



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:58 PM UTC

PDB ID : 2JHV / pdb_00002j hv
Title : CRYSTAL STRUCTURE OF RHOGDI E154A,E155A MUTANT
Authors : Cooper, D.R.; Pinkowska, M.; Derewenda, Z.S.
Deposited on : 2007-02-23
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

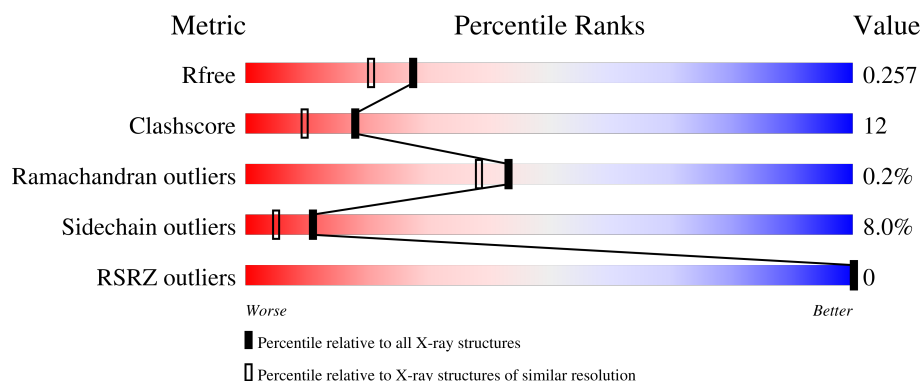
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	138	 71% 25% .
1	B	138	 67% 24% 7% .
1	C	138	 68% 29% ..
1	D	138	 68% 26% . .
1	E	138	 65% 29% . .

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Mol	Chain	Length	Quality of chain
1	F	138	58% 33% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7145 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 RHO GDP-DISSOCIATION INHIBITOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1102	707	184	206	5			
1	B	138	Total	C	N	O	S	0	0	0
			1102	707	184	206	5			
1	C	138	Total	C	N	O	S	0	0	0
			1102	707	184	206	5			
1	D	138	Total	C	N	O	S	0	0	0
			1102	707	184	206	5			
1	E	138	Total	C	N	O	S	0	0	0
			1102	707	184	206	5			
1	F	138	Total	C	N	O	S	0	0	0
			1102	707	184	206	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	ALA	GLU	engineered mutation	UNP P52565
A	155	ALA	GLU	engineered mutation	UNP P52565
B	154	ALA	GLU	engineered mutation	UNP P52565
B	155	ALA	GLU	engineered mutation	UNP P52565
C	154	ALA	GLU	engineered mutation	UNP P52565
C	155	ALA	GLU	engineered mutation	UNP P52565
D	154	ALA	GLU	engineered mutation	UNP P52565
D	155	ALA	GLU	engineered mutation	UNP P52565
E	154	ALA	GLU	engineered mutation	UNP P52565
E	155	ALA	GLU	engineered mutation	UNP P52565
F	154	ALA	GLU	engineered mutation	UNP P52565
F	155	ALA	GLU	engineered mutation	UNP P52565

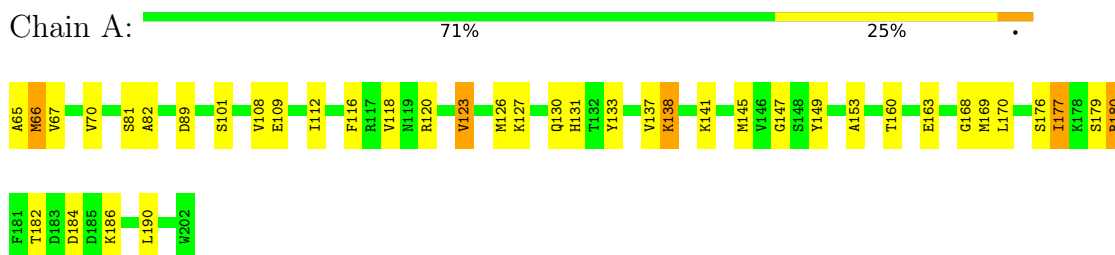
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total 91	O 91	0	0
2	B	87	Total 87	O 87	0	0
2	C	93	Total 93	O 93	0	0
2	D	84	Total 84	O 84	0	0
2	E	86	Total 86	O 86	0	0
2	F	92	Total 92	O 92	0	0

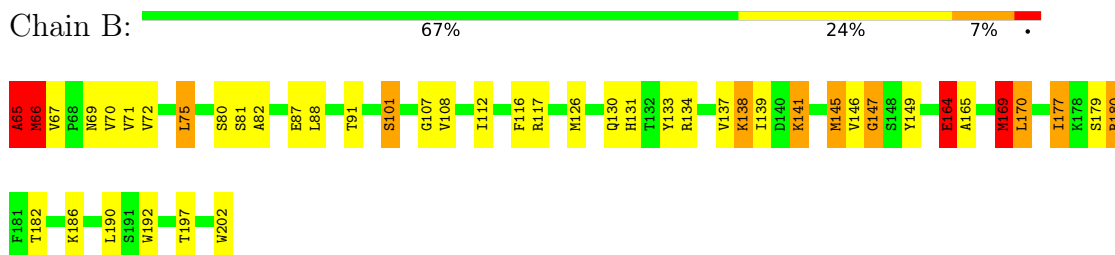
3 Residue-property plots

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.

