Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:03 pm BST

PDB ID	:	1OQS
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 following versions of software and data (see references ⓘ) were used in the production of this report:

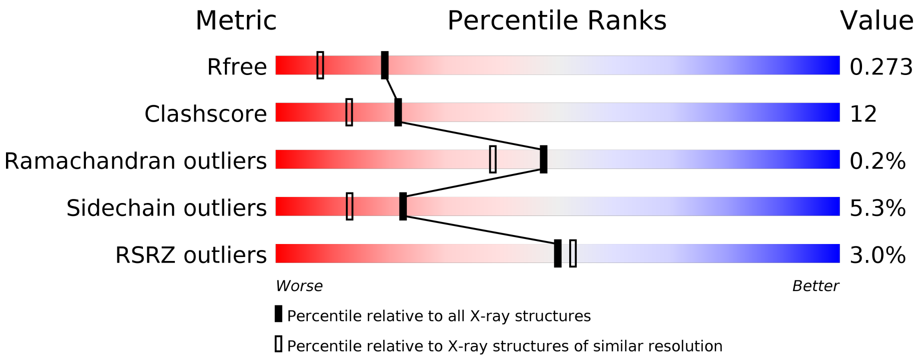
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

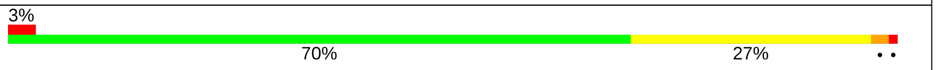
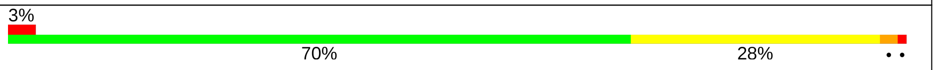
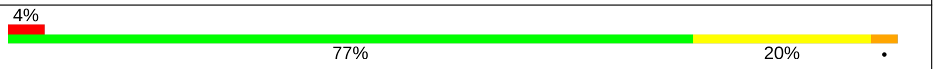
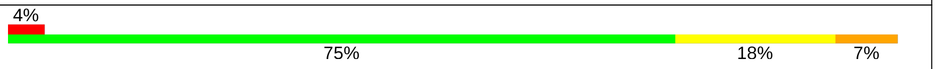
The reported resolution of this entry is 1.90 Å.

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	C	122	
1	E	122	
1	G	122	
2	B	122	
2	D	122	

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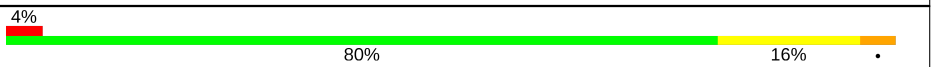
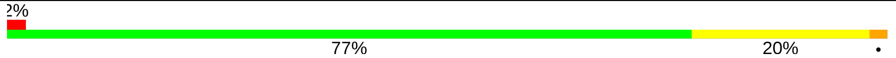
Mol	Chain	Length	Quality of chain
2	F	122	
2	H	122	

2 Entry composition ⓘ

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
			Total	C	N	O	S			
1	A	122	949	581	159	194	15	4	0	0
1	C	122	949	581	159	194	15	3	0	0
1	E	122	949	581	159	194	15	3	0	0
1	G	122	949	581	159	194	15	0	0	0

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
			Total	C	N	O	S			
2	B	122	976	604	184	173	15	6	3	0
2	D	122	961	596	177	173	15	3	0	0
2	F	122	961	596	177	173	15	0	0	0
2	H	122	961	596	177	173	15	3	0	0

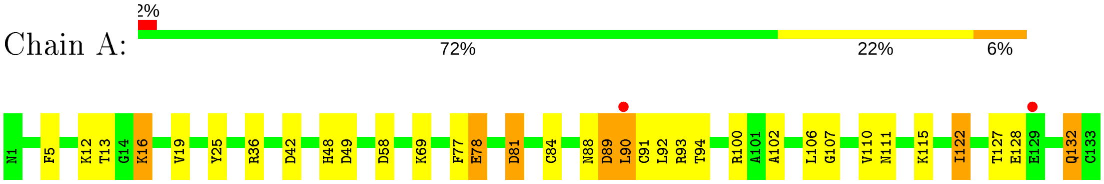
- Molecule 3 is water.

