



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:07 AM UTC

PDB ID : 6GWS / pdb_00006gws
Title : Crystal structure of human PCNA in complex with three p15 peptides
Authors : De March, M.; Merino, N.; Gonzalez-Magana, A.; Romano-Moreno, M.; Onesti, S.; Blanco, F.J.; De Biasio, A.
Deposited on : 2018-06-25
Resolution : 2.90 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

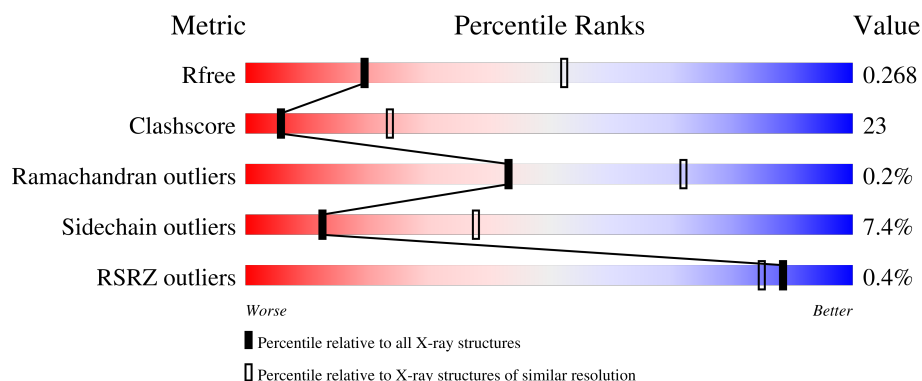
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	264	57% 34% 5% .
1	B	264	55% 34% 5% .
1	C	264	54% 37% 5% .
2	D	32	47% 16% . 34%
2	E	32	31% 31% . 31%

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Mol	Chain	Length	Quality of chain
2	F	32	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6430 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1963	1233	322	392	16			
1	B	255	Total	C	N	O	S	0	0	0
			1963	1233	322	392	16			
1	C	255	Total	C	N	O	S	0	0	0
			1956	1229	320	391	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12004
A	-1	PRO	-	expression tag	UNP P12004
A	0	HIS	-	expression tag	UNP P12004
B	-2	GLY	-	expression tag	UNP P12004
B	-1	PRO	-	expression tag	UNP P12004
B	0	HIS	-	expression tag	UNP P12004
C	-2	GLY	-	expression tag	UNP P12004
C	-1	PRO	-	expression tag	UNP P12004
C	0	HIS	-	expression tag	UNP P12004

- Molecule 2 is a protein called PCNA-associated factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	S	0	0	0
			174	115	32	26	1			
2	E	22	Total	C	N	O	S	0	0	0
			180	118	33	28	1			
2	F	23	Total	C	N	O	S	0	0	0
			184	120	34	29	1			

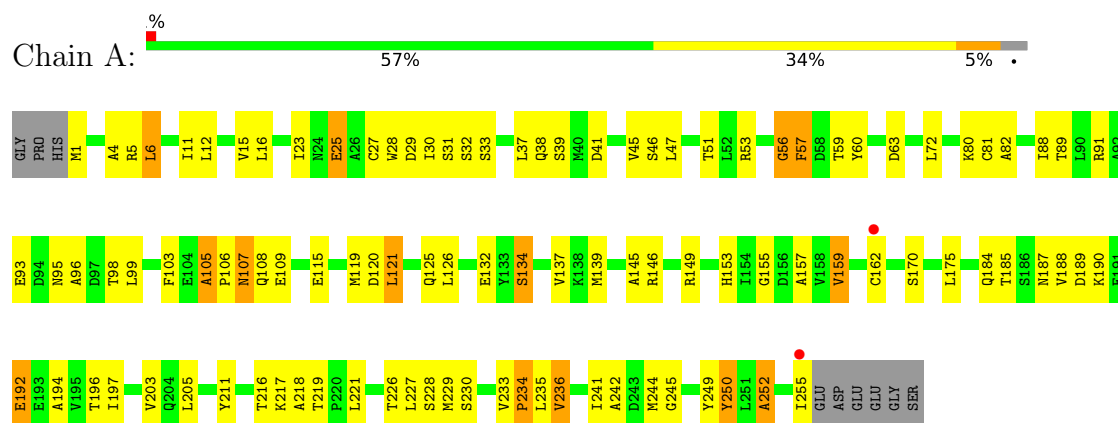
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	4	Total 4	O 4	0	0
3	C	2	Total 2	O 2	0	0
3	E	1	Total 1	O 1	0	0

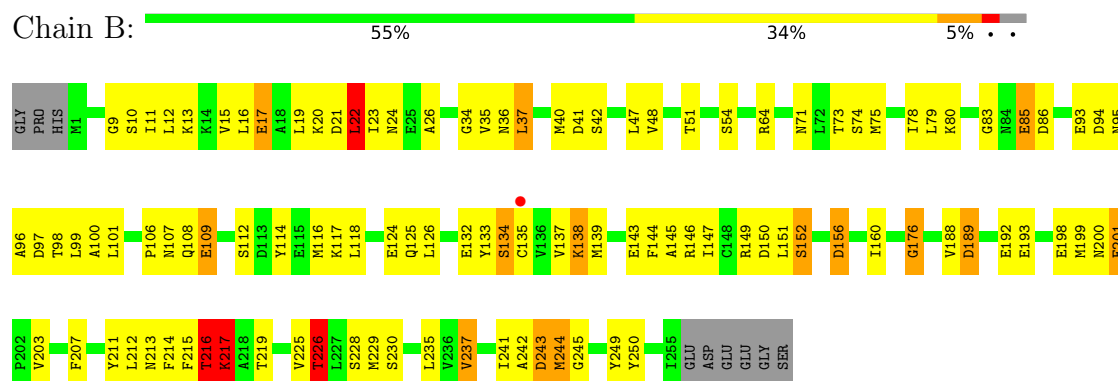
3 Residue-property plots [i](#)

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.