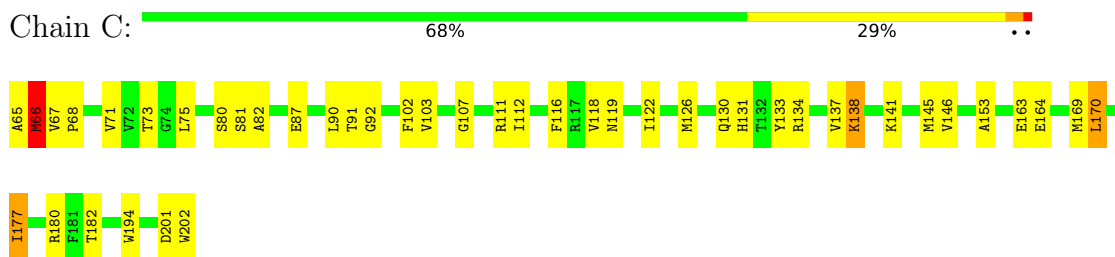
• Molecule 1: RHO GDP-DISSOCIATION INHIBITOR 1



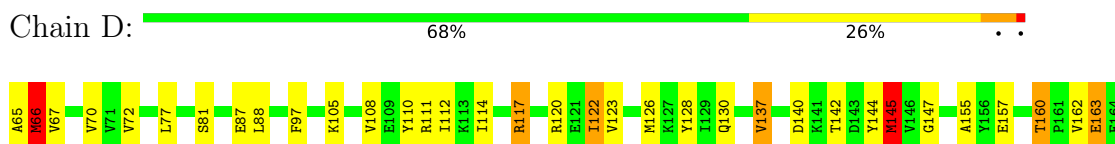
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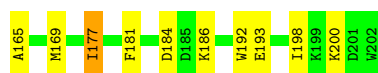


• Molecule 1: RHO GDP-DISSOCIATION INHIBITOR 1



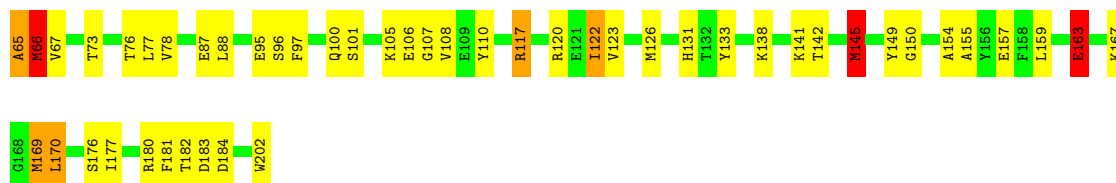
• Molecule 1: RHO GDP-DISSOCIATION INHIBITOR 1





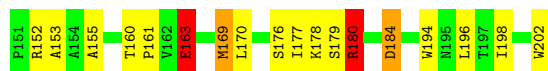
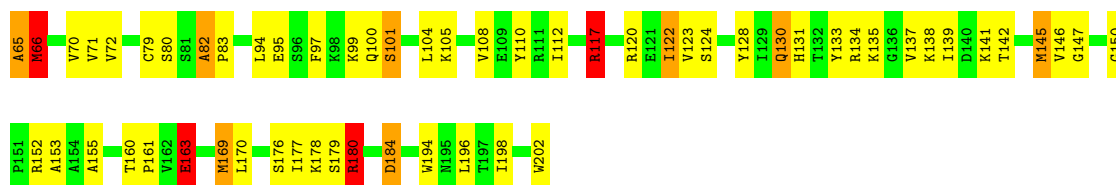
• Molecule 1: RHO GDP-DISSOCIATION INHIBITOR 1

Chain E: 65% 29% . .



