



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:52 AM UTC

PDB ID : 1OQS / pdb_00001oqs
Title : Crystal Structure of RV4/RV7 Complex
Authors : Perbandt, M.; Betzel, C.
Deposited on : 2003-03-11
Resolution : 1.90 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

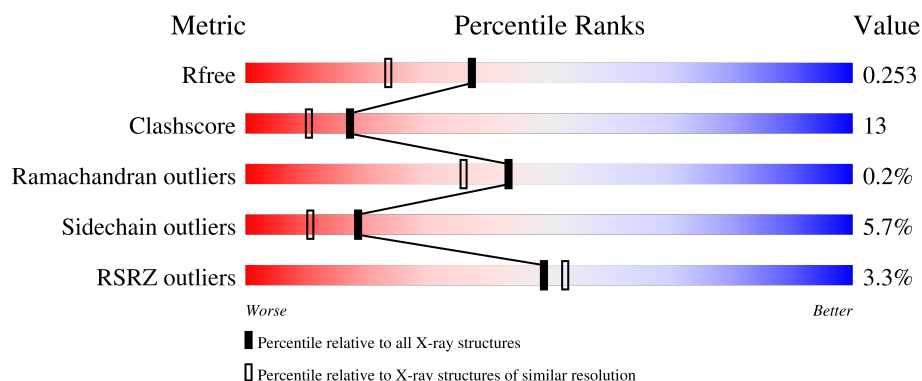
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	122	2% 66% 28% 5% .
1	C	122	2% 68% 23% 7% .
1	E	122	5% 62% 31% 7%
1	G	122	5% 66% 29% . .
2	B	122	5% 74% 23% .

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Mol	Chain	Length	Quality of chain
2	D	122	3% 72% 22% 5%
2	F	122	2% 76% 19% 5%
2	H	122	2% 74% 24%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8012 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 Phospholipase A2 RV-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	4	0	0
			949	581	159	194	15			
1	C	122	Total	C	N	O	S	3	0	0
			949	581	159	194	15			
1	E	122	Total	C	N	O	S	3	0	0
			949	581	159	194	15			
1	G	122	Total	C	N	O	S	0	0	0
			949	581	159	194	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLN	GLU	conflict	UNP P31100
C	11	GLN	GLU	conflict	UNP P31100
E	11	GLN	GLU	conflict	UNP P31100
G	11	GLN	GLU	conflict	UNP P31100

- Molecule 2 is a protein called Phospholipase A2 RV-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	6	3	0
			976	604	184	173	15			
2	D	122	Total	C	N	O	S	3	0	0
			961	596	177	173	15			
2	F	122	Total	C	N	O	S	0	0	0
			961	596	177	173	15			
2	H	122	Total	C	N	O	S	3	0	0
			961	596	177	173	15			

- Molecule 3 is water.

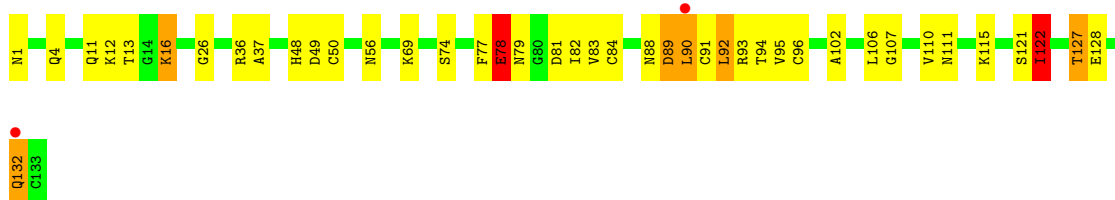
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	52	Total 52	O 52	0	0
3	C	58	Total 58	O 58	0	0
3	D	33	Total 33	O 33	1	0
3	E	39	Total 39	O 39	0	0
3	F	35	Total 35	O 35	0	0
3	G	42	Total 42	O 42	0	0
3	H	48	Total 48	O 48	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

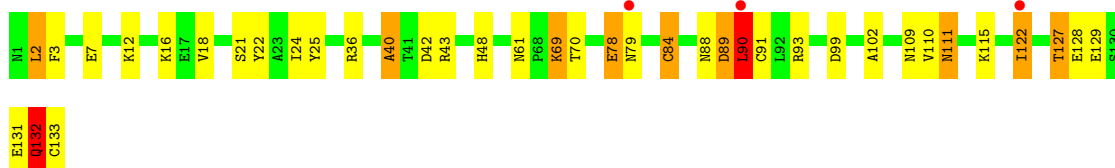
- Molecule 1: Phospholipase A2 RV-7

Chain A: 



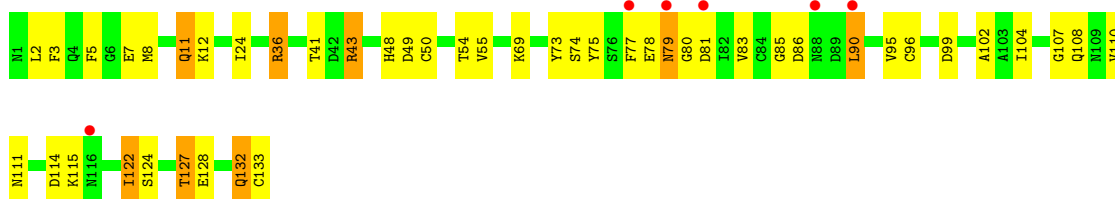
- Molecule 1: Phospholipase A2 RV-7

Chain C: 