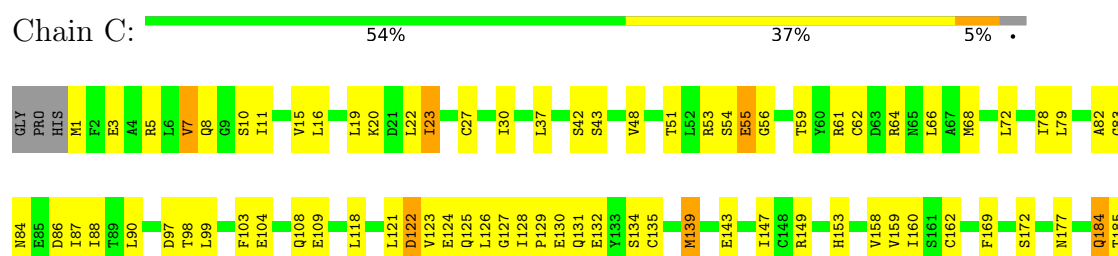
• Molecule 1: Proliferating cell nuclear antigen

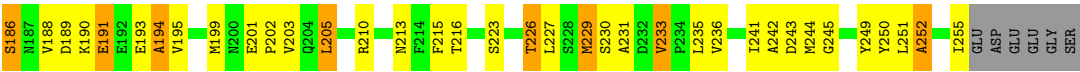


• Molecule 1: Proliferating cell nuclear antigen

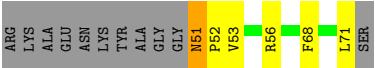


• Molecule 1: Proliferating cell nuclear antigen

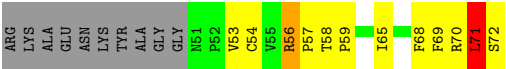




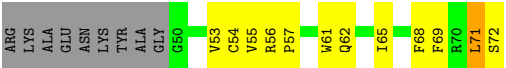
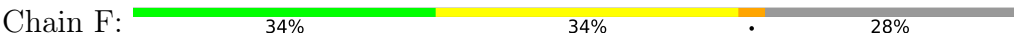
● Molecule 2: PCNA-associated factor



● Molecule 2: PCNA-associated factor



● Molecule 2: PCNA-associated factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.24Å 89.75Å 85.13Å 90.00° 117.25° 90.00°	Depositor
Resolution (Å)	75.69 – 2.90 75.68 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (75.69-2.90) 98.4 (75.68-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.200 , 0.263 0.215 , 0.268	Depositor DCC
R_{free} test set	1098 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	90.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6430	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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 [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	1.31	7/1989 (0.4%)	1.44	15/2687 (0.6%)
1	B	1.31	5/1989 (0.3%)	1.41	24/2687 (0.9%)
1	C	1.29	3/1982 (0.2%)	1.44	23/2679 (0.9%)
2	D	1.42	3/180 (1.7%)	1.36	1/243 (0.4%)
2	E	1.45	0/186	1.64	4/251 (1.6%)
2	F	1.30	2/190 (1.1%)	1.50	6/256 (2.3%)
All	All	1.31	20/6516 (0.3%)	1.44	73/8803 (0.8%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	ALA	CA-C	6.96	1.61	1.52
1	A	57	PHE	CA-C	6.56	1.61	1.52
1	C	55	GLU	CA-C	6.38	1.61	1.52
1	B	226	THR	N-CA	-5.91	1.38	1.46
1	A	153	HIS	CA-C	-5.58	1.45	1.52
1	B	212	LEU	C-O	5.57	1.31	1.24
1	A	250	TYR	CA-C	5.56	1.59	1.52
2	D	52	PRO	N-CA	5.53	1.52	1.46
1	B	230	SER	CA-C	-5.46	1.45	1.52
1	C	127	GLY	C-O	5.39	1.29	1.23
1	A	157	ALA	CA-C	5.37	1.59	1.52
1	B	237	VAL	CA-C	-5.35	1.46	1.52
2	D	53	VAL	CA-CB	5.34	1.60	1.53
1	B	201	GLU	N-CA	5.32	1.51	1.46
2	F	57	PRO	C-O	5.28	1.30	1.23
1	A	252	ALA	CA-C	5.21	1.58	1.52
1	A	88	ILE	CA-C	-5.13	1.46	1.52
1	C	213	ASN	CG-OD1	5.11	1.33	1.23
2	F	57	PRO	CA-C	5.06	1.58	1.52
2	D	51	ASN	C-N	5.06	1.39	1.33

