



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:56 PM UTC

PDB ID : 7VPH / pdb_00007vph
Title : Crystal structure of the C-terminal tail of SARS-CoV-2 Orf6 complex with human nucleoporin pair Rae1-Nup98
Authors : Li, T.; Guo, H.; Yang, T.; Wen, Y.; Ji, X.
Deposited on : 2021-10-17
Resolution : 2.80 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

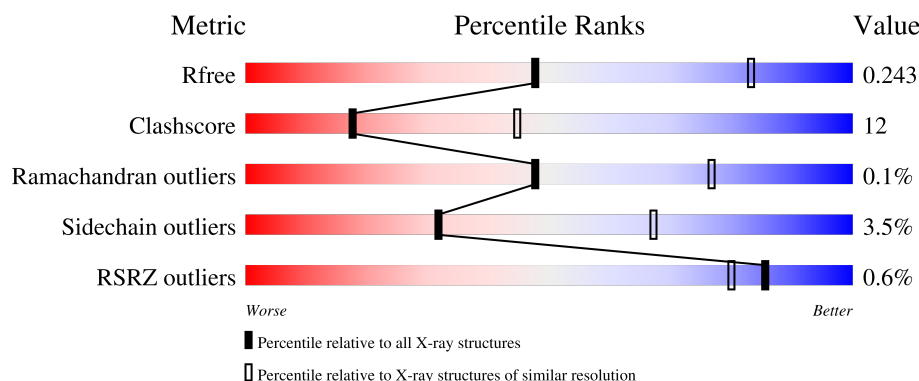
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	378	
1	C	378	
1	E	378	
1	G	378	
2	B	67	

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Mol	Chain	Length	Quality of chain
2	D	67	49%16%34%
2	F	67	70%10%19%
2	H	67	% 39%30%31%
3	I	21	29%10%5%57%
3	J	21	33%5%62%
3	K	21	29%14%57%
3	X	21	33%10%57%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12567 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 mRNA export factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2681	1693	470	500	18			
1	C	337	Total	C	N	O	S	0	1	0
			2674	1690	470	496	18			
1	E	336	Total	C	N	O	S	0	0	0
			2658	1681	465	494	18			
1	G	336	Total	C	N	O	S	0	0	0
			2656	1680	463	495	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	HIS	-	expression tag	UNP P78406
A	370	HIS	-	expression tag	UNP P78406
A	371	HIS	-	expression tag	UNP P78406
A	372	HIS	-	expression tag	UNP P78406
A	373	HIS	-	expression tag	UNP P78406
A	374	HIS	-	expression tag	UNP P78406
A	375	HIS	-	expression tag	UNP P78406
A	376	HIS	-	expression tag	UNP P78406
A	377	HIS	-	expression tag	UNP P78406
A	378	HIS	-	expression tag	UNP P78406
C	369	HIS	-	expression tag	UNP P78406
C	370	HIS	-	expression tag	UNP P78406
C	371	HIS	-	expression tag	UNP P78406
C	372	HIS	-	expression tag	UNP P78406
C	373	HIS	-	expression tag	UNP P78406
C	374	HIS	-	expression tag	UNP P78406
C	375	HIS	-	expression tag	UNP P78406
C	376	HIS	-	expression tag	UNP P78406
C	377	HIS	-	expression tag	UNP P78406
C	378	HIS	-	expression tag	UNP P78406
E	369	HIS	-	expression tag	UNP P78406

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Chain	Residue	Modelled	Actual	Comment	Reference
E	370	HIS	-	expression tag	UNP P78406
E	371	HIS	-	expression tag	UNP P78406
E	372	HIS	-	expression tag	UNP P78406
E	373	HIS	-	expression tag	UNP P78406
E	374	HIS	-	expression tag	UNP P78406
E	375	HIS	-	expression tag	UNP P78406
E	376	HIS	-	expression tag	UNP P78406
E	377	HIS	-	expression tag	UNP P78406
E	378	HIS	-	expression tag	UNP P78406
G	369	HIS	-	expression tag	UNP P78406
G	370	HIS	-	expression tag	UNP P78406
G	371	HIS	-	expression tag	UNP P78406
G	372	HIS	-	expression tag	UNP P78406
G	373	HIS	-	expression tag	UNP P78406
G	374	HIS	-	expression tag	UNP P78406
G	375	HIS	-	expression tag	UNP P78406
G	376	HIS	-	expression tag	UNP P78406
G	377	HIS	-	expression tag	UNP P78406
G	378	HIS	-	expression tag	UNP P78406