• Molecule 1: RHO GDP-DISSOCIATION INHIBITOR 1

Chain F: 58% 33% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.69Å 130.89Å 92.82Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	92.85 – 2.07 92.83 – 2.07	Depositor EDS
% Data completeness (in resolution range)	90.0 (92.85-2.07) 89.8 (92.83-2.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.257 0.214 , 0.257	Depositor DCC
R_{free} test set	1373 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l 0.014 for -k,-h,-l 0.013 for -1/2*h-1/2*k+l,1/2*h+1/2*k+l,-1/2*h+1/2*k 0.010 for -1/2*h-1/2*k-l,1/2*h+1/2*k-l,1/2*h-1/2*k 0.010 for -1/2*h+1/2*k-l,-1/2*h+1/2*k+l,1/2*h+1/2*k 0.007 for -1/2*h+1/2*k+l,-1/2*h+1/2*k-l,-1/2*h-1/2*k 0.408 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.417 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.006 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/2*h+1/2*k 0.015 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2*h-1/2*k 0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7145	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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	1.80	11/1127 (1.0%)	1.44	11/1522 (0.7%)
1	B	1.94	21/1127 (1.9%)	1.52	14/1522 (0.9%)
1	C	1.87	24/1127 (2.1%)	1.41	11/1522 (0.7%)
1	D	2.01	23/1127 (2.0%)	1.51	7/1522 (0.5%)
1	E	1.97	21/1127 (1.9%)	1.50	8/1522 (0.5%)
1	F	2.03	34/1127 (3.0%)	1.51	9/1522 (0.6%)
All	All	1.94	134/6762 (2.0%)	1.48	60/9132 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	MET	CG-SD	12.30	2.11	1.80
1	E	66	MET	CB-CG	11.17	1.85	1.52
1	E	66	MET	CG-SD	11.11	2.08	1.80
1	D	66	MET	CB-CG	10.77	1.84	1.52
1	F	66	MET	CG-SD	10.73	2.07	1.80
1	F	152	ARG	N-CA	-9.15	1.35	1.46
1	F	66	MET	CB-CG	8.98	1.79	1.52
1	B	182	THR	CA-CB	8.95	1.65	1.53
1	F	117	ARG	CG-CD	8.04	1.76	1.52
1	C	103	VAL	CA-CB	8.00	1.63	1.54
1	C	138	LYS	CE-NZ	7.45	1.71	1.49
1	F	123	VAL	CB-CG1	-7.43	1.28	1.52
1	E	155	ALA	CA-CB	7.42	1.66	1.53
1	A	137	VAL	CA-CB	7.05	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	182	THR	CA-CB	6.97	1.63	1.53
1	F	79	CYS	N-CA	-6.94	1.38	1.46
1	C	71	VAL	C-O	-6.88	1.16	1.24
1	D	117	ARG	CG-CD	6.88	1.73	1.52
1	B	80	SER	C-O	-6.85	1.16	1.24
1	E	66	MET	SD-CE	6.81	1.96	1.79
1	E	76	THR	C-O	6.80	1.32	1.24
1	D	181	PHE	C-O	-6.75	1.16	1.24
1	B	117	ARG	CA-C	-6.73	1.44	1.52
1	F	180	ARG	CG-CD	6.68	1.72	1.52
1	C	177	ILE	CA-CB	-6.66	1.46	1.54
1	E	78	VAL	CA-C	6.58	1.60	1.52
1	E	145	MET	CG-SD	6.57	1.97	1.80
1	F	153	ALA	CA-CB	6.53	1.63	1.53
1	D	163	GLU	CG-CD	6.49	1.68	1.52
1	D	72	VAL	CA-CB	-6.49	1.46	1.53
1	F	130	GLN	CA-C	-6.47	1.45	1.52
1	A	138	LYS	CE-NZ	6.43	1.68	1.49
1	F	178	LYS	N-CA	-6.32	1.38	1.46
1	C	180	ARG	CZ-NH1	6.32	1.41	1.32
1	B	192	TRP	N-CA	-6.15	1.38	1.46
1	C	194	TRP	C-O	6.06	1.30	1.23
1	F	123	VAL	C-O	6.06	1.30	1.24
1	B	138	LYS	CE-NZ	6.02	1.67	1.49
1	E	155	ALA	CA-C	-6.02	1.45	1.52
1	C	118	VAL	CA-CB	5.99	1.61	1.54
1	D	66	MET	SD-CE	5.97	1.94	1.79
1	F	176	SER	C-O	-5.96	1.17	1.24
1	D	193	GLU	CB-CG	5.93	1.70	1.52
1	E	65	ALA	N-CA	5.89	1.57	1.46
1	F	155	ALA	CA-C	-5.88	1.45	1.52
