22	2.03	0.41
1:M:197:ARG:O	1:M:330:THR:OG1	2.34	0.41
1:I:417:VAL:HA	1:I:420:ILE:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:181:THR:HA	1:N:282:GLY:HA3	2.03	0.41
1:A:18:ARG:CD	1:A:67:GLU:OE2	2.69	0.40
1:A:417:VAL:HA	1:A:420:ILE:HG22	2.03	0.40
1:A:18:ARG:HB2	1:A:18:ARG:NH1	2.26	0.40
1:H:417:VAL:HA	1:H:420:ILE:HG22	2.03	0.40
1:N:284:ARG:NE	1:N:364:LYS:HB3	2.32	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:MET:O	1:M:359:ASP:OD2[1_455]	2.09	0.11

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	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	B	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	C	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	D	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	E	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	F	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	G	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	H	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	I	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	J	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	K	522/547 (95%)	516 (99%)	6 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	M	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	N	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
All	All	7308/7658 (95%)	7224 (99%)	84 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	405/415 (98%)	400 (99%)	5 (1%)	63	79
1	B	405/415 (98%)	402 (99%)	3 (1%)	76	83
1	C	405/415 (98%)	401 (99%)	4 (1%)	68	80
1	D	405/415 (98%)	401 (99%)	4 (1%)	68	80
1	E	405/415 (98%)	401 (99%)	4 (1%)	68	80
1	F	405/415 (98%)	399 (98%)	6 (2%)	57	76
1	G	405/415 (98%)	401 (99%)	4 (1%)	68	80
1	H	405/415 (98%)	403 (100%)	2 (0%)	81	85
1	I	405/415 (98%)	402 (99%)	3 (1%)	76	83
1	J	405/415 (98%)	401 (99%)	4 (1%)	68	80
1	K	405/415 (98%)	402 (99%)	3 (1%)	76	83
1	L	405/415 (98%)	399 (98%)	6 (2%)	57	76
1	M	405/415 (98%)	400 (99%)	5 (1%)	63	79
1	N	405/415 (98%)	400 (99%)	5 (1%)	63	79
All	All	5670/5810 (98%)	5612 (99%)	58 (1%)	68	80

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	82	ASN
1	A	94	VAL
1	A	225	LYS
1	A	272	LYS
1	B	82	ASN
1	B	94	VAL
1	B	272	LYS
1	C	82	ASN
1	C	94	VAL
1	C	225	LYS
1	C	272	LYS
1	D	82	ASN
1	D	94	VAL
1	D	225	LYS
1	D	272	LYS
1	E	74	VAL
1	E	82	ASN
1	E	94	VAL
1	E	272	LYS
1	F	82	ASN
1	F	94	VAL
1	F	109	CYS
1	F	225	LYS
1	F	272	LYS
1	F	343	GLN
1	G	82	ASN
1	G	94	VAL
1	G	225	LYS
1	G	272	LYS
1	H	82	ASN
1	H	94	VAL
1	I	82	ASN
1	I	94	VAL
1	I	272	LYS
1	J	82	ASN
1	J	94	VAL
1	J	109	CYS
1	J	225	LYS
1	K	82	ASN