- Molecule 2 is a protein called Isoform 3 of Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	51	Total	C	N	O	S	0	0	0
			405	247	69	86	3			
2	D	44	Total	C	N	O	S	0	0	0
			353	217	61	73	2			
2	F	54	Total	C	N	O	S	0	0	0
			423	259	72	89	3			
2	H	46	Total	C	N	O	S	0	0	0
			369	227	64	76	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	MET	-	initiating methionine	UNP P52948
B	148	HIS	-	expression tag	UNP P52948
B	149	HIS	-	expression tag	UNP P52948
B	150	HIS	-	expression tag	UNP P52948
B	151	HIS	-	expression tag	UNP P52948
B	152	HIS	-	expression tag	UNP P52948
B	153	HIS	-	expression tag	UNP P52948

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Chain	Residue	Modelled	Actual	Comment	Reference
B	154	HIS	-	expression tag	UNP P52948
B	155	HIS	-	expression tag	UNP P52948
B	156	HIS	-	expression tag	UNP P52948
B	157	HIS	-	expression tag	UNP P52948
D	147	MET	-	initiating methionine	UNP P52948
D	148	HIS	-	expression tag	UNP P52948
D	149	HIS	-	expression tag	UNP P52948
D	150	HIS	-	expression tag	UNP P52948
D	151	HIS	-	expression tag	UNP P52948
D	152	HIS	-	expression tag	UNP P52948
D	153	HIS	-	expression tag	UNP P52948
D	154	HIS	-	expression tag	UNP P52948
D	155	HIS	-	expression tag	UNP P52948
D	156	HIS	-	expression tag	UNP P52948
D	157	HIS	-	expression tag	UNP P52948
F	147	MET	-	initiating methionine	UNP P52948
F	148	HIS	-	expression tag	UNP P52948
F	149	HIS	-	expression tag	UNP P52948
F	150	HIS	-	expression tag	UNP P52948
F	151	HIS	-	expression tag	UNP P52948
F	152	HIS	-	expression tag	UNP P52948
F	153	HIS	-	expression tag	UNP P52948
F	154	HIS	-	expression tag	UNP P52948
F	155	HIS	-	expression tag	UNP P52948
F	156	HIS	-	expression tag	UNP P52948
F	157	HIS	-	expression tag	UNP P52948
H	147	MET	-	initiating methionine	UNP P52948
H	148	HIS	-	expression tag	UNP P52948
H	149	HIS	-	expression tag	UNP P52948
H	150	HIS	-	expression tag	UNP P52948
H	151	HIS	-	expression tag	UNP P52948
H	152	HIS	-	expression tag	UNP P52948
H	153	HIS	-	expression tag	UNP P52948
H	154	HIS	-	expression tag	UNP P52948
H	155	HIS	-	expression tag	UNP P52948
H	156	HIS	-	expression tag	UNP P52948
H	157	HIS	-	expression tag	UNP P52948

- Molecule 3 is a protein called ORF6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	9	Total	C	N	O	S	0	0	0
			75	44	10	20	1			

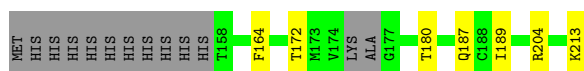
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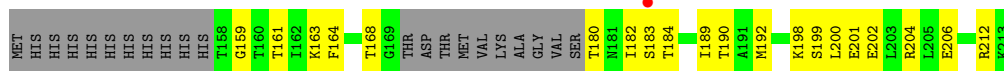
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	8	Total	C	N	O	S	0	0	0
			67	40	9	17	1			
3	K	9	Total	C	N	O	S	0	0	0
			75	44	10	20	1			
3	X	9	Total	C	N	O	S	0	0	0
			75	44	10	20	1			

- Molecule 4 is water.