1	E	117	ARG	C-O	-5.87	1.16	1.24
1	D	114	ILE	N-CA	-5.86	1.39	1.46
1	F	163	GLU	CG-CD	5.83	1.66	1.52
1	A	118	VAL	CA-CB	5.82	1.61	1.54
1	B	180	ARG	CZ-NH1	5.80	1.40	1.32
1	F	124	SER	C-O	-5.79	1.16	1.23
1	F	198	ILE	C-O	-5.77	1.17	1.24
1	B	180	ARG	C-O	-5.77	1.17	1.23
1	E	159	LEU	CG-CD2	-5.72	1.33	1.52
1	D	122	ILE	CA-CB	-5.71	1.48	1.54
1	F	145	MET	CG-SD	5.69	1.95	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	154	ALA	C-O	5.69	1.31	1.23
1	D	70	VAL	N-CA	-5.68	1.39	1.46
1	C	73	THR	CA-CB	5.68	1.62	1.54
1	D	145	MET	CG-SD	5.66	1.94	1.80
1	F	161	PRO	C-O	-5.66	1.17	1.23
1	B	134	ARG	CA-C	-5.65	1.45	1.52
1	C	92	GLY	C-O	5.65	1.29	1.23
1	D	165	ALA	CA-C	5.64	1.59	1.53
1	A	89	ASP	CA-C	5.64	1.59	1.52
1	F	71	VAL	C-O	-5.64	1.18	1.24
1	B	182	THR	C-O	-5.63	1.17	1.24
1	E	150	GLY	CA-C	-5.61	1.43	1.51
1	D	192	TRP	C-O	-5.59	1.16	1.23
1	F	65	ALA	C-O	5.59	1.34	1.23
1	A	67	VAL	CA-C	5.59	1.58	1.52
1	C	141	LYS	CD-CE	5.58	1.69	1.52
1	F	122	ILE	CB-CG1	-5.58	1.42	1.53
1	F	137	VAL	CA-C	-5.56	1.46	1.52
1	A	190	LEU	CA-C	-5.55	1.45	1.52
1	F	150	GLY	C-O	5.47	1.31	1.24
1	C	133	TYR	CA-C	-5.47	1.46	1.52
1	C	111	ARG	C-O	-5.46	1.16	1.23
1	E	122	ILE	CB-CG1	-5.44	1.42	1.53
1	F	82	ALA	C-O	-5.42	1.17	1.24
1	B	139	ILE	N-CA	-5.39	1.41	1.46
1	E	182	THR	CA-CB	5.38	1.62	1.53
1	C	145	MET	CG-SD	5.38	1.94	1.80
1	E	176	SER	C-O	-5.38	1.17	1.23
1	B	164	GLU	CA-C	-5.37	1.46	1.52
1	F	155	ALA	CA-CB	5.37	1.62	1.53
1	F	180	ARG	CD-NE	5.36	1.53	1.46
1	F	72	VAL	CA-CB	-5.35	1.47	1.54
1	D	77	LEU	N-CA	-5.34	1.39	1.46
1	C	141	LYS	CE-NZ	5.32	1.65	1.49
1	B	71	VAL	CA-CB	5.30	1.61	1.54
1	E	122	ILE	CA-CB	-5.30	1.48	1.54
1	E	149	TYR	C-O	-5.30	1.17	1.23
1	B	88	LEU	CG-CD2	5.30	1.70	1.52
1	D	160	THR	N-CA	-5.29	1.36	1.45
1	C	122	ILE	CA-CB	5.29	1.60	1.54
1	D	144	TYR	C-O	-5.29	1.18	1.24
1	D	177	ILE	CG1-CD1	-5.27	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	GLU	CG-CD	5.24	1.65	1.52
1	D	122	ILE	CB-CG1	-5.24	1.43	1.53
1	F	117	ARG	CB-CG	5.23	1.68	1.52
1	F	70	VAL	CA-CB	5.23	1.61	1.54
1	E	163	GLU	CD-OE2	5.22	1.35	1.25
1	A	180	ARG	CZ-NH1	5.21	1.40	1.32
1	F	146	VAL	CA-CB	-5.21	1.48	1.54
1	B	190	LEU	CA-C	-5.21	1.45	1.52
1	C	146	VAL	C-O	-5.20	1.18	1.23
1	B	65	ALA	CA-CB	5.20	1.69	1.52
1	B	146	VAL	C-O	-5.18	1.17	1.23
1	A	123	VAL	CA-CB	-5.17	1.47	1.54
1	C	68	PRO	C-O	5.16	1.29	1.23
1	B	70	VAL	C-O	-5.16	1.18	1.24
1	F	101	SER	C-O	-5.13	1.17	1.23
1	A	180	ARG	CG-CD	5.12	1.67	1.52
1	B	69	ASN	C-O	-5.12	1.18	1.24
1	D	137	VAL	CA-C	-5.12	1.46	1.52
1	D	145	MET	CA-C	5.11	1.59	1.52
1	B	108	VAL	C-O	-5.11	1.17	1.24
1	F	194	TRP	C-O	-5.10	1.17	1.23
1	D	160	THR	CA-CB	5.09	1.60	1.53
1	A	168	GLY	C-O	-5.08	1.17	1.23
1	C	102	PHE	N-CA	-5.08	1.39	1.46
1	F	94	LEU	CA-C	5.07	1.59	1.52
1	C	163	GLU	CG-CD	5.06	1.64	1.52
1	C	134	ARG	C-O	-5.06	1.18	1.24
1	F	66	MET	N-CA	5.05	1.55	1.46
1	B	101	SER	N-CA	-5.05	1.40	1.46
1	C	90	LEU	CA-C	5.03	1.59	1.52
1	C	137	VAL	CA-CB	5.03	1.60	1.54
1	E	77	LEU	CA-C	-5.03	1.46	1.52
1	A	116	PHE	C-O	-5.02	1.17	1.23
1	D	155	ALA	CA-C	-5.01	1.46	1.52
1	E	73	THR	C-O	-5.01	1.17	1.24
1	B	133	TYR	N-CA	-5.01	1.39	1.45