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	VAL	N-CA-C	-13.20	98.37	109.19
1	B	19	LEU	N-CA-C	11.91	124.34	111.36
1	A	219	THR	CA-C-N	-10.02	109.00	120.12
1	A	219	THR	C-N-CA	-10.02	109.00	120.12
1	B	219	THR	CA-C-N	-8.80	108.84	119.84
1	B	219	THR	C-N-CA	-8.80	108.84	119.84
1	C	233	VAL	CA-C-N	-8.48	111.41	120.66
1	C	233	VAL	C-N-CA	-8.48	111.41	120.66
1	C	194	ALA	N-CA-C	8.46	121.86	110.35
2	E	71	LEU	N-CA-C	-8.18	98.97	110.50
1	B	192	GLU	N-CA-C	-7.38	104.42	113.50
1	C	139	MET	CA-C-N	-7.38	112.32	120.14
1	C	139	MET	C-N-CA	-7.38	112.32	120.14
2	D	68	PHE	N-CA-C	-7.20	105.42	114.56
1	C	193	GLU	N-CA-C	7.15	121.26	112.54
1	C	233	VAL	CB-CA-C	7.06	116.25	109.33
1	A	185	THR	N-CA-C	7.05	120.42	109.07
1	B	189	ASP	N-CA-C	6.87	121.41	112.89
1	C	130	GLU	N-CA-C	-6.65	101.75	110.53
1	B	109	GLU	N-CA-C	6.61	118.49	111.28
1	B	22	LEU	N-CA-C	6.46	118.40	111.36
2	F	61	TRP	N-CA-C	6.43	120.84	113.19
1	C	84	ASN	N-CA-C	6.31	118.16	111.28
1	B	138	LYS	N-CA-C	-6.30	98.63	108.90
2	E	54	CYS	N-CA-C	-6.27	98.97	109.07
1	B	211	TYR	N-CA-C	6.21	119.33	111.69
1	C	124	GLU	N-CA-C	-6.15	99.17	109.07
1	A	63	ASP	N-CA-C	-6.13	105.45	113.12
1	C	189	ASP	N-CA-C	-6.05	104.60	111.07
1	B	229	MET	N-CA-C	5.97	118.93	109.50
1	B	176	GLY	N-CA-C	5.93	118.03	110.20
1	A	242	ALA	N-CA-C	5.92	118.91	110.10
1	A	28	TRP	N-CA-C	-5.89	99.13	108.73
1	C	97	ASP	N-CA-C	-5.84	98.36	110.80
1	C	131	GLN	N-CA-C	5.74	116.98	108.60
1	C	132	GLU	N-CA-C	-5.72	100.08	109.40
2	F	56	ARG	N-CA-C	5.70	117.86	110.40
1	C	188	VAL	N-CA-C	-5.68	103.79	110.21
1	A	205	LEU	N-CA-C	5.67	118.46	109.50
1	B	97	ASP	N-CA-C	5.65	118.10	109.62
2	F	54	CYS	N-CA-C	-5.65	101.28	109.59
1	C	186	SER	N-CA-C	5.64	117.43	111.28
1	C	23	ILE	CB-CA-C	-5.64	102.81	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	56	ARG	CA-C-N	-5.61	114.79	120.85
2	E	56	ARG	C-N-CA	-5.61	114.79	120.85
1	C	241	ILE	N-CA-C	-5.61	99.71	108.86
1	A	211	TYR	N-CA-C	5.57	117.16	111.14
2	F	56	ARG	CA-C-N	-5.56	114.87	120.21
2	F	56	ARG	C-N-CA	-5.56	114.87	120.21
1	B	156	ASP	N-CA-C	5.46	117.32	111.36
1	B	237	VAL	N-CA-C	-5.38	100.67	108.36
1	A	56	GLY	N-CA-C	5.36	120.56	114.67
1	B	244	MET	N-CA-C	-5.29	106.51	113.12
1	A	57	PHE	N-CA-C	5.25	118.78	109.96
1	A	155	GLY	N-CA-C	5.21	118.31	110.18
2	F	55	VAL	N-CA-CB	5.21	116.40	110.72
1	A	234	PRO	N-CA-C	5.21	123.19	112.47
1	B	217	LYS	N-CA-C	-5.20	106.94	113.28
1	B	54	SER	N-CA-C	5.19	118.40	111.75
1	A	121	LEU	N-CA-C	5.18	116.83	108.34
1	C	184	GLN	N-CA-C	5.14	117.69	110.23
1	B	34	GLY	N-CA-C	5.13	119.17	111.42
1	A	25	GLU	N-CA-C	5.13	116.09	108.60
1	B	75	MET	N-CA-C	-5.12	105.88	111.82
1	C	252	ALA	CA-C-N	5.12	126.46	120.98
1	C	252	ALA	C-N-CA	5.12	126.46	120.98
1	C	229	MET	N-CA-C	5.09	116.72	109.14
1	B	24	ASN	N-CA-C	5.08	116.90	111.36
1	B	201	GLU	CA-C-N	-5.08	115.13	120.66
1	B	201	GLU	C-N-CA	-5.08	115.13	120.66
1	B	242	ALA	N-CA-C	5.07	118.44	111.54
1	B	203	VAL	N-CA-C	-5.06	101.67	108.35
1	A	132	GLU	N-CA-C	-5.05	102.04	110.17