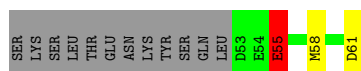
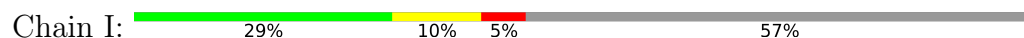
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	2	Total	O	0	0
			2	2		
4	C	8	Total	O	0	0
			8	8		
4	D	1	Total	O	0	0
			1	1		
4	E	17	Total	O	0	0
			17	17		
4	F	1	Total	O	0	0
			1	1		
4	G	4	Total	O	0	0
			4	4		
4	X	2	Total	O	0	0
			2	2		



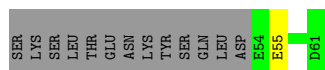
- Molecule 2: Isoform 3 of Nuclear pore complex protein Nup98-Nup96



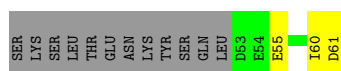
- Molecule 3: ORF6 protein



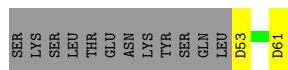
- Molecule 3: ORF6 protein



- Molecule 3: ORF6 protein



- Molecule 3: ORF6 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.66Å 103.32Å 136.59Å 90.00° 97.45° 90.00°	Depositor
Resolution (Å)	41.06 – 2.80 41.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.06-2.80) 99.5 (41.06-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.192 , 0.244 0.192 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12567	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.51	0/2758	0.74	2/3749 (0.1%)
1	C	0.52	2/2754 (0.1%)	0.96	19/3742 (0.5%)
1	E	0.45	0/2734	0.70	3/3714 (0.1%)
1	G	0.45	0/2732	0.77	9/3713 (0.2%)
2	B	0.58	1/409 (0.2%)	0.75	0/547
2	D	0.44	0/357	0.67	0/476
2	F	0.41	0/427	0.62	0/572
2	H	0.36	0/373	0.67	0/498
3	I	0.45	0/75	1.12	2/100 (2.0%)
3	J	0.41	0/67	0.71	0/89
3	K	0.33	0/75	0.68	0/100
3	X	0.69	0/75	0.95	0/100
All	All	0.48	3/12836 (0.0%)	0.79	35/17400 (0.2%)

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	C	0	3
1	G	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	360	GLU	CD-OE1	5.58	1.35	1.25
2	B	193	LYS	CE-NZ	5.32	1.65	1.49
1	C	328	ASN	CB-CG	5.29	1.65	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	GLU	N-CA-C	-14.41	94.07	112.23
1	C	360	GLU	CG-CD-OE2	-13.40	87.58	118.40
1	C	227	LYS	CA-CB-CG	12.55	139.21	114.10
1	G	196	GLN	CA-CB-CG	11.08	136.26	114.10
1	A	349	LYS	CG-CD-CE	-10.08	88.11	111.30
1	C	71	VAL	CA-C-N	10.03	137.47	122.93
1	C	71	VAL	C-N-CA	10.03	137.47	122.93
1	C	360	GLU	CG-CD-OE1	9.94	141.25	118.40
1	C	360	GLU	CA-C-N	8.23	132.82	120.31
1	C	360	GLU	C-N-CA	8.23	132.82	120.31
1	C	359	ALA	N-CA-C	-7.75	102.80	111.71
1	C	72	GLN	CA-CB-CG	7.24	128.57	114.10
1	C	360	GLU	CB-CG-CD	7.15	124.75	112.60
1	E	72	GLN	CB-CA-C	7.13	123.38	109.33
1	G	189	GLU	CA-CB-CG	-7.05	99.99	114.10
1	G	75	GLY	CA-C-N	-7.01	110.23	122.64
1	G	75	GLY	C-N-CA	-7.01	110.23	122.64
1	C	227	LYS	CD-CE-NZ	6.84	133.81	111.90
1	C	72	GLN	CB-CA-C	6.65	121.35	109.38
1	C	357	ASN	N-CA-C	6.61	124.88	110.80
1	E	72	GLN	CA-CB-CG	6.56	127.21	114.10
1	G	36	SER	CA-C-N	6.26	131.56	122.29
1	G	36	SER	C-N-CA	6.26	131.56	122.29
1	C	358	ALA	CA-C-N	-6.11	111.48	120.28
1	C	358	ALA	C-N-CA	-6.11	111.48	120.28
3	I	55	GLU	CA-CB-CG	6.04	126.17	114.10
1	C	328	ASN	CB-CA-C	5.92	121.19	112.07
1	G	196	GLN	N-CA-C	-5.84	100.18	109.59
1	C	359	ALA	CA-C-N	-5.83	110.78	120.68
1	C	359	ALA	C-N-CA	-5.83	110.78	120.68
3	I	55	GLU	CB-CA-C	5.59	118.95	109.84
1	A	349	LYS	CB-CG-CD	5.58	124.12	111.30
1	E	157	ASP	CB-CA-C	-5.38	99.23	109.95
1	G	196	GLN	CA-C-N	-5.06	114.39	122.29
1	G	196	GLN	C-N-CA	-5.06	114.39	122.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	328	ASN	Peptide
1	C	356	ARG	Peptide
1	C	359	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	G	26	HIS	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	2681	0	2575	68	0
1	C	2674	0	2575	70	0
1	E	2658	0	2555	62	0
1	G	2656	0	2547	83	0
2	B	405	0	397	10	0
2	D	353	0	348	6	0
2	F	423	0	418	7	0
2	H	369	0	365	17	0
3	I	75	0	60	5	0
3	J	67	0	56	1	0
3	K	75	0	60	2	0
3	X	75	0	60	3	0
4	A	21	0	0	1	0
4	B	2	0	0	1	0
4	C	8	0	0	0	0
4	D	1	0	0	0	0
4	E	17	0	0	2	0
4	F	1	0	0	0	0
4	G	4	0	0	0	0
4	X	2	0	0	0	0
All	All	12567	0	12016	303	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 12.