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	MET	CB-CG-SD	11.62	147.58	112.70
1	F	66	MET	CB-CG-SD	10.17	143.21	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	MET	CB-CG-SD	9.82	142.15	112.70
1	F	117	ARG	CG-CD-NE	-9.79	90.46	112.00
1	E	65	ALA	N-CA-C	-8.74	86.52	111.00
1	B	165	ALA	N-CA-C	-7.16	99.89	109.84
1	C	66	MET	CB-CG-SD	-7.09	91.42	112.70
1	A	147	GLY	N-CA-C	6.64	120.22	111.52
1	E	122	ILE	N-CA-CB	-6.56	99.11	110.13
1	C	146	VAL	N-CA-C	-6.41	106.30	111.81
1	D	122	ILE	CA-CB-CG2	6.39	121.36	110.50
1	C	82	ALA	CA-C-N	6.36	126.07	119.64
1	C	82	ALA	C-N-CA	6.36	126.07	119.64
1	E	65	ALA	CA-C-O	-6.32	110.05	120.80
1	A	108	VAL	CB-CA-C	-6.32	102.91	111.63
1	C	91	THR	CA-C-N	6.19	127.94	122.43
1	C	91	THR	C-N-CA	6.19	127.94	122.43
1	C	153	ALA	N-CA-C	6.18	117.68	111.07
1	F	180	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	B	72	VAL	CB-CA-C	6.08	118.19	111.08
1	E	66	MET	CG-SD-CE	5.99	114.07	100.90
1	B	145	MET	N-CA-C	-5.92	99.55	108.96
1	D	66	MET	CG-SD-CE	5.91	113.90	100.90
1	E	107	GLY	N-CA-C	5.88	122.88	115.42
1	B	180	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	A	82	ALA	CA-C-N	5.78	125.48	119.64
1	A	82	ALA	C-N-CA	5.78	125.48	119.64
1	C	180	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	B	82	ALA	CA-C-N	5.72	125.34	119.56
1	B	82	ALA	C-N-CA	5.72	125.34	119.56
1	B	87	GLU	CA-CB-CG	5.72	125.55	114.10
1	D	66	MET	CA-CB-CG	5.70	125.51	114.10
1	A	66	MET	CB-CG-SD	-5.69	95.62	112.70
1	C	119	ASN	N-CA-C	5.64	120.44	113.50
1	A	180	ARG	NE-CZ-NH2	-5.58	114.17	119.20
1	E	66	MET	CA-CB-CG	5.55	125.19	114.10
1	B	91	THR	N-CA-C	-5.54	106.52	113.28
1	F	66	MET	CA-CB-CG	5.53	125.17	114.10
1	A	180	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	F	80	SER	N-CA-C	5.50	118.79	111.75
1	F	184	ASP	N-CA-CB	5.49	120.00	110.39
1	B	186	LYS	CA-C-N	5.46	128.59	120.95
1	B	186	LYS	C-N-CA	5.46	128.59	120.95
1	C	141	LYS	CD-CE-NZ	5.45	129.34	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	ASP	N-CA-C	5.41	117.21	109.14
1	A	153	ALA	N-CA-C	5.38	116.82	111.07
1	B	169	MET	CG-SD-CE	5.34	112.65	100.90
1	A	184	ASP	CB-CA-C	5.32	121.02	110.17
1	E	184	ASP	CB-CA-C	5.28	120.45	109.95
1	D	184	ASP	N-CA-CB	5.23	118.93	110.40
1	D	163	GLU	CB-CA-C	5.23	120.66	110.30
1	B	117	ARG	CG-CD-NE	-5.16	100.65	112.00
1	D	162	VAL	CB-CA-C	-5.11	103.27	111.59
1	F	122	ILE	CA-CB-CG2	5.08	119.14	110.50
1	B	147	GLY	CA-C-N	5.06	129.70	122.72
1	B	147	GLY	C-N-CA	5.06	129.70	122.72
1	A	160	THR	CA-C-N	-5.05	114.51	119.92
1	A	160	THR	C-N-CA	-5.05	114.51	119.92
1	F	150	GLY	CA-C-N	-5.01	114.79	119.85
1	F	150	GLY	C-N-CA	-5.01	114.79	119.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	65	ALA	Peptide
1	B	66	MET	Peptide