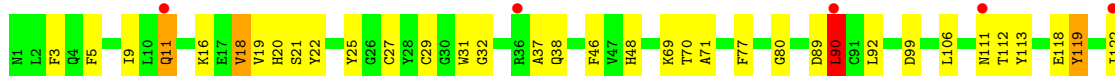
- Molecule 1: Phospholipase A2 RV-7

Chain E: 



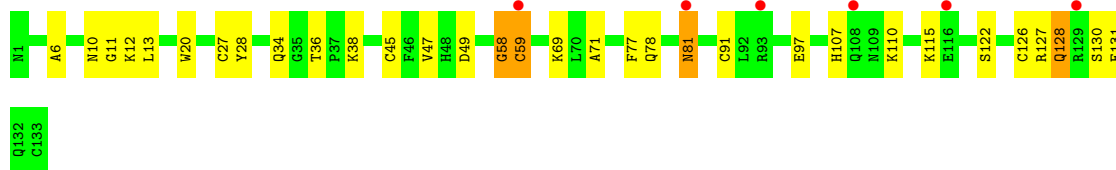
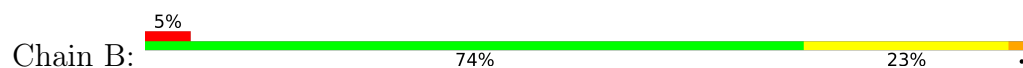
- Molecule 1: Phospholipase A2 RV-7

Chain G: 

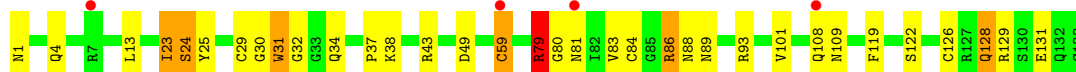
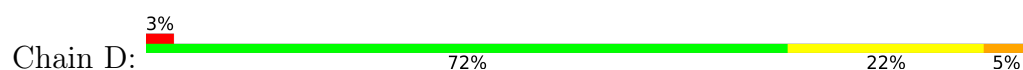




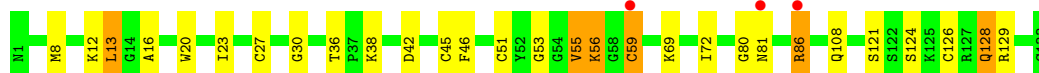
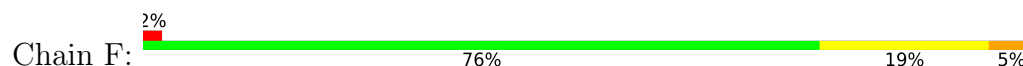
- Molecule 2: Phospholipase A2 RV-4



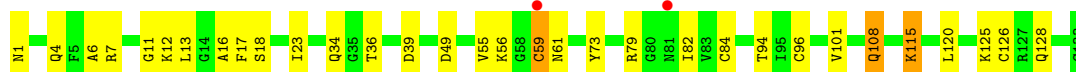
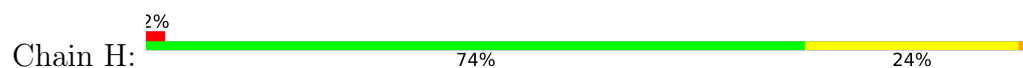
- Molecule 2: Phospholipase A2 RV-4