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

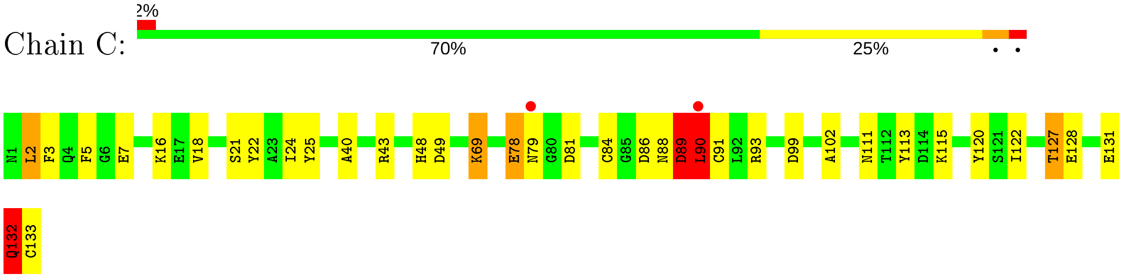
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

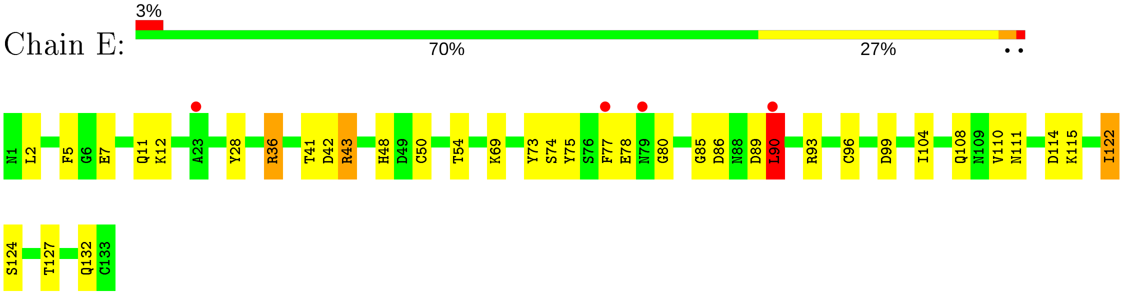
- Molecule 1: Phospholipase A2 RV-7



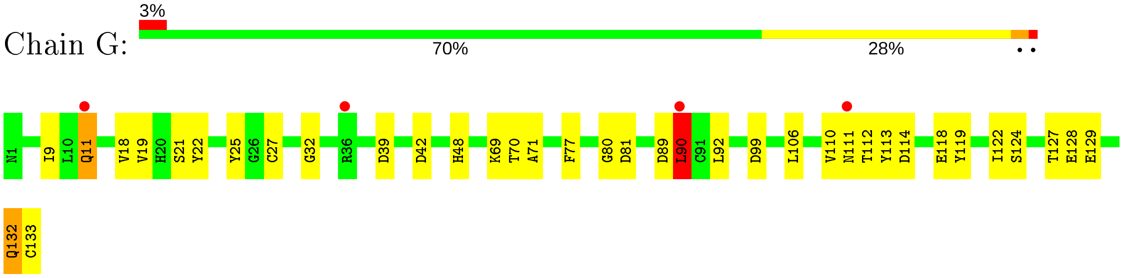
- Molecule 1: Phospholipase A2 RV-7



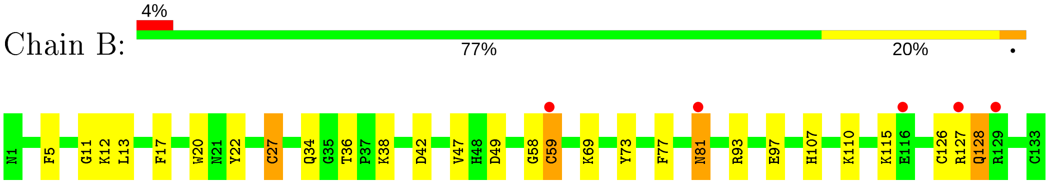
- Molecule 1: Phospholipase A2 RV-7



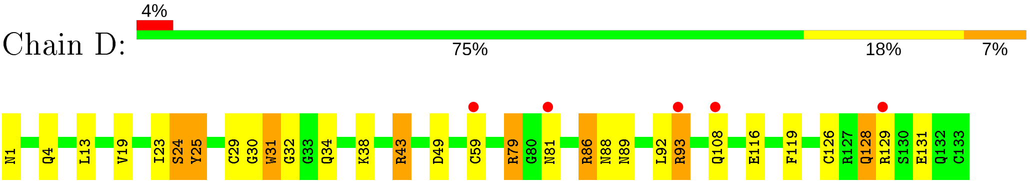
- Molecule 1: Phospholipase A2 RV-7



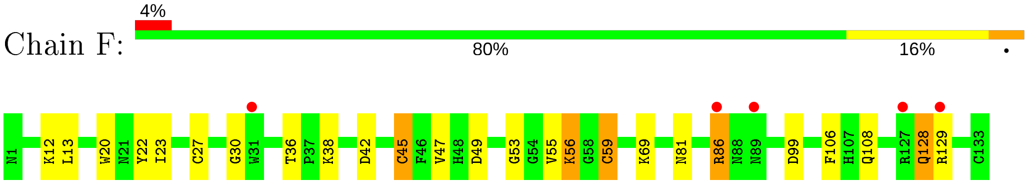
- Molecule 2: Phospholipase A2 RV-4



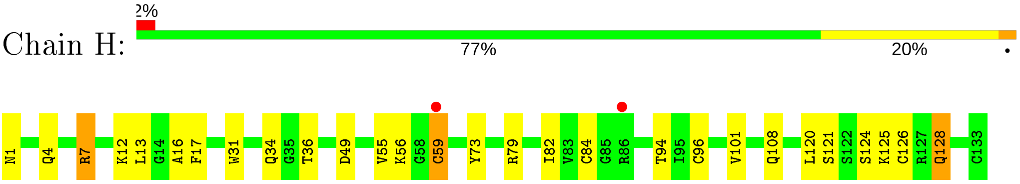
- Molecule 2: Phospholipase A2 RV-4



- 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 27.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 98.2 (27.42-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.16	Depositor
R, R_{free}	0.222 , 0.284 0.221 , 0.273	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)	0.32 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.37	6/968 (0.6%)	1.31	8/1310 (0.6%)
1	C	1.39	8/968 (0.8%)	1.44	10/1310 (0.8%)
1	E	1.31	4/968 (0.4%)	1.29	11/1310 (0.8%)
1	G	1.34	3/968 (0.3%)	1.22	7/1310 (0.5%)
2	B	1.44	8/1014 (0.8%)	1.19	5/1358 (0.4%)
2	D	1.36	4/983 (0.4%)	1.33	9/1319 (0.7%)
2	F	1.37	4/983 (0.4%)	1.20	4/1319 (0.3%)
2	H	1.42	4/983 (0.4%)	1.20	3/1319 (0.2%)
All	All	1.38	41/7835 (0.5%)	1.28	57/10555 (0.5%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	89	ASN	CB-CG	17.85	1.92	1.51
2	F	59	CYS	CB-SG	-11.97	1.61	1.82
2	F	22	TYR	CD1-CE1	-9.19	1.25	1.39
1	A	25	TYR	CD1-CE1	8.05	1.51	1.39
1	C	115	LYS	CG-CD	-7.97	1.25	1.52
1	A	132	GLN	CG-CD	7.86	1.69	1.51
2	H	101	VAL	CB-CG1	7.71	1.69	1.52
1	G	132	GLN	CG-CD	7.14	1.67	1.51
1	G	25	TYR	CD1-CE1	6.69	1.49	1.39
1	A	5	PHE	CE1-CZ	6.63	1.50	1.37
2	D	116	GLU	CD-OE2	6.63	1.32	1.25
2	B	73	TYR	CD2-CE2	6.35	1.48	1.39