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	1102	0	1107	18	0
1	B	1102	0	1107	25	0
1	C	1102	0	1107	16	0
1	D	1102	0	1107	31	0
1	E	1102	0	1107	30	0
1	F	1102	0	1107	42	1
2	A	91	0	0	4	0
2	B	87	0	0	4	0
2	C	93	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	84	0	0	7	0
2	E	86	0	0	9	1
2	F	92	0	0	11	0
All	All	7145	0	6642	161	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 12.

All (161) 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:F:117:ARG:CD	1:F:117:ARG:CG	1.76	1.60
1:F:66:MET:CB	1:F:66:MET:CG	1.79	1.59
1:A:138:LYS:CE	1:A:138:LYS:NZ	1.68	1.52
1:E:66:MET:CB	1:E:66:MET:CG	1.86	1.52
1:D:66:MET:CB	1:D:66:MET:CG	1.84	1.51
1:C:138:LYS:CE	1:C:138:LYS:NZ	1.71	1.49
1:F:66:MET:CG	1:F:66:MET:SD	2.07	1.42
1:E:66:MET:CG	1:E:66:MET:SD	2.08	1.41
1:D:66:MET:CG	1:D:66:MET:SD	2.11	1.39
1:D:65:ALA:HB1	1:D:66:MET:C	1.47	1.38
1:F:65:ALA:HB1	1:F:66:MET:C	1.62	1.24
1:F:65:ALA:HB1	1:F:66:MET:CA	1.72	1.19
1:E:65:ALA:N	2:E:2001:HOH:O	1.84	1.11
1:F:65:ALA:CB	1:F:66:MET:HA	1.84	1.07
1:F:120:ARG:NE	2:F:2035:HOH:O	1.87	1.05
1:F:65:ALA:HB1	1:F:66:MET:HA	1.39	1.02
1:B:116:PHE:CE2	1:B:126:MET:HE1	1.96	1.01
1:E:66:MET:HB2	2:E:2002:HOH:O	1.58	1.01
1:F:65:ALA:CB	1:F:66:MET:CA	2.40	0.98
1:D:66:MET:HB2	2:D:2004:HOH:O	1.61	0.98
1:F:117:ARG:CG	1:F:117:ARG:NE	2.27	0.97
1:F:66:MET:HB2	2:F:2004:HOH:O	1.62	0.96
1:B:65:ALA:HB1	1:B:66:MET:HA	1.45	0.96
1:D:65:ALA:HB1	1:D:66:MET:CA	1.97	0.93
1:E:126:MET:HE2	1:E:181:PHE:CE1	2.05	0.91
1:E:169:MET:HE2	1:E:170:LEU:HD13	1.52	0.91
1:E:126:MET:CE	1:E:181:PHE:CE1	2.55	0.89
1:F:120:ARG:NH2	2:F:2035:HOH:O	2.03	0.88
1:E:67:VAL:O	1:E:120:ARG:NH2	2.07	0.87
1:A:131:HIS:HD2	2:A:2081:HOH:O	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:HE2	1:B:170:LEU:HA	1.56	0.86
1:D:67:VAL:O	1:D:120:ARG:NH2	2.08	0.86
1:C:131:HIS:HD2	2:C:2087:HOH:O	1.58	0.85
1:D:65:ALA:CB	1:D:66:MET:C	2.42	0.85
1:D:65:ALA:CB	1:D:66:MET:CA	2.56	0.84
1:B:66:MET:SD	2:F:2053:HOH:O	2.38	0.81
1:F:202:TRP:C	2:F:2091:HOH:O	2.23	0.80
1:F:65:ALA:HA	2:F:2002:HOH:O	1.84	0.77
1:F:65:ALA:O	2:F:2001:HOH:O	2.03	0.77
1:C:65:ALA:HB1	1:C:66:MET:HA	1.67	0.76
1:F:65:ALA:HB3	1:F:66:MET:HA	1.66	0.76
1:C:116:PHE:CE2	1:C:126:MET:HE1	2.21	0.76
1:C:112:ILE:HD13	1:C:130:GLN:HE22	1.51	0.76
1:D:65:ALA:HB1	1:D:66:MET:O	1.85	0.76
1:F:163:GLU:HB3	2:F:2065:HOH:O	1.87	0.74
1:D:65:ALA:CB	1:D:66:MET:HA	2.18	0.73
1:D:65:ALA:HB2	2:D:2001:HOH:O	1.91	0.70
1:F:65:ALA:HB1	1:F:66:MET:O	1.92	0.69
1:F:117:ARG:CG	1:F:117:ARG:CZ	2.72	0.67
1:E:202:TRP:C	2:E:2085:HOH:O	2.37	0.67
1:B:101:SER:HG	1:B:197:THR:HG1	1.37	0.67
1:F:120:ARG:CZ	2:F:2035:HOH:O	2.22	0.67
1:D:65:ALA:HB3	1:D:66:MET:HA	1.78	0.64
1:E:163:GLU:HB3	2:E:2065:HOH:O	1.98	0.64
1:E:169:MET:HE3	2:E:2071:HOH:O	1.97	0.64
1:F:169:MET:HE3	2:F:2071:HOH:O	1.98	0.64
1:B:112:ILE:HD13	1:B:130:GLN:HE22	1.64	0.63
1:B:131:HIS:HD2	2:B:2076:HOH:O	1.81	0.62
1:D:117:ARG:HD2	2:D:2037:HOH:O	2.00	0.62
1:E:66:MET:HG3	1:E:67:VAL:HG23	1.82	0.62
1:D:123:VAL:HG11	1:D:126:MET:SD	2.40	0.62
1:D:128:TYR:OH	1:D:130:GLN:NE2	2.24	0.61
1:B:65:ALA:CB	1:B:66:MET:HA	2.24	0.61
1:D:105:LYS:O	1:D:108:VAL:HG22	1.99	0.61
1:A:131:HIS:CE1	1:A:141:LYS:HG3	2.36	0.61
1:C:169:MET:CE	1:C:170:LEU:HD13	2.31	0.60
1:C:169:MET:HE2	1:C:170:LEU:HD13	1.83	0.59
1:E:126:MET:HE1	1:E:181:PHE:CE1	2.37	0.59
1:D:112:ILE:HD13	1:D:130:GLN:HE22	1.68	0.59
1:E:123:VAL:HG11	1:E:126:MET:SD	2.43	0.59
1:B:131:HIS:CE1	1:B:141:LYS:HG3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:MET:HE2	1:B:170:LEU:CA	2.30	0.58
1:E:110:TYR:CZ	1:E:163:GLU:CG	2.87	0.58
1:E:126:MET:HE2	1:E:181:PHE:CZ	2.39	0.57
1:B:126:MET:HE2	1:B:149:TYR:CD2	2.39	0.57
1:F:104:LEU:HD12	1:F:196:LEU:HD11	1.85	0.57