- Molecule 2: Phospholipase A2 RV-4



- Molecule 2: Phospholipase A2 RV-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.92Å 85.12Å 78.16Å 90.00° 95.10° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 98.1 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.16	Depositor
R, R_{free}	0.222 , 0.284 (Not available) , 0.253	Depositor DCC
R_{free} test set	3805 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.933	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8012	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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	1.60	12/968 (1.2%)	1.59	10/1310 (0.8%)
1	C	1.68	10/968 (1.0%)	1.64	11/1310 (0.8%)
1	E	1.60	8/968 (0.8%)	1.63	18/1310 (1.4%)
1	G	1.59	7/968 (0.7%)	1.54	12/1310 (0.9%)
2	B	1.64	8/1014 (0.8%)	1.51	10/1358 (0.7%)
2	D	1.57	6/983 (0.6%)	1.52	10/1319 (0.8%)
2	F	1.55	7/983 (0.7%)	1.53	9/1319 (0.7%)
2	H	1.62	8/983 (0.8%)	1.49	6/1319 (0.5%)
All	All	1.61	66/7835 (0.8%)	1.56	86/10555 (0.8%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	89	ASN	CB-CG	16.02	1.92	1.52
1	E	8	MET	SD-CE	-11.19	1.51	1.79
1	C	115	LYS	CG-CD	-9.04	1.25	1.52
2	H	39	ASP	C-O	-8.39	1.16	1.24
1	A	132	GLN	CG-CD	6.83	1.69	1.52
1	G	37	ALA	CA-CB	-6.79	1.43	1.53
2	B	115	LYS	CG-CD	6.70	1.72	1.52
1	E	36	ARG	NE-CZ	6.60	1.40	1.33
1	C	111	ASN	C-O	-6.58	1.15	1.24
2	D	23	ILE	CA-CB	6.51	1.62	1.54
1	A	95	VAL	CA-C	6.45	1.60	1.52
2	F	59	CYS	CA-C	6.41	1.60	1.52
1	A	37	ALA	CA-CB	-6.33	1.43	1.53
1	G	132	GLN	CG-CD	6.17	1.67	1.52
2	F	72	ILE	C-O	6.08	1.30	1.24
1	C	122	ILE	CA-CB	6.03	1.62	1.54
2	F	51	CYS	C-O	5.97	1.31	1.24
1	E	24	ILE	CA-CB	5.96	1.61	1.54
1	A	11	GLN	CD-NE2	-5.93	1.20	1.33
2	F	59	CYS	CB-SG	-5.86	1.61	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	84	CYS	C-O	-5.85	1.16	1.24
1	E	102	ALA	N-CA	-5.78	1.38	1.46
1	E	95	VAL	N-CA	-5.78	1.40	1.46
1	A	82	ILE	CG1-CD1	5.76	1.74	1.51
2	B	6	ALA	CA-CB	5.75	1.62	1.53
2	B	6	ALA	N-CA	-5.73	1.39	1.46
2	D	101	VAL	CA-CB	5.66	1.61	1.54
1	C	61	ASN	C-O	-5.53	1.18	1.24
1	A	4	GLN	N-CA	5.45	1.53	1.46
1	A	16	LYS	CA-C	-5.43	1.46	1.52
1	C	132	GLN	CG-CD	5.42	1.65	1.52
2	D	83	VAL	CA-CB	5.42	1.61	1.54
2	H	101	VAL	CA-CB	5.42	1.60	1.54
1	G	18	VAL	C-O	-5.41	1.17	1.24
2	H	6	ALA	CA-CB	5.41	1.61	1.53
1	G	90	LEU	CA-C	5.40	1.59	1.52
1	A	78	GLU	CA-C	-5.39	1.46	1.52
2	F	8	MET	SD-CE	5.38	1.93	1.79
2	H	59	CYS	CA-C	5.37	1.59	1.52
2	B	47	VAL	N-CA	-5.36	1.40	1.46
1	E	128	GLU	N-CA	5.35	1.53	1.45
1	C	25	TYR	C-O	-5.31	1.17	1.23
1	C	90	LEU	CA-C	5.29	1.59	1.52
2	B	122	SER	CA-C	5.27	1.60	1.52
2	H	108	GLN	N-CA	-5.27	1.40	1.46
1	E	132	GLN	CG-CD	5.23	1.65	1.52
1	A	74	SER	CA-C	-5.23	1.46	1.52
2	H	61	ASN	C-O	-5.21	1.18	1.24
1	G	31	TRP	C-O	-5.21	1.17	1.23
2	H	11	GLY	C-O	5.18	1.30	1.23
2	B	78	GLN	C-O	5.17	1.29	1.23
2	B	10	ASN	C-O	5.11	1.30	1.24
1	G	70	THR	CA-CB	5.09	1.61	1.54
1	A	92	LEU	CA-C	-5.08	1.46	1.52
1	C	42	ASP	C-O	-5.08	1.17	1.24
2	H	115	LYS	CG-CD	5.07	1.67	1.52
1	A	50	CYS	N-CA	-5.07	1.40	1.46
2	F	16	ALA	N-CA	-5.07	1.39	1.46
1	E	55	VAL	CA-CB	-5.06	1.48	1.54
2	D	79	ARG	CD-NE	-5.05	1.39	1.46
2	F	46	PHE	CA-C	5.05	1.59	1.52
1	G	119	TYR	CA-C	-5.04	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	45	CYS	C-O	-5.03	1.18	1.24
1	A	96	CYS	C-O	5.02	1.29	1.24
2	D	84	CYS	CA-C	-5.02	1.46	1.52
1	C	40	ALA	C-O	-5.02	1.18	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	LYS	CB-CG-CD	12.79	140.71	111.30
2	F	59	CYS	CB-CA-C	10.02	131.99	110.45