1	K	94	VAL
1	K	272	LYS
1	L	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	94	VAL
1	L	109	CYS
1	L	272	LYS
1	L	366	GLN
1	L	524	LEU
1	M	74	VAL
1	M	82	ASN
1	M	94	VAL
1	M	188	ASP
1	M	272	LYS
1	N	82	ASN
1	N	94	VAL
1	N	225	LYS
1	N	272	LYS
1	N	339	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	97	GLN
1	A	453	GLN
1	B	37	ASN
1	B	453	GLN
1	C	37	ASN
1	C	453	GLN
1	D	37	ASN
1	D	229	ASN
1	D	453	GLN
1	E	37	ASN
1	E	453	GLN
1	F	37	ASN
1	G	453	GLN
1	H	37	ASN
1	H	453	GLN
1	I	37	ASN
1	J	37	ASN
1	J	453	GLN
1	K	37	ASN
1	K	453	GLN
1	L	37	ASN
1	L	366	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	37	ASN
1	M	453	GLN
1	N	37	ASN
1	N	453	GLN

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	524/547 (95%)	0.32	10 (1%) 66 46	35, 67, 147, 180	0
1	B	524/547 (95%)	0.40	8 (1%) 72 52	40, 76, 141, 161	0
1	C	524/547 (95%)	0.25	7 (1%) 75 55	36, 62, 122, 154	0
1	D	524/547 (95%)	0.49	33 (6%) 26 17	34, 71, 146, 176	0
1	E	524/547 (95%)	0.58	43 (8%) 17 11	37, 83, 158, 189	0
1	F	524/547 (95%)	0.32	12 (2%) 61 41	37, 64, 133, 176	0
1	G	524/547 (95%)	0.50	35 (6%) 24 15	39, 80, 145, 177	0
1	H	524/547 (95%)	0.29	6 (1%) 78 61	41, 77, 125, 147	0
1	I	524/547 (95%)	0.38	6 (1%) 78 61	40, 74, 134, 162	0
1	J	524/547 (95%)	0.42	12 (2%) 61 41	45, 84, 137, 158	0
1	K	524/547 (95%)	0.75	58 (11%) 10 7	45, 98, 151, 166	0
1	L	524/547 (95%)	0.49	18 (3%) 48 30	47, 89, 170, 196	0
1	M	524/547 (95%)	0.58	27 (5%) 33 21	42, 79, 160, 199	0
1	N	524/547 (95%)	0.76	64 (12%) 8 6	45, 90, 181, 215	0
All	All	7336/7658 (95%)	0.47	339 (4%) 37 23	34, 74, 149, 215	0

All (339) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	233	MET	6.0
1	E	210	THR	5.7
1	N	233	MET	5.3
1	N	237	LEU	5.0
1	D	489	ILE	4.7
1	K	218	PRO	4.7
1	M	359	ASP	4.5
1	K	317	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	210	THR	4.2
1	N	261	THR	4.2
1	K	44	PHE	4.2
1	N	240	VAL	4.1
1	E	237	LEU	3.8
1	D	492	GLY	3.8
1	D	270	ILE	3.8
1	N	263	VAL	3.7
1	N	317	LEU	3.7
1	E	240	VAL	3.6
1	K	316	ASP	3.6
1	M	251	ALA	3.6
1	K	270	ILE	3.6
1	B	234	LEU	3.6
1	N	301	ILE	3.5
1	K	228	SER	3.5
1	N	264	VAL	3.5
1	K	222	LEU	3.5
1	A	353	ILE	3.5
1	K	210	THR	3.5
1	K	223	ALA	3.5
1	E	259	LEU	3.5
1	G	301	ILE	3.5
1	N	243	ALA	3.4
1	N	314	LEU	3.4
1	N	254	VAL	3.3
1	M	262	LEU	3.3
1	N	234	LEU	3.3
1	N	262	LEU	3.2
1	G	240	VAL	3.2
1	N	300	VAL	3.2
1	N	266	THR	3.2
1	E	246	PRO	3.2
1	E	279	PRO	3.2
1	K	240	VAL	3.2
1	D	490	ASP	3.2
1	M	270	ILE	3.2
1	D	247	LEU	3.2
1	K	215	LEU	3.2
1	L	233	MET	3.1
1	E	270	ILE	3.1
1	K	227	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	316	ASP	3.1