All (303) 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)
2:H:182:ILE:HG22	2:H:183:SER:H	1.33	0.93
1:A:171:GLU:HG3	1:A:172:ARG:H	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:MET:HE1	1:G:158:THR:HB	1.54	0.89
1:C:328:ASN:HB2	1:C:357:ASN:OD1	1.74	0.88
1:C:34:VAL:HA	1:C:77:THR:HG21	1.56	0.86
1:C:272:ASP:HB3	1:C:274:TYR:HE2	1.40	0.85
1:C:72:GLN:OE1	1:C:73:ASP:N	2.13	0.81
1:A:171:GLU:HG2	1:A:188:ALA:HB3	1.63	0.81
1:G:293:SER:HA	1:G:317:PRO:HB3	1.64	0.80
1:A:171:GLU:HG3	1:A:172:ARG:N	2.00	0.76
1:C:62:TRP:HA	1:C:88:PRO:HB3	1.68	0.76
1:A:350:LYS:HD3	1:A:350:LYS:N	1.99	0.75
1:A:143:CYS:HB3	1:A:164:MET:HE1	1.68	0.74
1:G:56:PHE:CE2	1:G:70:GLU:HG3	2.24	0.73
1:C:244:TYR:OH	1:C:302:LYS:NZ	2.23	0.72
1:A:267:THR:HG22	1:A:269:ALA:H	1.53	0.72
1:C:211:LEU:HD13	1:C:235:SER:HB3	1.71	0.71
1:C:272:ASP:HB3	1:C:274:TYR:CE2	2.24	0.71
1:C:307:LYS:O	3:I:55:GLU:HA	1.92	0.70
1:E:110:ALA:HB3	1:E:124:ALA:HB3	1.74	0.70
1:A:88:PRO:HD2	1:A:106:CYS:HB2	1.74	0.69
1:A:165:MET:HE1	1:A:200:GLN:HG3	1.74	0.69
1:G:307:LYS:HE3	1:G:310:THR:OG1	1.92	0.69
1:E:88:PRO:HD2	1:E:106:CYS:HB2	1.75	0.69
1:G:165:MET:HE1	1:G:201:PRO:HD2	1.75	0.69
1:E:189:GLU:OE1	4:E:401:HOH:O	2.12	0.66
1:C:102:PHE:CE1	1:C:112:MET:HG3	2.31	0.66
1:G:29:MET:HE3	1:G:311:SER:HB2	1.78	0.66
2:D:163:LYS:NZ	2:F:213:LYS:O	2.23	0.66
1:C:357:ASN:ND2	1:C:360:GLU:OE2	2.28	0.66
1:G:34:VAL:HG13	1:G:77:THR:HG21	1.77	0.65
1:G:196:GLN:OE1	1:G:202:SER:OG	2.13	0.64
1:A:282:HIS:HD2	1:A:285:HIS:H	1.46	0.64
1:A:282:HIS:CD2	1:A:285:HIS:H	2.15	0.64
1:G:145:MET:HG3	1:G:155:PHE:CE2	2.33	0.63
1:G:182:MET:HE3	1:G:228:PRO:HB2	1.80	0.63
1:E:145:MET:HG3	1:E:155:PHE:CE2	2.33	0.62
1:G:69:TRP:CD1	1:G:77:THR:HG1	2.17	0.62
1:G:273:ILE:HD11	2:H:184:THR:HB	1.80	0.62
1:E:101:VAL:HG23	1:E:115:LEU:HD21	1.81	0.62
1:G:52:LEU:HD13	1:G:98:GLY:HA3	1.82	0.62
1:C:328:ASN:CG	1:C:359:ALA:HB2	2.25	0.62
1:G:337:ASP:O	2:H:200:LEU:HD23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:MET:HE1	1:C:200:GLN:HG3	1.81	0.62
1:C:85:HIS:CE1	1:C:111:LYS:HG3	2.34	0.62