2	H	59	CYS	CB-CA-C	9.21	130.34	110.07
2	F	16	ALA	N-CA-C	-8.25	99.52	110.24
1	G	38	GLN	N-CA-C	8.13	121.25	111.82
1	G	133	CYS	CA-C-O	-8.04	107.14	120.80
1	C	133	CYS	CA-C-O	-8.02	107.17	120.80
1	E	5	PHE	N-CA-C	-7.82	102.83	111.36
1	E	132	GLN	CB-CG-CD	7.77	125.80	112.60
1	A	132	GLN	CB-CG-CD	7.66	125.62	112.60
1	E	115	LYS	CB-CG-CD	7.62	128.82	111.30
2	B	49	ASP	N-CA-C	-7.36	103.34	111.36
2	D	79	ARG	NE-CZ-NH2	-7.27	112.66	119.20
1	E	85	GLY	N-CA-C	7.25	127.28	115.46
2	H	18	SER	N-CA-C	7.16	119.08	111.28
2	D	37	PRO	CA-C-O	-6.97	113.72	121.32
1	C	69	LYS	CD-CE-NZ	-6.94	89.69	111.90
1	C	109	ASN	N-CA-C	6.92	121.81	112.88
1	C	115	LYS	CG-CD-CE	6.92	127.22	111.30
2	B	59	CYS	N-CA-C	6.89	117.13	108.45
1	G	46	PHE	N-CA-C	-6.84	103.75	111.07
1	E	86	ASP	N-CA-C	6.71	119.48	110.35
2	D	109	ASN	N-CA-C	6.68	121.14	112.92
2	B	58	GLY	CA-C-O	6.66	126.42	119.02
1	G	5	PHE	N-CA-C	-6.63	104.06	111.28
2	B	81	ASN	CB-CA-C	6.56	122.26	109.33
1	C	2	LEU	N-CA-C	6.50	118.36	111.28
1	E	11	GLN	N-CA-C	6.41	119.08	111.71
1	A	26	GLY	N-CA-C	6.39	123.44	111.80
1	E	3	PHE	N-CA-C	-6.39	104.40	111.36
1	E	83	VAL	N-CA-C	6.37	117.09	108.17
1	C	132	GLN	CB-CG-CD	6.22	123.17	112.60
1	E	43	ARG	CG-CD-NE	-6.21	98.33	112.00
2	D	59	CYS	N-CA-C	6.14	116.67	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	THR	N-CA-CB	-6.12	101.37	110.61
2	B	115	LYS	CB-CG-CD	-6.11	97.25	111.30
1	A	115	LYS	CB-CG-CD	6.08	125.29	111.30
2	H	115	LYS	CG-CD-CE	6.05	125.21	111.30
2	D	79	ARG	NE-CZ-NH1	5.93	127.44	121.50
1	G	3	PHE	CB-CA-C	-5.93	100.95	110.79
1	E	81	ASP	CA-C-N	-5.89	114.77	122.37
1	E	81	ASP	C-N-CA	-5.89	114.77	122.37
2	D	79	ARG	CG-CD-NE	-5.86	99.10	112.00
2	F	13	LEU	N-CA-C	5.85	120.58	113.38
1	E	79	ASN	CB-CA-C	-5.83	102.20	111.48
1	G	127	THR	N-CA-CB	-5.83	101.52	110.44
1	G	25	TYR	N-CA-C	5.80	118.70	109.24
2	B	91	CYS	N-CA-C	5.78	118.36	111.71
1	A	121	SER	CA-C-N	-5.72	112.29	120.42
1	A	121	SER	C-N-CA	-5.72	112.29	120.42
1	E	127	THR	N-CA-CB	-5.67	102.09	110.49
2	F	55	VAL	CA-C-N	-5.65	114.47	122.94
2	F	55	VAL	C-N-CA	-5.65	114.47	122.94
1	G	29	CYS	N-CA-C	-5.63	105.22	111.36
1	E	115	LYS	CG-CD-CE	5.62	124.24	111.30
1	G	70	THR	OG1-CB-CG2	-5.61	98.08	109.30
1	G	20	HIS	CB-CA-C	-5.53	102.07	111.02
1	E	24	ILE	N-CA-C	5.51	117.50	111.77
1	E	49	ASP	N-CA-C	-5.47	105.31	111.28
2	D	79	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	83	VAL	N-CA-C	5.38	115.60	107.80
2	D	122	SER	N-CA-C	-5.37	104.87	111.75
1	C	90	LEU	N-CA-CB	-5.33	102.29	110.12
1	E	133	CYS	CA-C-O	-5.32	111.76	120.80
1	E	43	ARG	CB-CG-CD	5.30	123.50	111.30
1	C	36	ARG	N-CA-C	5.30	118.26	109.46
2	F	59	CYS	N-CA-CB	-5.29	102.83	111.66
2	F	126	CYS	CA-C-N	-5.29	114.69	122.83
2	F	126	CYS	C-N-CA	-5.29	114.69	122.83
2	D	31	TRP	CA-CB-CG	-5.27	103.59	113.60
1	A	79	ASN	CB-CA-C	-5.25	104.13	111.80
1	G	132	GLN	CB-CG-CD	5.25	121.53	112.60
2	B	28	TYR	CA-C-N	-5.25	113.61	120.95
2	B	28	TYR	C-N-CA	-5.25	113.61	120.95
2	F	80	GLY	N-CA-C	-5.22	108.51	115.40
1	G	16	LYS	N-CA-C	5.21	118.56	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ASN	N-CA-C	5.20	119.61	113.12
2	H	84	CYS	CA-C-N	-5.18	116.12	122.75
2	H	84	CYS	C-N-CA	-5.18	116.12	122.75
1	C	12	LYS	N-CA-C	5.18	119.31	112.89
1	C	70	THR	OG1-CB-CG2	-5.08	99.14	109.30
2	B	71	ALA	CA-C-N	-5.07	116.53	123.12
2	B	71	ALA	C-N-CA	-5.07	116.53	123.12
1	A	122	ILE	CA-CB-CG2	5.06	119.10	110.50
2	H	59	CYS	CA-C-O	-5.06	115.68	121.40
2	D	80	GLY	N-CA-C	-5.05	108.28	115.30