1	C	132	GLN	CG-CD	6.33	1.65	1.51
2	H	59	CYS	CB-SG	-6.29	1.71	1.82
1	C	113	TYR	CG-CD2	6.21	1.47	1.39
1	E	132	GLN	CG-CD	6.12	1.65	1.51
2	B	115	LYS	CG-CD	5.91	1.72	1.52
1	C	25	TYR	CD1-CE1	5.77	1.48	1.39
1	A	19	VAL	CB-CG2	5.70	1.64	1.52
1	C	113	TYR	CD1-CE1	5.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	ARG	NE-CZ	5.59	1.40	1.33
2	F	47	VAL	CB-CG2	5.58	1.64	1.52
2	H	31	TRP	CB-CG	-5.53	1.40	1.50
1	E	28	TYR	CD2-CE2	-5.51	1.31	1.39
2	H	101	VAL	CB-CG2	5.51	1.64	1.52
2	B	5	PHE	CD1-CE1	5.50	1.50	1.39
2	B	27	CYS	CB-SG	-5.47	1.72	1.81
2	B	47	VAL	CB-CG2	5.45	1.64	1.52
1	A	132	GLN	CB-CG	5.44	1.67	1.52
1	G	110	VAL	CB-CG1	-5.44	1.41	1.52
2	D	25	TYR	CZ-OH	5.44	1.47	1.37
2	D	19	VAL	CB-CG1	5.44	1.64	1.52
1	A	25	TYR	CD2-CE2	5.35	1.47	1.39
2	B	17	PHE	CE1-CZ	5.30	1.47	1.37
1	E	5	PHE	CE1-CZ	5.25	1.47	1.37
1	C	5	PHE	CE1-CZ	5.21	1.47	1.37
2	B	59	CYS	CB-SG	-5.20	1.73	1.81
2	F	106	PHE	CE2-CZ	5.20	1.47	1.37
1	C	120	TYR	CE2-CZ	-5.17	1.31	1.38
1	C	128	GLU	CD-OE1	-5.15	1.20	1.25
2	B	22	TYR	CD2-CE2	5.02	1.46	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	79	ARG	NE-CZ-NH2	-15.28	112.66	120.30
2	D	79	ARG	NE-CZ-NH1	14.27	127.44	120.30
1	C	81	ASP	CB-CG-OD2	12.09	129.18	118.30
1	C	115	LYS	CB-CG-CD	11.20	140.71	111.60
2	F	59	CYS	CB-CA-C	10.80	131.99	110.40
2	H	59	CYS	CB-CA-C	9.97	130.34	110.40
1	C	69	LYS	CD-CE-NZ	-9.57	89.69	111.70
1	C	89	ASP	CB-CG-OD1	9.39	126.75	118.30
2	F	49	ASP	CB-CG-OD1	8.42	125.88	118.30
2	D	43	ARG	NE-CZ-NH2	-8.05	116.28	120.30
2	D	93	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	49	ASP	CB-CG-OD1	7.53	125.08	118.30
1	E	86	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	81	ASP	CB-CG-OD2	7.26	124.83	118.30
1	G	90	LEU	CB-CG-CD2	6.91	122.74	111.00
1	C	2	LEU	CB-CG-CD1	-6.80	99.43	111.00