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	1963	0	1973	111	0
1	B	1963	0	1973	99	0
1	C	1956	0	1958	77	0
2	D	174	0	178	9	0
2	E	180	0	183	11	0
2	F	184	0	186	27	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	E	1	0	0	0	0
All	All	6430	0	6451	297	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (297) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD13	1:B:79:LEU:CD1	1.63	1.26
1:B:12:LEU:O	1:B:16:LEU:HD12	1.43	1.17
1:C:149:ARG:HD2	2:D:51:ASN:O	1.46	1.14
1:B:85:GLU:HB2	1:B:106:PRO:HG3	1.29	1.13
1:A:1:MET:SD	1:A:93:GLU:HG2	1.89	1.12
1:A:250:TYR:O	2:F:65:ILE:HD11	1.50	1.10
1:B:16:LEU:HD13	1:B:79:LEU:HD13	1.33	1.10
2:F:71:LEU:HD12	2:F:71:LEU:H	1.18	1.09
1:A:134:SER:OG	1:A:230:SER:HA	1.60	1.01
1:A:6:LEU:HD11	1:A:244:MET:HE1	1.38	1.00
2:F:68:PHE:C	2:F:69:PHE:HD1	1.69	1.00
1:C:191:GLU:OE1	1:C:191:GLU:N	1.95	0.99
1:B:109:GLU:N	1:B:109:GLU:OE1	1.95	0.99
1:B:11:ILE:O	1:B:15:VAL:HG23	1.62	0.98
1:C:190:LYS:CB	1:C:194:ALA:HB2	1.92	0.97
1:A:187:ASN:HB3	1:A:188:VAL:C	1.90	0.95
1:B:99:LEU:HD12	1:B:100:ALA:N	1.82	0.94
1:A:12:LEU:O	1:A:16:LEU:HD23	1.69	0.93
1:A:46:SER:C	2:F:65:ILE:HD12	1.95	0.92
1:B:99:LEU:HD12	1:B:100:ALA:H	1.34	0.91
1:C:185:THR:HG22	1:C:185:THR:O	1.68	0.90
1:C:139:MET:HE1	1:C:169:PHE:CZ	2.07	0.90
1:A:51:THR:O	1:A:245:GLY:HA3	1.72	0.89
1:C:199:MET:HE3	1:C:202:PRO:N	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:CD1	1:A:244:MET:HE1	2.02	0.88
1:A:120:ASP:O	1:A:121:LEU:HD23	1.74	0.87
1:B:16:LEU:CD1	1:B:79:LEU:CD1	2.53	0.86
1:A:107:ASN:HD22	1:A:109:GLU:CG	1.88	0.86
1:C:51:THR:O	1:C:245:GLY:HA3	1.76	0.86
1:B:74:SER:O	1:B:78:ILE:HG13	1.77	0.85
2:E:70:ARG:HG2	2:E:71:LEU:O	1.75	0.85
1:A:47:LEU:N	2:F:65:ILE:HD12	1.93	0.84
1:A:162:CYS:SG	1:A:203:VAL:HG22	2.19	0.83
1:A:47:LEU:N	2:F:65:ILE:CD1	2.41	0.83
1:B:107:ASN:HB2	1:B:109:GLU:CD	2.03	0.82
1:C:199:MET:HE3	1:C:201:GLU:C	2.05	0.81
2:F:68:PHE:O	2:F:69:PHE:HD1	1.64	0.81
1:A:107:ASN:HB2	1:A:109:GLU:HG2	1.61	0.80
1:C:121:LEU:HD12	1:C:122:ASP:H	1.47	0.79
1:B:16:LEU:HD13	1:B:79:LEU:HD11	1.61	0.79
1:B:93:GLU:OE1	1:B:96:ALA:HB2	1.83	0.79
1:C:184:GLN:HE21	1:C:186:SER:HB3	1.46	0.78
1:A:134:SER:OG	1:A:230:SER:CA	2.32	0.78
1:B:143:GLU:O	1:B:147:ILE:HG13	1.84	0.78
1:B:85:GLU:HB2	1:B:106:PRO:CG	2.12	0.78
1:C:205:LEU:HD21	1:C:231:ALA:HA	1.66	0.78
1:A:107:ASN:HD22	1:A:109:GLU:HG2	1.49	0.77
1:A:134:SER:OG	1:A:230:SER:CB	2.32	0.77
1:B:12:LEU:O	1:B:16:LEU:CD1	2.28	0.76
1:C:139:MET:HE1	1:C:169:PHE:HZ	1.48	0.76
1:B:22:LEU:HD23	1:B:41:ASP:HB3	1.66	0.76
1:A:187:ASN:HD21	1:A:194:ALA:HA	1.49	0.76
1:C:185:THR:HB	1:C:195:VAL:H	1.51	0.76
1:B:23:ILE:CG2	1:B:41:ASP:HA	2.15	0.75
1:A:37:LEU:HD23	1:A:38:GLN:N	2.01	0.75
2:F:71:LEU:H	2:F:71:LEU:CD1	1.97	0.75
1:B:85:GLU:CB	1:B:106:PRO:HG3	2.13	0.74
1:A:11:ILE:O	1:A:15:VAL:HG23	1.88	0.74
2:F:71:LEU:HD12	2:F:71:LEU:N	2.00	0.74
1:A:45:VAL:O	2:F:65:ILE:HG13	1.87	0.74
1:A:187:ASN:HB3	1:A:188:VAL:CA	2.17	0.73
1:C:87:ILE:HB	1:C:104:GLU:CG	2.19	0.73
1:C:126:LEU:HD23	2:D:71:LEU:HD23	1.69	0.73
1:C:172:SER:HB2	1:C:177:ASN:OD1	1.89	0.72
1:A:107:ASN:ND2	1:A:109:GLU:HB2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:PHE:C	2:F:69:PHE:CD1	2.61	0.72
1:C:172:SER:CB	1:C:177:ASN:OD1	2.38	0.72
1:C:53:ARG:NH2	1:C:243:ASP:O	2.23	0.72
1:C:135:CYS:SG	1:C:203:VAL:HG22	2.31	0.71
1:C:19:LEU:HD22	1:C:48:VAL:HG11	1.70	0.71