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	949	0	842	27	0
1	C	949	0	842	22	3
1	E	949	0	842	36	7
1	G	949	0	842	35	2
2	B	976	0	921	19	0
2	D	961	0	898	34	3
2	F	961	0	898	20	8
2	H	961	0	898	19	3
3	A	50	0	0	3	0
3	B	52	0	0	3	0
3	C	58	0	0	1	0
3	D	33	0	0	3	0
3	E	39	0	0	5	0
3	F	35	0	0	3	0
3	G	42	0	0	6	0
3	H	48	0	0	1	0
All	All	8012	0	6983	183	13

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 13.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:ARG:HD3	3:E:172:HOH:O	1.23	1.30
1:E:122:ILE:CD1	1:G:124:SER:HB3	1.63	1.27
2:F:81:ASN:HB2	3:F:138:HOH:O	1.10	1.22
1:G:90:LEU:H	1:G:90:LEU:CD2	1.51	1.20
1:E:122:ILE:HD12	1:G:124:SER:HB3	1.21	1.14
1:G:90:LEU:H	1:G:90:LEU:HD23	1.10	1.12
1:E:122:ILE:HD12	1:G:124:SER:CB	1.83	1.08
1:G:111:ASN:HB3	3:G:164:HOH:O	1.52	1.08
1:A:90:LEU:HD23	1:A:90:LEU:H	1.25	1.02
1:E:122:ILE:CD1	1:G:124:SER:CB	2.37	1.01
1:G:111:ASN:CB	3:G:164:HOH:O	2.07	0.99
2:F:55:VAL:O	2:F:56:LYS:HD3	1.66	0.95
2:B:38:LYS:HE2	3:B:165:HOH:O	1.66	0.95
1:E:122:ILE:HD11	1:G:124:SER:HB3	1.46	0.94
2:D:59:CYS:HB2	3:D:144:HOH:O	1.67	0.94
1:E:43:ARG:CD	3:E:172:HOH:O	1.89	0.94
1:C:48:HIS:CD2	1:C:102:ALA:HB2	2.02	0.92
1:G:90:LEU:HD23	1:G:90:LEU:N	1.86	0.91
1:C:48:HIS:HD2	1:C:102:ALA:HB2	1.33	0.89
1:E:90:LEU:HD23	1:E:90:LEU:H	1.39	0.87
1:G:90:LEU:CD2	1:G:90:LEU:N	2.37	0.87
2:D:86:ARG:NH1	2:D:86:ARG:HB3	1.94	0.81
1:A:90:LEU:H	1:A:90:LEU:CD2	1.90	0.81
2:D:86:ARG:NH1	2:D:86:ARG:CB	2.47	0.78
1:E:90:LEU:H	1:E:90:LEU:CD2	1.93	0.77
1:E:104:ILE:HG22	1:E:108:GLN:HE21	1.49	0.77
2:B:107:HIS:O	2:B:110:LYS:HG2	1.86	0.75
2:B:34:GLN:HE22	2:B:127[B]:ARG:HE	1.37	0.73
1:A:88:ASN:O	1:A:89:ASP:C	2.30	0.73
1:E:122:ILE:HG13	1:E:124:SER:N	2.05	0.71
1:C:48:HIS:CD2	1:C:102:ALA:CB	2.73	0.70
1:A:107:GLY:O	2:F:108:GLN:NE2	2.26	0.69
1:C:90:LEU:H	1:C:90:LEU:HD23	1.58	0.69
2:D:86:ARG:CZ	2:D:86:ARG:HB2	2.22	0.69
1:G:9:ILE:HD12	1:G:18:VAL:HG11	1.74	0.68
1:E:104:ILE:CG2	1:E:108:GLN:HE21	2.07	0.67
1:C:16:LYS:HE2	3:C:164:HOH:O	1.94	0.67
1:E:7:GLU:OE1	1:E:75:TYR:OH	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:H	1:C:90:LEU:CD2	1.88	0.66
1:E:122:ILE:CG2	2:F:20:TRP:HZ2	2.09	0.66
1:G:9:ILE:CD1	1:G:18:VAL:HG11	2.26	0.66
1:A:78:GLU:HB2	2:D:129:ARG:NH2	2.12	0.65
2:D:86:ARG:HB3	2:D:86:ARG:HH11	1.59	0.65
2:D:86:ARG:CB	2:D:86:ARG:CZ	2.74	0.65
2:D:108:GLN:CG	1:G:80:GLY:HA2	2.28	0.63
1:E:48:HIS:HE1	1:E:99:ASP:OD1	1.82	0.62
1:E:104:ILE:HG22	1:E:108:GLN:NE2	2.15	0.62
2:B:59:CYS:HB2	3:B:162:HOH:O	2.00	0.62
1:C:90:LEU:HD23	1:C:90:LEU:N	2.15	0.61
1:A:49:ASP:OD1	2:B:69:LYS:NZ	2.33	0.61
1:C:90:LEU:CD2	1:C:90:LEU:N	2.62	0.61
1:G:48:HIS:HE1	1:G:99:ASP:OD1	1.84	0.61
1:G:11:GLN:HG3	1:G:77:PHE:CZ	2.37	0.60
2:D:86:ARG:CB	2:D:86:ARG:HH11	2.13	0.60
2:B:34:GLN:HE22	2:B:127[B]:ARG:NE	1.98	0.59
2:H:108:GLN:OE1	3:H:134:HOH:O	2.16	0.59
1:G:11:GLN:HG3	1:G:77:PHE:CE2	2.37	0.59
1:C:78:GLU:O	1:C:79:ASN:HB2	2.02	0.59
2:F:55:VAL:C	2:F:56:LYS:HD3	2.28	0.58
2:H:36:THR:H	2:H:128:GLN:HE21	1.51	0.58
2:H:12:LYS:CB	2:H:13:LEU:HD12	2.34	0.57
1:A:89:ASP:C	1:A:89:ASP:OD1	2.46	0.57
1:E:114:ASP:OD2	3:E:137:HOH:O	2.18	0.57
1:G:89:ASP:HA	1:G:90:LEU:HD23	1.86	0.56
1:A:90:LEU:HD23	1:A:90:LEU:N	2.09	0.56
1:G:18:VAL:HG13	3:G:172:HOH:O	2.05	0.56
2:H:16:ALA:O	2:H:17:PHE:HB2	2.05	0.56
2:H:120:LEU:HD22	2:H:125:LYS:HG3	1.88	0.56
1:E:48:HIS:HD2	3:E:145:HOH:O	1.89	0.56
2:F:81:ASN:CB	3:F:138:HOH:O	1.90	0.56
2:F:81:ASN:CG	3:F:138:HOH:O	2.30	0.55
1:G:22:TYR:CE1	1:G:106:LEU:HD22	2.42	0.55
1:C:48:HIS:NE2	1:C:99:ASP:HA	2.22	0.55
2:H:34:GLN:HG3	2:H:126:CYS:O	2.06	0.55
2:F:27:CYS:SG	2:F:38:LYS:HE2	2.47	0.55
1:E:11:GLN:HG3	1:E:77:PHE:CE2	2.41	0.54
1:G:19:VAL:HG22	3:G:157:HOH:O	2.06	0.54
2:B:36:THR:H	2:B:128:GLN:NE2	2.05	0.54
1:A:16:LYS:HE2	3:A:152:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:CYS:HB3	2:B:34:GLN:O	2.07	0.54
2:B:36:THR:H	2:B:128:GLN:HE21	1.54	0.54
1:G:128:GLU:OE2	3:G:135:HOH:O	2.19	0.53
1:E:36:ARG:HD2	3:E:167:HOH:O	2.09	0.53
2:D:24:SER:OG	2:D:119:PHE:HA	2.08	0.53
1:A:77:PHE:C	1:A:78:GLU:HG2	2.35	0.52
1:A:89:ASP:OD1	1:A:91:CYS:N	2.40	0.52