1	C	86	ASP	CB-CG-OD2	6.68	124.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	LYS	CB-CG-CD	6.62	128.82	111.60
1	A	100	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	C	90	LEU	CB-CG-CD2	6.48	122.02	111.00
1	A	58	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	16	LYS	CD-CE-NZ	6.45	126.54	111.70
1	G	114	ASP	CB-CG-OD1	6.43	124.09	118.30
1	E	43	ARG	CG-CD-NE	-6.42	98.33	111.80
2	H	7	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	E	90	LEU	CB-CG-CD2	6.37	121.82	111.00
2	B	49	ASP	CB-CG-OD1	6.30	123.97	118.30
1	G	81	ASP	CB-CG-OD2	6.22	123.90	118.30
1	G	133	CYS	CA-C-O	-6.17	107.14	120.10
1	C	133	CYS	CA-C-O	-6.16	107.17	120.10
2	D	93	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	F	45	CYS	CA-CB-SG	-6.11	103.00	114.00
1	A	42	ASP	CB-CG-OD2	6.08	123.77	118.30
2	D	79	ARG	CG-CD-NE	-6.05	99.10	111.80
1	E	42	ASP	CB-CG-OD2	6.03	123.73	118.30
2	D	79	ARG	CD-NE-CZ	6.03	132.04	123.60
1	E	89	ASP	CB-CG-OD2	6.01	123.71	118.30
2	B	81	ASN	CB-CA-C	5.93	122.26	110.40
1	E	85	GLY	N-CA-C	5.67	127.28	113.10
2	B	42	ASP	CB-CG-OD1	5.63	123.37	118.30
2	H	84	CYS	CA-CB-SG	-5.53	104.04	114.00
2	B	115	LYS	CB-CG-CD	-5.52	97.25	111.60
1	E	43	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	E	132	GLN	CB-CG-CD	5.46	125.80	111.60
2	D	92	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	G	42	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	132	GLN	CB-CG-CD	5.39	125.62	111.60
2	F	99	ASP	CB-CG-OD2	5.37	123.13	118.30
1	G	39	ASP	CB-CG-OD2	5.34	123.11	118.30
2	D	31	TRP	CA-CB-CG	-5.32	103.59	113.70
1	A	81	ASP	OD1-CG-OD2	-5.28	113.27	123.30
1	A	115	LYS	CB-CG-CD	5.26	125.29	111.60
1	E	36	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	G	70	THR	OG1-CB-CG2	-5.18	98.08	110.00
1	C	115	LYS	CG-CD-CE	5.11	127.22	111.90
1	E	93	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	B	5	PHE	CB-CG-CD2	-5.06	117.25	120.80