1:C:110:ALA:HB3	1:C:124:ALA:HB3	1.82	0.62
1:E:198:GLU:O	1:E:200:GLN:N	2.33	0.62
1:A:41:SER:HG	2:B:204:ARG:HH22	1.49	0.61
1:G:174:TYR:CZ	2:H:199:SER:HB3	2.36	0.61
1:G:299:PHE:HB3	1:G:362:LEU:HD21	1.83	0.60
1:A:171:GLU:CG	1:A:188:ALA:HB3	2.30	0.60
1:A:58:ILE:HD13	1:A:68:CYS:HB2	1.83	0.59
1:E:154:LYS:HG2	1:E:166:VAL:HG22	1.83	0.59
1:C:193:ILE:HG12	1:C:206[A]:ARG:HD3	1.84	0.59
1:C:282:HIS:HE1	1:C:284:VAL:HB	1.67	0.59
2:D:167:PRO:HD2	2:D:186:HIS:HB2	1.84	0.59
1:A:41:SER:OG	2:B:204:ARG:NH2	2.29	0.59
1:G:291:VAL:HB	1:G:318:ILE:HB	1.85	0.58
1:A:66:VAL:HG23	1:A:89:VAL:HG21	1.85	0.58
1:G:132:THR:OG1	1:G:134:HIS:NE2	2.37	0.58
1:C:316:GLN:HB2	1:C:317:PRO:HD2	1.84	0.58
1:C:31:ASP:OD1	1:C:356:ARG:NH1	2.37	0.57
1:A:51:THR:OG1	1:A:96:ASP:O	2.19	0.57
1:G:239:ARG:NH1	3:K:61:ASP:OD2	2.37	0.57
1:A:282:HIS:NE2	1:A:284:VAL:HG22	2.19	0.57
2:D:198:LYS:NZ	2:D:206:GLU:OE2	2.38	0.57
1:G:83:GLN:HG2	1:G:113:TRP:CE2	2.40	0.57
1:A:205:ARG:HG2	1:A:207:ILE:HD13	1.87	0.57
1:E:106:CYS:HA	1:E:129:PRO:HB3	1.85	0.56
1:E:133:ILE:HD12	1:E:146:THR:HG22	1.86	0.56
1:A:40:ASP:HB2	1:A:63:ALA:HB2	1.86	0.56
1:E:252:LYS:O	1:E:252:LYS:HD3	2.05	0.56
1:E:351:ASN:OD1	4:E:402:HOH:O	2.17	0.56
1:A:239:ARG:NH1	3:X:61:ASP:OD2	2.35	0.56
1:E:112:MET:O	1:E:120:ALA:HA	2.06	0.56
1:E:340:LYS:HG2	2:F:164:PHE:CE2	2.41	0.56
1:G:100:LYS:HD2	1:G:112:MET:SD	2.46	0.55
1:E:56:PHE:CZ	1:E:70:GLU:HG3	2.41	0.55
1:C:337:ASP:OD1	1:C:339:SER:OG	2.21	0.55
2:H:182:ILE:HG22	2:H:183:SER:N	2.14	0.55
1:C:328:ASN:CB	1:C:359:ALA:HB2	2.36	0.55
1:E:214:GLN:HB3	1:E:236:ILE:HD13	1.88	0.55
1:G:29:MET:O	1:G:30:LYS:HG2	2.06	0.55
1:G:32:ILE:HG21	1:G:75:GLY:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASP:OD1	1:C:294:ASP:N	2.38	0.55
1:G:66:VAL:HG13	1:G:89:VAL:HG21	1.89	0.55
1:G:76:GLN:HG3	1:G:77:THR:N	2.22	0.55
1:C:190:ARG:NH1	1:C:211:LEU:O	2.36	0.54
1:C:365:ARG:HD2	1:C:365:ARG:N	2.22	0.54
1:G:216:ARG:NH2	2:H:200:LEU:HB2	2.22	0.54
1:G:157:ASP:O	1:G:158:THR:OG1	2.20	0.54
1:E:282:HIS:CE1	1:E:284:VAL:HG13	2.43	0.54