1:C:127:THR:CG2	1:C:127:THR:O	2.57	0.52
1:E:122:ILE:HD11	1:G:124:SER:CB	2.23	0.52
1:A:48:HIS:HB2	1:A:102:ALA:HB2	1.92	0.52
1:E:124:SER:O	2:H:7:ARG:NH2	2.43	0.52
2:H:12:LYS:HG2	2:H:82:ILE:HD11	1.92	0.52
1:E:78:GLU:C	1:E:80:GLY:N	2.66	0.52
2:F:128:GLN:NE2	2:F:128:GLN:H	2.07	0.52
2:D:129:ARG:HD2	3:D:161:HOH:O	2.08	0.52
1:G:48:HIS:CE1	1:G:99:ASP:OD1	2.64	0.51
2:B:12[A]:LYS:HB3	2:B:13:LEU:HD12	1.92	0.51
1:C:69:LYS:HE2	2:D:49:ASP:OD2	2.11	0.51
1:A:78:GLU:O	2:D:129:ARG:NH2	2.42	0.51
1:A:49:ASP:CG	2:B:69:LYS:HZ3	2.18	0.51
1:A:88:ASN:O	1:A:90:LEU:N	2.43	0.51
1:A:78:GLU:HB2	2:D:129:ARG:HH22	1.74	0.50
2:F:12:LYS:HB3	2:F:13:LEU:HD12	1.94	0.50
2:B:97:GLU:OE1	3:B:147:HOH:O	2.19	0.49
2:D:43:ARG:NH2	2:D:131:GLU:OE2	2.36	0.49
2:H:16:ALA:O	2:H:17:PHE:CB	2.60	0.49
2:B:58:GLY:O	2:B:59:CYS:HB3	2.13	0.49
1:E:90:LEU:HD23	1:E:90:LEU:N	2.18	0.48
2:F:42:ASP:O	2:F:45:CYS:HB2	2.13	0.48
2:D:25:TYR:HB3	2:D:29:CYS:HB2	1.94	0.48
2:H:12:LYS:HB2	2:H:13:LEU:HD12	1.94	0.48
1:A:12:LYS:HE2	3:A:159:HOH:O	2.13	0.48
1:C:131:GLU:O	1:C:132:GLN:NE2	2.46	0.48
1:E:122:ILE:CG2	2:F:20:TRP:CZ2	2.95	0.48
2:F:23:ILE:O	2:F:30:GLY:HA3	2.13	0.48
2:F:53:GLY:O	2:F:56:LYS:HE2	2.14	0.47
1:C:40:ALA:HA	1:C:43:ARG:NH1	2.29	0.47
2:D:126:CYS:HA	2:D:128:GLN:HE22	1.77	0.47
2:D:128:GLN:NE2	2:D:128:GLN:H	2.13	0.47
1:E:69:LYS:O	1:E:69:LYS:CG	2.62	0.47
1:A:13:THR:HB	1:A:110:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:CYS:HB3	1:A:93:ARG:HD2	1.96	0.46
1:C:84:CYS:HB3	1:C:93:ARG:HD2	1.97	0.46
1:A:122:ILE:HD11	3:A:177:HOH:O	2.14	0.46
2:B:34:GLN:NE2	2:B:127[B]:ARG:HD2	2.31	0.46
1:E:50:CYS:O	1:E:54:THR:HG23	2.15	0.46
2:B:34:GLN:HG3	2:B:126:CYS:O	2.15	0.46
2:D:23:ILE:O	2:D:30:GLY:HA3	2.15	0.46
2:H:13:LEU:HD12	2:H:13:LEU:N	2.32	0.45
2:D:34:GLN:HG3	2:D:126:CYS:O	2.15	0.45
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.65	0.45
1:G:112:THR:O	1:G:113:TYR:C	2.60	0.45
2:F:36:THR:H	2:F:128:GLN:NE2	2.15	0.45
2:D:108:GLN:HG3	1:G:80:GLY:HA2	1.98	0.44
2:D:108:GLN:HE21	1:G:80:GLY:HA2	1.81	0.44
2:H:12:LYS:HB3	2:H:13:LEU:HD12	2.00	0.44
1:G:71:ALA:HB1	1:G:92:LEU:HD23	1.99	0.44
2:H:55:VAL:HG22	2:H:94:THR:CG2	2.48	0.44
2:D:88:ASN:HB2	2:D:93:ARG:HA	1.99	0.44
1:E:2:LEU:HD23	1:E:2:LEU:HA	1.50	0.44
1:A:78:GLU:C	2:D:129:ARG:HH22	2.25	0.44
2:D:108:GLN:HG3	3:G:171:HOH:O	2.18	0.44
2:D:23:ILE:HD13	2:D:23:ILE:HA	1.78	0.43
2:B:97:GLU:O	2:B:97:GLU:HG3	2.14	0.43
1:C:18:VAL:HG23	1:C:22:TYR:HB2	2.00	0.43
1:A:106:LEU:O	1:A:110:VAL:HG13	2.18	0.43
1:C:2:LEU:HD23	1:C:2:LEU:HA	1.87	0.43
1:G:118:GLU:O	1:G:119:TYR:HB2	2.18	0.43
2:H:36:THR:H	2:H:128:GLN:NE2	2.16	0.43
2:H:128:GLN:H	2:H:128:GLN:CD	2.26	0.43
1:C:3:PHE:O	1:C:7:GLU:HG3	2.19	0.43
1:C:21:SER:O	1:C:24:ILE:HG12	2.19	0.43
2:H:1:ASN:OD1	2:H:4:GLN:HG3	2.19	0.42
1:A:78:GLU:CB	2:D:129:ARG:NH2	2.81	0.42
1:A:122:ILE:HG22	2:B:20:TRP:HZ2	1.84	0.42
1:C:89:ASP:OD1	1:C:91:CYS:N	2.53	0.42
1:E:110:VAL:HG23	1:E:111:ASN:N	2.34	0.42
1:E:122:ILE:HG21	2:F:20:TRP:HZ2	1.81	0.42
2:B:11:GLY:HA3	2:B:77:PHE:CZ	2.55	0.42
1:E:73:TYR:CG	1:E:96:CYS:HB2	2.55	0.42
2:H:55:VAL:HG22	2:H:94:THR:HG21	2.02	0.41
2:H:73:TYR:CG	2:H:96:CYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASN:OD1	1:A:1:ASN:C	2.63	0.41
1:E:78:GLU:O	1:E:80:GLY:N	2.53	0.41
1:G:9:ILE:HG21	1:G:18:VAL:HG12	2.02	0.41
1:E:78:GLU:O	1:E:79:ASN:C	2.63	0.41
1:G:27:CYS:O	1:G:32:GLY:HA3	2.21	0.41
1:A:81:ASP:HB2	2:D:129:ARG:HH12	1.86	0.41
2:B:130:SER:O	2:B:131:GLU:C	2.63	0.41
1:C:2:LEU:HB2	2:D:32:GLY:O	2.21	0.41
2:D:1:ASN:OD1	2:D:4:GLN:HG3	2.21	0.41
2:D:38:LYS:HD3	3:D:135:HOH:O	2.20	0.41
2:D:108:GLN:HG2	1:G:80:GLY:HA2	1.99	0.41
1:E:107:GLY:O	1:E:108:GLN:C	2.62	0.41
1:C:128:GLU:O	1:C:129:GLU:C	2.64	0.40
2:F:69:LYS:O	2:F:69:LYS:HD2	2.21	0.40
1:G:69:LYS:HE2	2:H:49:ASP:OD2	2.21	0.40
1:E:122:ILE:HD12	1:G:124:SER:HB2	1.89	0.40
2:F:13:LEU:HD12	2:F:13:LEU:N	2.36	0.40
2:D:128:GLN:H	2:D:128:GLN:CD	2.29	0.40
1:E:122:ILE:CD1	1:G:124:SER:OG	2.68	0.40
2:F:121:SER:C	2:F:124:SER:N	2.79	0.40
2:D:13:LEU:N	2:D:13:LEU:HD12	2.37	0.40
2:F:121:SER:C	2:F:124:SER:H	2.28	0.40