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	949	0	842	24	0
1	C	949	0	842	21	3
1	E	949	0	842	34	7
1	G	949	0	842	35	2
2	B	976	0	921	17	0
2	D	961	0	898	33	3
2	F	961	0	898	18	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	174	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 12.

All (174) 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:CD2	1:G:90:LEU:H	1.51	1.20
1:E:122:ILE:HD12	1:G:124:SER:HB3	1.21	1.14
1:G:90:LEU:HD23	1:G:90:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:G:90:LEU:HD23	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:N	1:G:90:LEU:CD2	2.37	0.87
2:D:86:ARG:NH1	2:D:86:ARG:HB3	1.94	0.81
1:A:90:LEU:CD2	1:A:90:LEU:H	1.90	0.81
2:D:86:ARG:NH1	2:D:86:ARG:CB	2.47	0.78
1:E:90:LEU:CD2	1:E:90:LEU:H	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: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:HD23	1:C:90:LEU:H	1.58	0.69
1:A:88:ASN:O	1:A:89:ASP:C	2.30	0.69
2:D:86:ARG:HB2	2:D:86:ARG:CZ	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
1:C:90:LEU:CD2	1:C:90:LEU:H	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:HH11	2:D:86:ARG:HB3	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:N	1:C:90:LEU:HD23	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	2:D:86:ARG:CB	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
1:A:49:ASP:OD1	2:B:69:LYS:NZ	2.33	0.59
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: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
2:F:81:ASN:CB	3:F:138:HOH:O	1.90	0.56
1:G:18:VAL:HG13	3:G:172:HOH:O	2.05	0.56
1:A:90:LEU:HD23	1:A:90:LEU:N	2.09	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
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
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
2:F:55:VAL:C	2:F:56:LYS:HD3	2.28	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:89:ASP:OD1	1:A:89:ASP:C	2.46	0.53
1:A:89:ASP:OD1	1:A:91:CYS:N	2.40	0.52
1:C:127:THR:O	1:C:127:THR:CG2	2.57	0.52
2:F:81:ASN:CG	3:F:138:HOH:O	2.30	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
2:H:12:LYS:HG2	2:H:82:ILE:HD11	1.92	0.52
1:E:124:SER:O	2:H:7:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:GLN:NE2	2:F:128:GLN:H	2.07	0.52
1:A:88:ASN:O	1:A:90:LEU:N	2.43	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: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
2:D:86:ARG:HH11	2:D:86:ARG:CG	2.26	0.48
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
1:A:77:PHE:C	1:A:78:GLU:HG2	2.35	0.47
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:CG	1:E:69:LYS:O	2.62	0.47
1:E:78:GLU:C	1:E:80:GLY:N	2.66	0.47
1:A:13:THR:HB	1:A:110:VAL:HG11	1.97	0.47
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:B:97:GLU:HG3	2:B:97:GLU:O	2.14	0.45
2:D:34:GLN:HG3	2:D:126:CYS:O	2.15	0.45
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:THR:H	2:F:128:GLN:NE2	2.15	0.45
2:D:108:GLN:HE21	1:G:80:GLY:HA2	1.81	0.44
2:D:108:GLN:HG3	1:G:80:GLY:HA2	1.98	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:HA	1:E:2:LEU:HD23	1.50	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
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
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:122:ILE:HG22	2:B:20:TRP:HZ2	1.84	0.42
1:A:78:GLU:CB	2:D:129:ARG:NH2	2.81	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
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
2:H:121:SER:HG	2:H:124:SER:HG	1.66	0.41
1:G:27:CYS:O	1:G:32:GLY:HA3	2.21	0.41
2:D:108:GLN:HG2	1:G:80:GLY:HA2	1.99	0.41
1:A:81:ASP:HB2	2:D:129:ARG:HH12	1.86	0.41
2:D:38:LYS:HD3	3:D:135:HOH:O	2.20	0.41
2:D:1:ASN:OD1	2:D:4:GLN:HG3	2.21	0.41
1:C:2:LEU:HB2	2:D:32:GLY:O	2.21	0.41
2:F:69:LYS:HD2	2:F:69:LYS:O	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:N	2:F:13:LEU:HD12	2.36	0.40
1:E:122:ILE:CD1	1:G:124:SER:OG	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:LEU:HD12	2:D:13:LEU:N	2.37	0.40
1:G:112:THR:O	1:G:113:TYR:C	2.60	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
2:D:79:ARG:CD	2:F:53:GLY:O[1_554]	2.04	0.16
1:C:78:GLU:CD	2:H:79:ARG:NH1[1_655]	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%)	19	9
2	B	123/122 (101%)	119 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	9
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%)	47	38