1:G:31:ASP:CG	1:G:356:ARG:HG3	2.32	0.54
1:A:65:ASP:HB3	1:A:84:MET:HE2	1.89	0.54
1:C:274:TYR:HB3	1:C:293:SER:HB3	1.89	0.54
1:E:144:VAL:O	1:E:155:PHE:HA	2.07	0.54
1:E:157:ASP:HB2	1:E:159:ARG:HG2	1.89	0.54
1:G:300:TRP:CZ3	1:G:307:LYS:HB2	2.43	0.54
1:G:190:ARG:HA	1:G:215:HIS:CE1	2.43	0.53
1:C:307:LYS:NZ	1:C:310:THR:OG1	2.30	0.53
1:G:261:ARG:HG2	1:G:273:ILE:HG23	1.90	0.53
1:C:192:LEU:O	1:C:206[A]:ARG:HD2	2.08	0.53
2:H:202:GLU:O	2:H:206:GLU:HG3	2.09	0.53
1:A:356:ARG:NH2	1:A:361:GLU:OE2	2.41	0.53
1:E:92:VAL:HG12	1:E:103:THR:HA	1.90	0.53
1:G:106:CYS:HA	1:G:129:PRO:HB3	1.90	0.53
1:G:85:HIS:CE1	1:G:111:LYS:HG3	2.44	0.52
1:A:46:SER:HB2	1:A:92:VAL:HG23	1.91	0.52
1:E:180:TYR:CD2	1:E:181:PRO:HA	2.44	0.52
1:A:183:ALA:HB3	1:A:195:TYR:HB2	1.91	0.52
1:A:348:GLN:O	1:A:350:LYS:NZ	2.43	0.52
1:C:42:ILE:HD12	1:C:333:ALA:HB1	1.92	0.52
1:C:106:CYS:HA	1:C:129:PRO:HB3	1.91	0.52
1:A:165:MET:HE1	1:A:200:GLN:CG	2.38	0.52
2:H:189:ILE:O	2:H:192:MET:HB2	2.10	0.52
1:G:85:HIS:NE2	1:G:103:THR:OG1	2.30	0.52
1:A:309:LYS:HD2	3:X:53:ASP:HB2	1.90	0.51
1:C:58:ILE:HD11	1:C:94:TRP:CZ2	2.44	0.51
1:E:112:MET:HE2	1:E:123:ILE:HG21	1.92	0.51
1:G:58:ILE:HD13	1:G:94:TRP:CZ2	2.44	0.51
1:G:62:TRP:CZ3	2:H:204:ARG:HG2	2.44	0.51
1:A:174:TYR:CZ	1:A:188:ALA:HB2	2.45	0.51
1:G:81:ALA:HB1	1:G:118:ASN:OD1	2.10	0.51
1:G:165:MET:HE1	1:G:201:PRO:CD	2.39	0.51
1:G:211:LEU:HD13	1:G:235:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:TYR:CD2	1:G:181:PRO:HA	2.46	0.51
1:A:144:VAL:O	1:A:155:PHE:HA	2.10	0.51
1:A:211:LEU:HD13	1:A:235:SER:HB3	1.92	0.51
1:C:308:LEU:HD23	3:I:55:GLU:HG3	1.92	0.51
1:E:252:LYS:HD3	1:E:252:LYS:C	2.35	0.51
1:A:171:GLU:OE2	1:A:172:ARG:NH1	2.44	0.51
1:A:217:CYS:SG	1:A:279:ILE:HG13	2.51	0.51
1:G:72:GLN:CD	1:G:78:ILE:HD11	2.36	0.51
2:H:182:ILE:CG2	2:H:183:SER:H	2.14	0.51
1:G:29:MET:CE	1:G:312:GLU:H	2.24	0.50
1:E:258:LYS:NZ	2:F:172:THR:O	2.45	0.50
1:A:190:ARG:HD3	1:A:212:LYS:HA	1.94	0.50
1:C:182:MET:HE1	1:C:245:ILE:HG13	1.93	0.49
1:C:26:HIS:HA	1:C:315:ASP:OD1	2.12	0.49