All (13) 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:E:11:GLN:O	2:F:86:ARG:NH1[2_546]	1.14	1.06
1:C:78:GLU:OE1	2:H:79:ARG:NH1[1_655]	1.24	0.96
2:D:86:ARG:NH1	1:G:129:GLU:OE2[2_545]	1.51	0.69
1:E:11:GLN:O	2:F:86:ARG:CZ[2_546]	1.89	0.31
1:E:11:GLN:C	2:F:86:ARG:NH1[2_546]	1.89	0.31
1:E:12:LYS:CA	2:F:86:ARG:NH1[2_546]	1.92	0.28
1:C:78:GLU:OE1	2:H:79:ARG:CZ[1_655]	1.96	0.24
1:E:11:GLN:O	2:F:86:ARG:CD[2_546]	2.01	0.19
1:C:78:GLU:CD	2:H:79:ARG:NH1[1_655]	2.04	0.16
2:D:79:ARG:CD	2:F:53:GLY:O[1_554]	2.04	0.16
2:D:86:ARG:CZ	1:G:129:GLU:OE2[2_545]	2.18	0.02
1:E:11:GLN:O	2:F:86:ARG:NE[2_546]	2.18	0.02
1:E:12:LYS:N	2:F:86:ARG:NH1[2_546]	2.19	0.01