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%)	96 (92%)	8 (8%)	13	5
1	E	104/104 (100%)	99 (95%)	5 (5%)	25	16
1	G	104/104 (100%)	99 (95%)	5 (5%)	25	16
2	B	106/103 (103%)	103 (97%)	3 (3%)	43	36
2	D	103/103 (100%)	99 (96%)	4 (4%)	32	23
2	F	103/103 (100%)	98 (95%)	5 (5%)	25	15
2	H	103/103 (100%)	100 (97%)	3 (3%)	42	35
All	All	831/828 (100%)	787 (95%)	44 (5%)	22	13

All (44) 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

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Mol	Chain	Res	Type
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	93	ARG
2	B	128	GLN
1	C	78	GLU
1	C	88	ASN
1	C	89	ASP
1	C	90	LEU
1	C	111	ASN
1	C	122	ILE
1	C	127	THR
1	C	132	GLN
2	D	24	SER
2	D	81	ASN
2	D	86	ARG
2	D	128	GLN
1	E	41	THR
1	E	74	SER
1	E	90	LEU
1	E	122	ILE
1	E	127	THR
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	56	LYS
2	H	59	CYS
2	H	128	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
2	B	111	ASN
2	B	128	GLN
1	C	132	GLN
2	D	78	GLN
2	D	81	ASN
2	D	128	GLN
1	E	48	HIS
1	E	108	GLN
2	F	111	ASN
2	F	128	GLN
1	G	20	HIS
1	G	48	HIS
1	G	132	GLN
2	H	111	ASN
2	H	128	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (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	122/122 (100%)	-0.13	2 (1%)	72	74	14, 22, 38, 45	4 (3%)
1	C	122/122 (100%)	-0.04	2 (1%)	72	74	15, 22, 32, 41	3 (2%)
1	E	122/122 (100%)	0.11	4 (3%)	46	49	19, 25, 36, 53	2 (1%)
1	G	122/122 (100%)	0.02	4 (3%)	46	49	19, 24, 37, 44	0
2	B	122/122 (100%)	0.02	5 (4%)	37	40	15, 22, 35, 46	3 (2%)
2	D	122/122 (100%)	0.11	5 (4%)	37	40	18, 26, 37, 48	3 (2%)
2	F	122/122 (100%)	0.05	5 (4%)	37	40	15, 24, 40, 52	1 (0%)
2	H	122/122 (100%)	-0.12	2 (1%)	72	74	16, 23, 33, 45	3 (2%)
All	All	976/976 (100%)	0.00	29 (2%)	50	53	14, 24, 38, 53	19 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	4.3
1	G	90	LEU	3.2
1	E	90	LEU	3.1
2	F	86	ARG	3.0
2	D	81	ASN	2.9
2	F	89	ASN	2.8
1	C	90	LEU	2.7
2	H	59	CYS	2.7
1	G	111	ASN	2.7
2	F	129	ARG	2.6
2	F	127	ARG	2.6
2	B	59	CYS	2.5
2	D	59	CYS	2.5
2	D	108	GLN	2.4
2	B	127[A]	ARG	2.4
2	B	129	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	79	ASN	2.4
1	E	77	PHE	2.4
2	B	81	ASN	2.4
1	G	36	ARG	2.3
1	C	79	ASN	2.3
1	G	11	GLN	2.3
2	B	116	GLU	2.3
2	F	31	TRP	2.2
2	D	93	ARG	2.2
1	E	23	ALA	2.1
1	A	129	GLU	2.1
2	D	129	ARG	2.0
2	H	86	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.