1:E:224:LYS:HD3	1:E:224:LYS:N	2.27	0.49
1:E:272:ASP:HB3	2:F:187:GLN:HG3	1.94	0.49
1:G:184:VAL:HG12	1:G:220:ILE:HD11	1.94	0.49
2:B:193:LYS:HD2	2:B:193:LYS:O	2.11	0.49
1:G:26:HIS:ND1	1:G:27:ASN:N	2.61	0.49
2:H:159:GLY:HA3	2:H:212:ARG:NH1	2.28	0.49
1:C:72:GLN:HB3	1:C:76:GLN:O	2.13	0.49
1:C:359:ALA:O	1:C:360:GLU:C	2.55	0.49
1:E:104:ALA:HB1	1:E:130:VAL:HG12	1.94	0.49
1:G:62:TRP:HA	1:G:88:PRO:HB3	1.94	0.49
1:A:85:HIS:NE2	1:A:103:THR:OG1	2.38	0.48
1:G:196:GLN:O	1:G:197:LEU:HD23	2.12	0.48
1:E:358:ALA:HB1	1:E:361:GLU:HB2	1.95	0.48
1:A:31:ASP:OD2	1:A:356:ARG:HD2	2.14	0.48
1:C:225:GLN:N	1:C:225:GLN:OE1	2.46	0.48
1:A:221:PHE:CD1	1:A:302:LYS:HE2	2.49	0.48
1:A:282:HIS:CD2	1:A:284:VAL:H	2.30	0.48
1:G:216:ARG:NH2	2:H:201:GLU:OE2	2.47	0.48
2:H:163:LYS:O	2:H:192:MET:HE1	2.14	0.48
1:C:291:VAL:HG11	1:C:321:CYS:HB3	1.96	0.48
1:A:41:SER:HB3	1:A:335:SER:HB3	1.96	0.48
1:C:343:GLU:HG2	1:E:346:ASN:CG	2.39	0.48
1:G:69:TRP:HB3	1:G:77:THR:HB	1.95	0.48
2:B:173:MET:HE2	2:B:182:ILE:HD13	1.95	0.47
1:E:128:ALA:HB1	1:E:129:PRO:HD2	1.96	0.47
1:G:237:GLU:O	1:G:239:ARG:N	2.47	0.47
1:A:62:TRP:HA	1:A:88:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:GLN:HG2	1:C:83:GLN:N	2.30	0.47
1:C:144:VAL:O	1:C:155:PHE:HA	2.14	0.47
1:A:26:HIS:HD2	1:A:352:TYR:CZ	2.32	0.47
1:A:282:HIS:HD2	1:A:284:VAL:H	1.61	0.47
1:C:282:HIS:CD2	1:C:327:GLY:O	2.67	0.47
1:E:62:TRP:HA	1:E:88:PRO:HB3	1.95	0.47
1:G:78:ILE:HB	1:G:80:LYS:HZ2	1.78	0.47
1:C:282:HIS:CE1	1:C:284:VAL:HB	2.48	0.47
1:C:306:THR:HB	3:I:55:GLU:HG2	1.97	0.47
1:C:180:TYR:CD2	1:C:181:PRO:HA	2.50	0.47
1:E:84:MET:HE3	1:E:84:MET:HB3	1.67	0.47
1:E:140:ASN:OD1	1:E:140:ASN:N	2.48	0.47
1:C:336:TYR:CE2	1:C:338:TRP:HA	2.50	0.47
1:E:113:TRP:HA	1:E:119:GLN:O	2.15	0.47
1:A:300:TRP:CZ3	1:A:307:LYS:HG3	2.50	0.46
1:C:165:MET:HE1	1:C:201:PRO:HD2	1.98	0.46
1:E:91:ASP:HB3	1:E:133:ILE:HG22	1.97	0.46
1:A:126:HIS:CD2	1:A:130:VAL:HG22	2.50	0.46
1:C:324:ASN:ND2	1:C:326:ASN:OD1	2.48	0.46
1:C:343:GLU:HG2	1:E:346:ASN:OD1	2.15	0.46