1:A:37:LEU:HD23	1:A:37:LEU:C	2.17	0.69
1:A:187:ASN:HB3	1:A:188:VAL:O	1.93	0.69
1:B:243:ASP:OD1	1:B:243:ASP:C	2.35	0.69
1:A:109:GLU:HA	1:A:109:GLU:OE1	1.93	0.68
1:A:134:SER:HG	1:A:230:SER:HA	1.59	0.67
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.25	0.67
1:C:185:THR:O	1:C:185:THR:CG2	2.42	0.66
1:A:46:SER:HA	2:F:65:ILE:CD1	2.26	0.66
1:A:107:ASN:HD22	1:A:109:GLU:CB	2.07	0.66
1:B:93:GLU:HB3	1:B:96:ALA:HB3	1.78	0.66
1:C:87:ILE:HB	1:C:104:GLU:HG2	1.77	0.66
1:C:79:LEU:O	1:C:82:ALA:HB3	1.95	0.66
1:C:83:GLY:O	1:C:86:ASP:HB2	1.95	0.66
1:A:252:ALA:HB3	2:F:62:GLN:NE2	2.11	0.66
2:F:68:PHE:O	2:F:69:PHE:CD1	2.48	0.66
1:B:101:LEU:HD12	1:B:101:LEU:N	2.10	0.65
1:B:16:LEU:CD1	1:B:79:LEU:HD11	2.23	0.65
1:A:115:GLU:O	1:B:176:GLY:HA3	1.96	0.65
1:C:153:HIS:CE1	2:D:51:ASN:OD1	2.50	0.65
1:A:107:ASN:HD22	1:A:109:GLU:HB2	1.61	0.65
1:B:26:ALA:HB1	1:B:37:LEU:HD21	1.78	0.64
1:B:108:GLN:N	1:B:109:GLU:OE1	2.31	0.64
1:A:137:VAL:CG1	1:A:139:MET:HE2	2.28	0.64
1:C:27:CYS:SG	1:C:123:VAL:CG2	2.86	0.64
1:C:30:ILE:HD11	1:C:68:MET:HE2	1.78	0.64
1:C:3:GLU:OE1	1:C:59:THR:HG21	1.97	0.63
1:B:188:VAL:HG11	1:B:193:GLU:OE1	1.98	0.63
1:C:48:VAL:HG22	1:C:249:TYR:CD1	2.34	0.63
1:A:149:ARG:HG3	2:F:53:VAL:HG22	1.81	0.62
1:B:107:ASN:O	1:B:108:GLN:HB2	1.99	0.62
1:B:80:LYS:CB	2:D:51:ASN:HD22	2.11	0.62
1:A:81:CYS:SG	1:B:150:ASP:HB3	2.39	0.62
1:B:135:CYS:SG	1:B:201:GLU:O	2.59	0.61
1:B:47:LEU:HD13	1:B:126:LEU:HD12	1.81	0.61
1:C:56:GLY:O	1:C:244:MET:HE2	2.00	0.61
1:B:23:ILE:HG22	1:B:41:ASP:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HB2	1:C:61:ARG:HH21	1.66	0.61
1:B:99:LEU:HB2	1:B:118:LEU:HD21	1.82	0.61
1:B:149:ARG:O	1:B:152:SER:HB2	2.01	0.60
1:A:175:LEU:CD2	1:C:78:ILE:HD11	2.32	0.60
1:A:38:GLN:HE22	1:A:126:LEU:H	1.48	0.59
1:B:47:LEU:HB2	2:E:65:ILE:HG21	1.85	0.59
1:B:241:ILE:O	1:B:241:ILE:HG22	2.01	0.59
1:C:88:ILE:HG12	1:C:103:PHE:HD1	1.66	0.59
1:A:46:SER:CA	2:F:65:ILE:HD12	2.31	0.59
1:C:11:ILE:O	1:C:15:VAL:HG23	2.03	0.59
1:B:93:GLU:CD	1:B:96:ALA:HB2	2.27	0.59
1:C:121:LEU:HD12	1:C:122:ASP:N	2.17	0.59
1:A:190:LYS:HD3	1:A:192:GLU:OE1	2.03	0.59
1:A:56:GLY:O	1:A:244:MET:HE2	2.03	0.58
1:C:3:GLU:OE1	1:C:59:THR:CG2	2.51	0.58
1:B:80:LYS:HB3	2:D:51:ASN:HD22	1.67	0.58
1:A:53:ARG:CZ	1:A:244:MET:O	2.51	0.58
1:B:83:GLY:N	1:B:86:ASP:OD2	2.34	0.58
1:B:51:THR:O	1:B:245:GLY:HA3	2.05	0.57
1:B:114:TYR:HA	1:C:177:ASN:O	2.04	0.57
1:C:199:MET:HG3	1:C:201:GLU:O	2.04	0.57
1:B:107:ASN:HB2	1:B:109:GLU:OE2	2.04	0.56
1:C:199:MET:HE1	1:C:202:PRO:HG3	1.86	0.56
1:B:137:VAL:O	1:B:226:THR:HA	2.06	0.56
1:B:139:MET:HE3	1:B:144:PHE:HB2	1.86	0.56
1:B:237:VAL:HB	1:B:249:TYR:HB2	1.87	0.56
2:E:68:PHE:O	2:E:69:PHE:HD1	1.87	0.56
1:A:187:ASN:CB	1:A:188:VAL:HA	2.36	0.56
1:A:1:MET:SD	1:A:93:GLU:CG	2.80	0.56
1:A:250:TYR:O	2:F:65:ILE:CD1	2.40	0.55
1:C:139:MET:CE	1:C:169:PHE:HZ	2.19	0.55
1:A:108:GLN:O	1:A:108:GLN:HG2	2.07	0.55
1:A:137:VAL:HG12	1:A:139:MET:HE2	1.89	0.55
1:A:187:ASN:CB	1:A:188:VAL:CA	2.83	0.55
1:C:172:SER:HB3	1:C:177:ASN:OD1	2.06	0.55
1:A:184:GLN:HE21	1:A:196:THR:HA	1.72	0.55
1:B:47:LEU:HB3	1:B:250:TYR:HB2	1.89	0.55
1:A:46:SER:HA	2:F:65:ILE:HD11	1.89	0.55
1:A:29:ASP:C	1:A:30:ILE:HD13	2.33	0.54
1:B:107:ASN:HB2	1:B:109:GLU:OE1	2.06	0.54
1:A:6:LEU:HD11	1:A:244:MET:CE	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLU:HA	1:B:20:LYS:HE2	1.89	0.54