1:D:65:ALA:HB1	1:D:67:VAL:N	2.12	0.57
1:D:66:MET:CB	1:D:66:MET:HG2	2.22	0.56
1:D:117:ARG:CD	2:D:2037:HOH:O	2.52	0.56
1:A:112:ILE:HD13	1:A:130:GLN:HE22	1.71	0.55
1:A:123:VAL:HG12	1:A:126:MET:HG3	1.88	0.55
1:C:202:TRP:C	2:C:2093:HOH:O	2.50	0.54
1:E:131:HIS:CE1	1:E:141:LYS:HG3	2.42	0.54
1:F:117:ARG:NE	1:F:117:ARG:CB	2.71	0.54
1:F:104:LEU:CD1	1:F:196:LEU:HD11	2.38	0.54
1:C:116:PHE:HE2	1:C:126:MET:HE1	1.70	0.53
1:B:202:TRP:C	2:B:2084:HOH:O	2.52	0.53
1:F:66:MET:CB	1:F:66:MET:HG2	2.19	0.53
1:A:126:MET:CE	1:A:149:TYR:CD2	2.92	0.53
1:F:110:TYR:CZ	1:F:163:GLU:HG3	2.44	0.53
1:B:66:MET:N	2:B:2002:HOH:O	2.40	0.52
1:F:66:MET:CB	1:F:66:MET:HG3	2.19	0.52
1:B:112:ILE:HD13	1:B:130:GLN:NE2	2.25	0.51
1:F:179:SER:C	1:F:180:ARG:HD2	2.36	0.51
1:F:128:TYR:OH	1:F:130:GLN:NE2	2.31	0.51
1:B:116:PHE:HE2	1:B:126:MET:HE1	1.65	0.51
1:A:180:ARG:HD3	2:A:2081:HOH:O	2.11	0.51
1:D:66:MET:CB	1:D:66:MET:HG3	2.22	0.50
1:F:145:MET:HE1	1:F:147:GLY:HA2	1.93	0.49
1:B:116:PHE:CE2	1:B:126:MET:CE	2.83	0.48
1:C:107:GLY:O	1:C:164:GLU:HG2	2.13	0.48
1:F:134:ARG:HG3	1:F:139:ILE:HD13	1.95	0.48
1:A:65:ALA:HB1	1:A:66:MET:HA	1.96	0.47
1:E:133:TYR:CE2	1:E:138:LYS:HB2	2.49	0.47
1:E:117:ARG:NH1	2:E:2032:HOH:O	2.46	0.47
1:E:110:TYR:CZ	1:E:163:GLU:HG3	2.50	0.47
1:B:180:ARG:N	1:B:180:ARG:HD3	2.30	0.47
1:E:117:ARG:HD2	2:E:2033:HOH:O	2.15	0.47
1:D:145:MET:HE1	1:D:147:GLY:HA2	1.98	0.46
1:A:120:ARG:NH2	2:A:2051:HOH:O	2.40	0.46
1:B:138:LYS:NZ	2:B:2057:HOH:O	2.48	0.46
1:A:109:GLU:HA	1:A:163:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:C	1:B:75:LEU:HD23	2.40	0.46
1:F:82:ALA:HA	1:F:83:PRO:HD3	1.87	0.46
1:E:88:LEU:HD22	1:E:97:PHE:CG	2.52	0.45
1:D:140:ASP:OD1	1:D:142:THR:OG1	2.33	0.45
1:E:163:GLU:CB	2:E:2065:HOH:O	2.61	0.45
1:F:131:HIS:CE1	1:F:141:LYS:HG3	2.52	0.45
1:F:145:MET:HE1	2:F:2054:HOH:O	2.17	0.45
1:A:176:SER:C	1:A:177:ILE:HG12	2.38	0.45
1:C:116:PHE:CE2	1:C:126:MET:CE	2.98	0.45
1:B:107:GLY:O	1:B:164:GLU:HG2	2.16	0.45
1:D:110:TYR:CE2	1:D:163:GLU:HG2	2.52	0.45
1:F:133:TYR:CE2	1:F:138:LYS:HB2	2.52	0.45
1:E:145:MET:HE1	2:E:2053:HOH:O	2.16	0.44
1:B:179:SER:C	1:B:180:ARG:HD3	2.43	0.44
1:C:131:HIS:CD2	2:C:2087:HOH:O	2.47	0.44
1:A:70:VAL:CG2	1:A:123:VAL:HG21	2.47	0.44
1:A:112:ILE:HD13	1:A:130:GLN:NE2	2.32	0.44
1:C:112:ILE:HD13	1:C:130:GLN:NE2	2.26	0.44
1:B:126:MET:HB2	1:B:147:GLY:O	2.18	0.43
1:D:120:ARG:HD2	2:D:2040:HOH:O	2.18	0.43
1:E:110:TYR:CZ	1:E:163:GLU:HG2	2.52	0.43
1:B:65:ALA:HA	1:B:67:VAL:C	2.43	0.43
1:C:65:ALA:HA	1:C:67:VAL:N	2.34	0.43
1:A:179:SER:C	1:A:180:ARG:HD2	2.44	0.43
1:E:105:LYS:O	1:E:108:VAL:HG22	2.18	0.43
1:F:105:LYS:O	1:F:108:VAL:HG22	2.19	0.43
1:F:97:PHE:HA	1:F:100:GLN:HG3	2.01	0.43
1:C:65:ALA:CB	1:C:66:MET:HA	2.44	0.42
1:D:110:TYR:CZ	1:D:163:GLU:HG2	2.54	0.42
1:F:112:ILE:H	1:F:160:THR:HG1	1.66	0.42
1:B:177:ILE:HG21	1:B:177:ILE:HD12	1.72	0.42
1:A:133:TYR:CD1	1:A:133:TYR:N	2.88	0.42
1:E:106:GLU:HB2	1:E:167:LYS:HA	2.00	0.42
1:F:180:ARG:HD2	1:F:180:ARG:N	2.34	0.42
1:A:127:LYS:HB3	1:A:182:THR:CG2	2.49	0.42
1:E:66:MET:CB	1:E:66:MET:HG2	2.25	0.42
1:A:127:LYS:HB3	1:A:182:THR:HG22	2.02	0.42
1:F:128:TYR:HE1	1:F:179:SER:HB3	1.85	0.42
1:D:88:LEU:HD22	1:D:97:PHE:CG	2.55	0.41
1:B:137:VAL:HG21	1:D:137:VAL:HG21	2.02	0.41
1:D:111:ARG:HD3	1:D:160:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:PHE:HB3	1:E:100:GLN:OE1	2.20	0.41
1:D:145:MET:HE1	2:D:2056:HOH:O	2.20	0.41
1:C:75:LEU:C	1:C:75:LEU:HD23	2.45	0.41
1:F:65:ALA:CB	1:F:66:MET:C	2.58	0.41
1:E:183:ASP:C	1:E:183:ASP:OD1	2.62	0.40
1:F:110:TYR:CZ	1:F:163:GLU:CG	3.04	0.40
1:A:138:LYS:NZ	2:A:2061:HOH:O	2.53	0.40
1:D:163:GLU:CB	2:D:2069:HOH:O	2.69	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:F:66:MET:CE	2:E:2080:HOH:O[4_555]	1.83	0.37