1	E	181	THR	3.1
1	G	261	THR	3.1
1	E	213	VAL	3.1
1	N	273	VAL	3.1
1	K	279	PRO	3.1
1	D	475	ASN	3.0
1	M	284	ARG	3.0
1	G	243	ALA	3.0
1	N	272	LYS	3.0
1	M	353	ILE	3.0
1	N	289	LEU	3.0
1	E	44	PHE	3.0
1	G	237	LEU	2.9
1	E	251	ALA	2.9
1	I	167	ASP	2.9
1	D	137	PRO	2.9
1	J	44	PHE	2.9
1	M	357	THR	2.9
1	N	313	THR	2.9
1	E	325	ILE	2.9
1	G	213	VAL	2.9
1	G	44	PHE	2.9
1	G	275	ALA	2.9
1	M	264	VAL	2.8
1	N	265	ASN	2.8
1	F	234	LEU	2.8
1	M	234	LEU	2.8
1	D	243	ALA	2.8
1	E	333	ILE	2.8
1	G	219	PHE	2.8
1	K	249	ILE	2.8
1	N	246	PRO	2.8
1	D	266	THR	2.8
1	K	254	VAL	2.8
1	K	263	VAL	2.8
1	K	314	LEU	2.8
1	L	259	LEU	2.8
1	N	198	GLY	2.8
1	D	109	CYS	2.8
1	C	272	LYS	2.8
1	H	272	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	218	PRO	2.8
1	K	220	ILE	2.8
1	N	387	VAL	2.8
1	M	243	ALA	2.7
1	D	234	LEU	2.7
1	E	324	VAL	2.7
1	G	246	PRO	2.7
1	N	332	ILE	2.7
1	K	273	VAL	2.7
1	N	202	PRO	2.7
1	E	172	GLU	2.7
1	D	302	SER	2.7
1	K	262	LEU	2.7
1	G	209	GLU	2.7
1	G	302	SER	2.7
1	E	221	LEU	2.7
1	F	314	LEU	2.7
1	K	213	VAL	2.7
1	N	205	ILE	2.6
1	B	255	GLU	2.6
1	D	210	THR	2.6
1	E	264	VAL	2.6
1	L	237	LEU	2.6
1	E	199	TYR	2.6
1	E	330	THR	2.6
1	N	201	SER	2.6
1	F	44	PHE	2.6
1	K	233	MET	2.6
1	G	328	ASP	2.6
1	J	262	LEU	2.6
1	N	259	LEU	2.6
1	L	302	SER	2.6
1	A	44	PHE	2.6
1	H	44	PHE	2.6
1	D	176	THR	2.6
1	G	266	THR	2.6
1	N	210	THR	2.6
1	B	270	ILE	2.6
1	K	43	SER	2.6
1	K	219	PHE	2.6
1	M	44	PHE	2.6
1	L	234	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	212	ALA	2.6
1	G	270	ILE	2.5
1	G	183	LEU	2.5
1	C	270	ILE	2.5
1	F	266	THR	2.5
1	K	176	THR	2.5
1	L	360	TYR	2.5
1	G	319	GLN	2.5
1	F	243	ALA	2.5
1	F	270	ILE	2.5
1	K	301	ILE	2.5
1	K	288	MET	2.5
1	L	44	PHE	2.5
1	L	262	LEU	2.5
1	N	295	LEU	2.5
1	B	275	ALA	2.5
1	E	223	ALA	2.5
1	N	249	ILE	2.5
1	G	233	MET	2.5
1	K	313	THR	2.5
1	G	272	LYS	2.5
1	E	236	VAL	2.5
1	G	254	VAL	2.5
1	D	301	ILE	2.5
1	K	305	ILE	2.5
1	L	270	ILE	2.5
1	N	292	ILE	2.5
1	H	329	THR	2.5
1	M	259	LEU	2.5
1	A	243	ALA	2.4
1	L	305	ILE	2.4
1	K	221	LEU	2.4
1	M	210	THR	2.4
1	K	271	VAL	2.4
1	N	219	PHE	2.4
1	N	248	LEU	2.4
1	L	218	PRO	2.4
1	M	305	ILE	2.4
1	D	305	ILE	2.4
1	N	220	ILE	2.4
1	D	259	LEU	2.4
1	K	309	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	300	VAL	2.4
1	E	381	VAL	2.4
1	G	182	GLY	2.4
1	D	274	ALA	2.4
1	M	275	ALA	2.4
1	G	314	LEU	2.4
1	J	264	VAL	2.4
1	E	211	GLY	2.3
1	N	299	THR	2.3
1	E	384	ALA	2.3
1	J	249	ILE	2.3
1	N	230	ILE	2.3
1	K	328	ASP	2.3
1	G	262	LEU	2.3
1	K	204	PHE	2.3
1	F	172	GLU	2.3
1	G	264	VAL	2.3
1	H	271	VAL	2.3
1	A	266	THR	2.3
1	D	313	THR	2.3
1	L	243	ALA	2.3
1	B	233	MET	2.3