1:A:25:GLU:CD	1:A:119:MET:HE1	2.33	0.54
1:A:5:ARG:CB	1:A:59:THR:HB	2.38	0.54
1:A:187:ASN:HB3	1:A:188:VAL:HA	1.88	0.53
1:A:221:LEU:HD22	1:A:241:ILE:HD12	1.89	0.53
1:C:226:THR:C	1:C:227:LEU:HD23	2.33	0.53
1:A:16:LEU:N	1:A:16:LEU:HD22	2.24	0.53
1:B:139:MET:HE2	1:B:144:PHE:CD1	2.44	0.53
1:C:158:VAL:HG22	1:C:159:VAL:N	2.24	0.53
1:B:188:VAL:CG1	1:B:189:ASP:N	2.73	0.52
1:B:139:MET:CE	1:B:144:PHE:HB2	2.40	0.52
1:A:105:ALA:HB1	1:A:106:PRO:HD2	1.91	0.52
1:A:229:MET:CG	1:A:235:LEU:HD13	2.40	0.52
1:B:93:GLU:CG	1:B:94:ASP:N	2.72	0.52
1:C:7:VAL:HA	1:C:87:ILE:HD12	1.92	0.52
1:A:184:GLN:NE2	1:A:197:ILE:H	2.08	0.51
1:A:95:ASN:CG	1:A:95:ASN:O	2.52	0.51
1:A:235:LEU:O	1:A:250:TYR:HA	2.10	0.51
1:A:47:LEU:H	2:F:65:ILE:CD1	2.21	0.51
1:A:25:GLU:OE2	1:A:119:MET:HE1	2.10	0.51
1:A:46:SER:CA	2:F:65:ILE:CD1	2.89	0.51
1:C:5:ARG:HB3	1:C:59:THR:HB	1.92	0.51
1:C:135:CYS:SG	1:C:162:CYS:HB2	2.50	0.51
1:A:107:ASN:ND2	1:A:109:GLU:HG2	2.23	0.51
1:A:137:VAL:HG11	1:A:139:MET:HE2	1.90	0.51
1:C:54:SER:OG	1:C:55:GLU:N	2.44	0.51
1:A:119:MET:HE2	1:A:121:LEU:HD21	1.93	0.50
1:B:21:ASP:OD1	1:B:214:PHE:CD1	2.64	0.50
2:E:70:ARG:CG	2:E:71:LEU:O	2.54	0.50
1:A:139:MET:HE3	1:A:227:LEU:HD12	1.92	0.50
1:B:93:GLU:CG	1:B:96:ALA:HB3	2.41	0.50
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.46	0.50
1:A:134:SER:OG	1:A:230:SER:HB2	2.10	0.50
1:C:22:LEU:HD23	1:C:48:VAL:HG21	1.93	0.50
1:B:93:GLU:CD	1:B:96:ALA:CB	2.85	0.49
1:A:91:ARG:O	1:A:99:LEU:HD12	2.12	0.49
1:C:88:ILE:HG12	1:C:103:PHE:CD1	2.47	0.49
1:A:47:LEU:HB3	2:F:65:ILE:HD13	1.95	0.49
1:B:80:LYS:HB2	2:D:51:ASN:HD22	1.77	0.49
1:B:125:GLN:O	2:E:72:SER:HA	2.12	0.49
1:C:56:GLY:O	1:C:244:MET:CE	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LEU:CD2	1:C:231:ALA:HA	2.40	0.49
2:F:69:PHE:CD1	2:F:69:PHE:N	2.77	0.49
1:A:47:LEU:CB	2:F:65:ILE:HD13	2.42	0.49
1:A:37:LEU:C	1:A:37:LEU:CD2	2.85	0.48
1:B:93:GLU:CB	1:B:96:ALA:HB3	2.42	0.48
1:A:80:LYS:O	1:B:146:ARG:NH1	2.45	0.48
1:B:156:ASP:OD1	2:E:56:ARG:NH1	2.46	0.48
1:B:22:LEU:C	1:B:23:ILE:HG23	2.39	0.48
1:B:23:ILE:HG21	1:B:40:MET:O	2.13	0.48
1:A:23:ILE:HB	1:A:72:LEU:HD12	1.96	0.48
1:A:25:GLU:OE2	1:A:119:MET:CE	2.62	0.48
1:A:162:CYS:SG	1:A:203:VAL:CG2	2.98	0.48
1:B:152:SER:OG	1:B:213:ASN:ND2	2.44	0.48
1:B:93:GLU:CG	1:B:96:ALA:CB	2.92	0.47
1:B:100:ALA:C	1:B:101:LEU:HD12	2.39	0.47
1:A:230:SER:OG	1:A:233:VAL:HB	2.14	0.47
1:B:139:MET:CE	1:B:144:PHE:CD1	2.98	0.47
1:A:23:ILE:HD13	1:A:41:ASP:HA	1.97	0.47
1:A:125:GLN:HB2	2:F:72:SER:HB3	1.97	0.47
1:B:215:PHE:C	1:B:217:LYS:H	2.22	0.47
1:C:199:MET:HE3	1:C:202:PRO:CA	2.45	0.47
1:A:46:SER:C	2:F:65:ILE:CD1	2.76	0.47
1:A:107:ASN:O	1:A:108:GLN:HB3	2.15	0.47
1:B:85:GLU:N	1:B:85:GLU:CD	2.73	0.47
1:C:23:ILE:HB	1:C:72:LEU:HD12	1.96	0.46
2:E:68:PHE:C	2:E:69:PHE:CD1	2.93	0.46
1:A:31:SER:O	1:A:60:TYR:OH	2.32	0.46
1:A:120:ASP:C	1:A:121:LEU:HD23	2.38	0.46
1:C:87:ILE:HB	1:C:104:GLU:HG3	1.97	0.46
1:B:145:ALA:HA	1:B:216:THR:HG21	1.97	0.46
1:C:108:GLN:O	1:C:109:GLU:HG3	2.16	0.46
1:C:134:SER:H	1:C:230:SER:HG	1.64	0.46
1:B:17:GLU:HG3	1:B:20:LYS:HE2	1.98	0.45
1:A:5:ARG:HB3	1:A:59:THR:HB	1.99	0.45
1:B:22:LEU:C	1:B:23:ILE:CG2	2.90	0.45
1:B:149:ARG:HG3	2:E:53:VAL:HG22	1.98	0.45
1:C:10:SER:O	1:C:11:ILE:C	2.60	0.45
1:C:199:MET:HE3	1:C:202:PRO:CD	2.46	0.45
2:E:68:PHE:C	2:E:69:PHE:HD1	2.24	0.45
1:A:189:ASP:HA	1:A:190:LYS:HA	1.72	0.45