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	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
1	B	136/138 (99%)	132 (97%)	3 (2%)	1 (1%)	18	10
1	C	136/138 (99%)	132 (97%)	3 (2%)	1 (1%)	18	10
1	D	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
1	E	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
1	F	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
All	All	816/828 (99%)	794 (97%)	20 (2%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	MET
1	B	66	MET

5.3.2 Protein sidechains [i](#)

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	121/121 (100%)	114 (94%)	7 (6%)	18	11
1	B	121/121 (100%)	113 (93%)	8 (7%)	15	8
1	C	121/121 (100%)	117 (97%)	4 (3%)	33	28
1	D	121/121 (100%)	110 (91%)	11 (9%)	9	3
1	E	121/121 (100%)	107 (88%)	14 (12%)	5	1
1	F	121/121 (100%)	107 (88%)	14 (12%)	5	1
All	All	726/726 (100%)	668 (92%)	58 (8%)	11	5

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

Mol	Chain	Res	Type
1	A	81	SER
1	A	101	SER
1	A	145	MET
1	A	169	MET
1	A	170	LEU
1	A	177	ILE
1	A	186	LYS
1	B	75	LEU
1	B	81	SER
1	B	141	LYS
1	B	145	MET
1	B	164	GLU
1	B	169	MET
1	B	170	LEU
1	B	177	ILE
1	C	80	SER
1	C	81	SER

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Mol	Chain	Res	Type
1	C	170	LEU
1	C	177	ILE
1	D	66	MET
1	D	81	SER
1	D	87	GLU
1	D	122	ILE
1	D	145	MET
1	D	157	GLU
1	D	169	MET
1	D	177	ILE
1	D	186	LYS
1	D	198	ILE
1	D	200	LYS
1	E	66	MET
1	E	87	GLU
1	E	95	GLU
1	E	96	SER
1	E	101	SER
1	E	122	ILE
1	E	142	THR
1	E	145	MET
1	E	157	GLU
1	E	163	GLU
1	E	169	MET
1	E	170	LEU
1	E	177	ILE
1	E	180	ARG
1	F	66	MET
1	F	95	GLU
1	F	99	LYS
1	F	101	SER
1	F	117	ARG
1	F	122	ILE
1	F	135	LYS
1	F	142	THR
1	F	163	GLU
1	F	169	MET
1	F	170	LEU
1	F	177	ILE
1	F	180	ARG
1	F	184	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	130	GLN
1	A	131	HIS
1	B	130	GLN
1	B	131	HIS
1	C	130	GLN
1	C	131	HIS
1	D	130	GLN
1	E	130	GLN
1	F	130	GLN
1	F	131	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	138/138 (100%)	-1.34	0 100 100	20, 32, 46, 58	0
1	B	138/138 (100%)	-1.35	0 100 100	21, 32, 43, 52	0
1	C	138/138 (100%)	-1.36	0 100 100	22, 32, 44, 56	0
1	D	138/138 (100%)	-1.33	0 100 100	23, 32, 46, 61	0
1	E	138/138 (100%)	-1.37	0 100 100	25, 33, 47, 61	0
1	F	138/138 (100%)	-1.34	0 100 100	24, 33, 47, 61	0
All	All	828/828 (100%)	-1.35	0 100 100	20, 32, 46, 61	0

There are no RSRZ outliers to report.

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.