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	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	C	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	E	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	G	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	16	8
2	B	123/122 (101%)	119 (97%)	4 (3%)	0	100	100
2	D	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	8
2	F	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
2	H	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
All	All	963/976 (99%)	923 (96%)	38 (4%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	31	TRP
1	G	21	SER

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	104/104 (100%)	93 (89%)	11 (11%)	6	2
1	C	104/104 (100%)	95 (91%)	9 (9%)	9	4
1	E	104/104 (100%)	98 (94%)	6 (6%)	18	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	104/104 (100%)	99 (95%)	5 (5%)	23	15
2	B	106/103 (103%)	104 (98%)	2 (2%)	50	47
2	D	103/103 (100%)	98 (95%)	5 (5%)	22	14
2	F	103/103 (100%)	98 (95%)	5 (5%)	22	14
2	H	103/103 (100%)	99 (96%)	4 (4%)	28	21
All	All	831/828 (100%)	784 (94%)	47 (6%)	18	11

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	69	LYS
1	A	78	GLU
1	A	89	ASP
1	A	90	LEU
1	A	94	THR
1	A	111	ASN
1	A	122	ILE
1	A	127	THR
1	A	128	GLU
1	A	132	GLN
2	B	81	ASN
2	B	128	GLN
1	C	78	GLU
1	C	88	ASN
1	C	89	ASP
1	C	90	LEU
1	C	110	VAL
1	C	111	ASN
1	C	122	ILE
1	C	127	THR
1	C	132	GLN
2	D	24	SER
2	D	79	ARG
2	D	81	ASN
2	D	86	ARG
2	D	128	GLN
1	E	41	THR
1	E	74	SER
1	E	90	LEU

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Mol	Chain	Res	Type
1	E	122	ILE
1	E	127	THR
1	E	132	GLN
2	F	56	LYS
2	F	59	CYS
2	F	86	ARG
2	F	128	GLN
2	F	129	ARG
1	G	11	GLN
1	G	90	LEU
1	G	122	ILE
1	G	127	THR
1	G	132	GLN
2	H	23	ILE
2	H	56	LYS
2	H	59	CYS
2	H	115	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
2	B	34	GLN
2	B	107	HIS
2	B	111	ASN
2	B	128	GLN
1	C	132	GLN
2	D	128	GLN
1	E	20	HIS
1	E	48	HIS
1	E	108	GLN
1	E	116	ASN
2	F	111	ASN
2	F	128	GLN
1	G	48	HIS
1	G	132	GLN
2	H	111	ASN
2	H	128	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	122/122 (100%)	0.04	2 (1%)	70	74	14, 22, 37, 39	4 (3%)
1	C	122/122 (100%)	0.07	3 (2%)	58	62	15, 22, 32, 41	3 (2%)
1	E	122/122 (100%)	0.37	6 (4%)	35	37	18, 25, 36, 53	2 (1%)
1	G	122/122 (100%)	0.18	6 (4%)	35	37	19, 24, 37, 44	0
2	B	122/122 (100%)	0.11	6 (4%)	35	37	13, 22, 35, 46	6 (4%)
2	D	122/122 (100%)	0.32	4 (3%)	49	52	18, 25, 37, 48	3 (2%)
2	F	122/122 (100%)	0.10	3 (2%)	58	62	15, 24, 39, 52	1 (0%)
2	H	122/122 (100%)	0.00	2 (1%)	70	74	16, 23, 33, 45	3 (2%)
All	All	976/976 (100%)	0.15	32 (3%)	49	52	13, 24, 37, 53	22 (2%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	4.8
1	C	90	LEU	4.4
2	H	59	CYS	4.0
1	E	90	LEU	3.9
2	B	59	CYS	3.5
2	B	108	GLN	3.5
2	D	108	GLN	3.4
1	G	111	ASN	3.4
2	H	81	ASN	3.2
2	B	81	ASN	3.2
1	G	11	GLN	3.2
2	F	59	CYS	3.0
1	G	90	LEU	3.0
1	E	79	ASN	3.0
2	F	86	ARG	2.9
2	B	129	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	122	ILE	2.8
2	D	81	ASN	2.7
1	E	88	ASN	2.7
2	F	81	ASN	2.6
1	E	81	ASP	2.5
1	G	132	GLN	2.4
2	D	59	CYS	2.4
2	B	116	GLU	2.3
1	C	122	ILE	2.3
2	B	93	ARG	2.3
1	A	132	GLN	2.2
1	C	79	ASN	2.2
2	D	7	ARG	2.2
1	G	36	ARG	2.1
1	E	116	ASN	2.0
1	E	77	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.