1	D	44	PHE	2.3
1	G	215	LEU	2.3
1	I	44	PHE	2.3
1	K	40	LEU	2.3
1	A	271	VAL	2.3
1	E	254	VAL	2.3
1	N	278	ALA	2.3
1	L	109	CYS	2.3
1	N	109	CYS	2.3
1	D	314	LEU	2.3
1	E	262	LEU	2.3
1	M	314	LEU	2.3
1	G	387	VAL	2.3
1	N	245	LYS	2.3
1	E	208	PRO	2.3
1	H	305	ILE	2.3
1	K	246	PRO	2.3
1	K	318	GLY	2.3
1	K	332	ILE	2.3
1	M	180	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	260	ALA	2.3
1	C	261	THR	2.3
1	K	266	THR	2.3
1	M	313	THR	2.3
1	A	209	GLU	2.3
1	C	172	GLU	2.3
1	N	315	GLU	2.3
1	K	193	MET	2.3
1	M	266	THR	2.3
1	K	217	SER	2.3
1	M	242	LYS	2.3
1	M	381	VAL	2.3
1	N	275	ALA	2.2
1	N	44	PHE	2.2
1	B	203	TYR	2.2
1	K	199	TYR	2.2
1	F	229	ASN	2.2
1	L	10	ASN	2.2
1	M	361	ASP	2.2
1	B	243	ALA	2.2
1	K	201	SER	2.2
1	D	254	VAL	2.2
1	N	250	ILE	2.2
1	D	262	LEU	2.2
1	K	247	LEU	2.2
1	K	259	LEU	2.2
1	K	225	LYS	2.2
1	E	266	THR	2.2
1	N	296	THR	2.2
1	D	271	VAL	2.2
1	C	232	GLU	2.2
1	D	233	MET	2.2
1	N	193	MET	2.2
1	J	246	PRO	2.2
1	B	210	THR	2.2
1	N	330	THR	2.2
1	N	305	ILE	2.2
1	J	237	LEU	2.2
1	E	267	MET	2.2
1	E	243	ALA	2.2
1	K	253	ASP	2.2
1	M	188	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	203	TYR	2.1
1	E	301	ILE	2.1
1	C	267	MET	2.1
1	J	278	ALA	2.1
1	N	209	GLU	2.1
1	L	244	GLY	2.1
1	E	224	ASP	2.1
1	N	224	ASP	2.1
1	D	264	VAL	2.1
1	G	313	THR	2.1
1	D	360	TYR	2.1
1	E	249	ILE	2.1
1	G	249	ILE	2.1
1	H	270	ILE	2.1
1	N	333	ILE	2.1
1	E	234	LEU	2.1
1	N	221	LEU	2.1
1	E	201	SER	2.1
1	N	182	GLY	2.1
1	G	326	ASN	2.1
1	A	109	CYS	2.1
1	K	236	VAL	2.1
1	A	270	ILE	2.1
1	I	176	THR	2.1
1	J	270	ILE	2.1
1	K	330	THR	2.1
1	L	266	THR	2.1
1	D	267	MET	2.1
1	F	267	MET	2.1
1	I	267	MET	2.1
1	K	275	ALA	2.1
1	A	208	PRO	2.1
1	C	271	VAL	2.1
1	K	237	LEU	2.1
1	L	250	ILE	2.1
1	E	239	ALA	2.1
1	G	258	ALA	2.1
1	J	319	GLN	2.1
1	K	208	PRO	2.1
1	F	272	LYS	2.1
1	E	248	LEU	2.1
1	M	199	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	218	PRO	2.1
1	K	74	VAL	2.0
1	M	226	LYS	2.0
1	D	206	ASN	2.0
1	E	265	ASN	2.0
1	N	231	ARG	2.0
1	N	270	ILE	2.0
1	J	233	MET	2.0
1	G	176	THR	2.0
1	K	224	ASP	2.0
1	K	299	THR	2.0
1	M	299	THR	2.0
1	D	138	CYS	2.0
1	E	219	PHE	2.0
1	I	264	VAL	2.0
1	J	271	VAL	2.0
1	D	222	LEU	2.0
1	E	200	LEU	2.0
1	E	322	ARG	2.0
1	J	247	LEU	2.0
1	K	524	LEU	2.0
1	N	309	LEU	2.0
1	D	217	SER	2.0
1	K	267	MET	2.0
1	F	275	ALA	2.0
1	G	212	ALA	2.0
1	N	335	GLY	2.0
1	I	246	PRO	2.0
1	M	272	LYS	2.0
1	N	242	LYS	2.0
1	G	323	VAL	2.0
1	N	255	GLU	2.0
1	N	336	VAL	2.0
1	F	317	LEU	2.0
1	A	230	ILE	2.0
1	L	227	ILE	2.0
1	N	227	ILE	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 [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.