1:A:149:ARG:HG3	2:F:53:VAL:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HB2	1:C:118:LEU:HD21	1.98	0.45
1:C:235:LEU:O	1:C:250:TYR:HA	2.17	0.45
1:A:145:ALA:HA	1:A:216:THR:HG21	1.99	0.45
1:C:215:PHE:CD1	1:C:249:TYR:CD1	3.05	0.45
1:A:89:THR:HG21	1:A:91:ARG:NH2	2.33	0.44
1:B:243:ASP:O	1:B:243:ASP:CG	2.57	0.44
1:C:199:MET:CE	1:C:202:PRO:HG3	2.47	0.44
1:C:7:VAL:HG22	1:C:87:ILE:HD12	1.99	0.44
1:A:218:ALA:HB2	1:A:249:TYR:OH	2.18	0.44
1:C:160:ILE:HG21	1:C:229:MET:HE1	1.98	0.44
1:A:5:ARG:HB2	1:A:59:THR:HB	1.98	0.44
1:A:252:ALA:HB3	2:F:62:GLN:HE22	1.81	0.44
1:A:107:ASN:OD1	1:A:107:ASN:N	2.51	0.43
1:C:27:CYS:SG	1:C:123:VAL:HG22	2.58	0.43
1:A:82:ALA:HB2	1:A:103:PHE:CD2	2.53	0.43
1:A:119:MET:CE	1:A:121:LEU:HD21	2.48	0.43
1:A:139:MET:CE	1:A:227:LEU:HD12	2.49	0.43
1:B:78:ILE:HD12	1:B:116:MET:HB2	2.00	0.43
1:A:4:ALA:HB1	1:A:57:PHE:CD2	2.54	0.43
2:E:58:THR:HA	2:E:59:PRO:HD3	1.86	0.43
1:B:80:LYS:CB	2:D:51:ASN:ND2	2.81	0.43
1:A:47:LEU:HB3	1:A:250:TYR:HB2	2.00	0.43
1:B:134:SER:HB3	1:B:201:GLU:HB2	2.00	0.43
1:B:160:ILE:HD12	1:B:207:PHE:CD2	2.54	0.43
1:C:242:ALA:C	1:C:243:ASP:CG	2.86	0.43
1:A:96:ALA:HB1	1:A:98:THR:O	2.19	0.42
1:A:134:SER:H	1:A:230:SER:HB3	1.84	0.42
1:B:64:ARG:HD3	1:B:94:ASP:OD2	2.20	0.42
1:B:135:CYS:SG	1:B:199:MET:HG3	2.59	0.42
1:B:93:GLU:HG2	1:B:94:ASP:N	2.34	0.42
1:B:244:MET:HE3	1:B:244:MET:HB2	1.78	0.42
1:C:135:CYS:SG	1:C:203:VAL:CG2	3.04	0.42
1:B:9:GLY:O	1:B:10:SER:C	2.62	0.42
1:B:99:LEU:HD12	1:B:99:LEU:C	2.39	0.42
1:B:13:LYS:HE2	1:B:13:LYS:HB3	1.65	0.42
1:B:200:ASN:O	1:B:201:GLU:HG3	2.20	0.42
1:C:27:CYS:SG	1:C:123:VAL:HG21	2.58	0.42
1:B:139:MET:CE	1:B:144:PHE:HD1	2.33	0.42
1:C:123:VAL:HG12	1:C:125:GLN:HG3	2.02	0.42
1:A:233:VAL:HA	1:A:234:PRO:HD2	1.94	0.42
1:B:71:ASN:HD22	1:B:74:SER:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:CG	1:B:228:SER:HB3	2.54	0.42
1:A:16:LEU:N	1:A:16:LEU:CD2	2.83	0.41
1:B:139:MET:HE3	1:B:144:PHE:CB	2.50	0.41
1:B:225:VAL:HG22	1:B:226:THR:N	2.34	0.41
1:C:128:ILE:HA	1:C:129:PRO:HD3	1.82	0.41
1:C:210:ARG:HD2	2:D:56:ARG:O	2.20	0.41
1:A:159:VAL:O	1:A:159:VAL:HG12	2.19	0.41
2:E:65:ILE:O	2:E:65:ILE:HG13	2.20	0.41
1:B:93:GLU:HG2	1:B:96:ALA:CB	2.51	0.41
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.88	0.41
1:B:71:ASN:ND2	1:B:74:SER:H	2.18	0.41
1:A:6:LEU:HD13	1:A:244:MET:HE1	1.98	0.41
1:C:62:CYS:SG	1:C:64:ARG:O	2.79	0.41
1:C:143:GLU:O	1:C:147:ILE:HG13	2.20	0.41
1:A:39:SER:O	1:A:47:LEU:HD12	2.21	0.41
1:B:116:MET:HG2	1:B:117:LYS:O	2.21	0.41
1:A:89:THR:HG21	1:A:91:ARG:HH21	1.86	0.41
1:A:162:CYS:HB2	1:A:203:VAL:H	1.84	0.41
1:B:86:ASP:OD1	1:B:86:ASP:N	2.53	0.41
1:A:16:LEU:HD13	1:A:16:LEU:HA	1.90	0.41
1:A:228:SER:HB2	1:A:236:VAL:HG22	2.03	0.41
1:B:94:ASP:O	1:B:95:ASN:HB3	2.21	0.41
1:C:149:ARG:CD	2:D:51:ASN:O	2.39	0.41
1:B:151:LEU:O	1:B:152:SER:C	2.61	0.40
1:B:23:ILE:O	1:B:23:ILE:HG13	2.22	0.40
1:C:16:LEU:O	1:C:20:LYS:HB3	2.21	0.40
1:C:251:LEU:HG	1:C:252:ALA:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/264 (96%)	242 (96%)	11 (4%)	0	100	100
1	B	253/264 (96%)	242 (96%)	9 (4%)	2 (1%)	16	44
1	C	253/264 (96%)	237 (94%)	16 (6%)	0	100	100
2	D	19/32 (59%)	17 (90%)	2 (10%)	0	100	100
2	E	20/32 (62%)	19 (95%)	1 (5%)	0	100	100
2	F	21/32 (66%)	20 (95%)	1 (5%)	0	100	100
All	All	819/888 (92%)	777 (95%)	40 (5%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	152	SER
1	B	216	THR

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	223/230 (97%)	209 (94%)	14 (6%)	16	45
1	B	223/230 (97%)	203 (91%)	20 (9%)	9	28
1	C	221/230 (96%)	204 (92%)	17 (8%)	12	35
2	D	19/26 (73%)	19 (100%)	0	100	100
2	E	20/26 (77%)	18 (90%)	2 (10%)	7	24
2	F	20/26 (77%)	19 (95%)	1 (5%)	22	53
All	All	726/768 (94%)	672 (93%)	54 (7%)	13	38

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	27	CYS
1	A	32	SER

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Mol	Chain	Res	Type
1	A	33	SER
1	A	107	ASN
1	A	134	SER
1	A	146	ARG
1	A	159	VAL
1	A	170	SER
1	A	192	GLU
1	A	217	LYS
1	A	226	THR
1	A	236	VAL
1	A	255	ILE
1	B	17	GLU
1	B	22	LEU
1	B	35	VAL
1	B	36	ASN
1	B	37	LEU
1	B	42	SER
1	B	48	VAL
1	B	73	THR
1	B	85	GLU
1	B	98	THR
1	B	112	SER
1	B	124	GLU
1	B	132	GLU
1	B	134	SER
1	B	138	LYS
1	B	198	GLU
1	B	216	THR
1	B	217	LYS
1	B	226	THR
1	B	243	ASP
1	C	7	VAL
1	C	8	GLN
1	C	37	LEU
1	C	42	SER
1	C	43	SER
1	C	66	LEU
1	C	90	LEU
1	C	98	THR
1	C	122	ASP
1	C	191	GLU
1	C	205	LEU

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Mol	Chain	Res	Type
1	C	216	THR
1	C	223	SER
1	C	226	THR
1	C	233	VAL
1	C	236	VAL
1	C	255	ILE
2	E	57	PRO
2	E	71	LEU
2	F	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	38	GLN
1	A	49	GLN
1	A	107	ASN
1	A	125	GLN
1	A	153	HIS
1	A	184	GLN
1	A	187	ASN
1	B	8	GLN
1	B	49	GLN
1	B	65	ASN
1	B	71	ASN
1	B	131	GLN
1	B	246	HIS
1	C	24	ASN
1	C	38	GLN
1	C	153	HIS
1	C	179	ASN
1	C	184	GLN
2	D	51	ASN
2	F	62	GLN

5.3.3 RNA ⓘ

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	255/264 (96%)	-0.34	2 (0%) 82 77	65, 97, 150, 191	0
1	B	255/264 (96%)	-0.39	1 (0%) 88 85	64, 90, 133, 180	0
1	C	255/264 (96%)	-0.39	0 100 100	62, 91, 147, 200	0
2	D	21/32 (65%)	-0.45	0 100 100	78, 91, 119, 121	0
2	E	22/32 (68%)	-0.48	0 100 100	73, 88, 109, 126	0
2	F	23/32 (71%)	-0.26	0 100 100	74, 103, 127, 136	0
All	All	831/888 (93%)	-0.38	3 (0%) 88 85	62, 94, 145, 200	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	CYS	2.4
1	A	162	CYS	2.3
1	A	255	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.