1:E:58:ILE:HD13	1:E:94:TRP:CZ2	2.50	0.46
1:G:260:HIS:ND1	1:G:294:ASP:OD1	2.46	0.46
1:G:293:SER:HB3	1:G:337:ASP:OD2	2.15	0.46
1:G:37:SER:HA	1:G:69:TRP:HZ2	1.79	0.46
1:A:145:MET:HG3	1:A:155:PHE:CE2	2.50	0.46
2:B:204:ARG:NH1	4:B:301:HOH:O	2.37	0.46
1:A:221:PHE:HB3	1:A:281:PHE:CE2	2.50	0.46
1:C:331:ALA:HA	1:C:354:PHE:O	2.16	0.46
1:E:96:ASP:OD1	1:E:135:TRP:NE1	2.49	0.46
1:E:306:THR:HB	3:J:55:GLU:HG3	1.97	0.46
1:C:358:ALA:HB1	1:C:361:GLU:HB2	1.98	0.46
1:C:38:PRO:HA	1:C:67:ARG:NH1	2.31	0.45
1:G:255:PHE:CD2	3:K:60:ILE:HG12	2.51	0.45
1:E:274:TYR:CD1	1:E:294:ASP:HB3	2.51	0.45
1:G:96:ASP:OD1	1:G:137:LYS:HD3	2.16	0.45
1:A:110:ALA:HB3	1:A:124:ALA:HB3	1.99	0.45
1:E:101:VAL:CG2	1:E:115:LEU:HD21	2.46	0.45
1:A:34:VAL:HG13	1:A:77:THR:HG21	1.99	0.45
1:A:112:MET:O	1:A:120:ALA:HA	2.16	0.45
1:A:126:HIS:CE1	1:A:154:LYS:HD2	2.52	0.45
1:C:258:LYS:NZ	3:I:61:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:SER:OG	2:F:204:ARG:NH2	2.40	0.45
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.83	0.45
2:H:198:LYS:NZ	2:H:206:GLU:OE2	2.43	0.45
1:G:141:TYR:OH	1:G:201:PRO:HD3	2.17	0.44
1:A:67:ARG:HB2	1:A:69:TRP:CH2	2.51	0.44
1:E:65:ASP:OD2	1:E:67:ARG:NE	2.50	0.44
1:G:84:MET:HE3	1:G:84:MET:HB2	1.78	0.44
2:B:167:PRO:HD2	2:B:186:HIS:HB2	1.99	0.44
1:G:315:ASP:OD1	1:G:315:ASP:N	2.47	0.44
1:G:34:VAL:HG23	1:G:353:ILE:O	2.16	0.44
2:H:189:ILE:HG23	2:H:190:THR:HG23	1.99	0.44
1:C:274:TYR:CD1	1:C:294:ASP:HA	2.52	0.44
2:D:205:LEU:O	2:D:209:GLN:HG3	2.18	0.44
1:A:338:TRP:CD2	2:B:204:ARG:HG3	2.53	0.44
1:G:80:LYS:HD3	1:G:80:LYS:HA	1.72	0.44
2:H:164:PHE:HD1	2:H:189:ILE:HD12	1.83	0.44
1:G:211:LEU:HD21	1:G:241:ALA:HB2	1.99	0.43
1:C:305:ARG:C	3:I:58:MET:HG3	2.43	0.43
1:E:336:TYR:CE2	1:E:338:TRP:HA	2.52	0.43
1:C:194:VAL:HG23	1:C:204:PHE:HB3	2.00	0.43
1:C:295:GLY:O	1:C:314:LEU:HD23	2.17	0.43
1:G:151:LYS:HG2	1:G:171:GLU:C	2.42	0.43
1:A:34:VAL:HG23	1:A:353:ILE:O	2.18	0.43
1:E:32:ILE:HD12	1:E:32:ILE:N	2.33	0.43
1:E:119:GLN:HA	1:E:119:GLN:OE1	2.17	0.43
1:G:118:ASN:O	1:G:118:ASN:ND2	2.48	0.43
1:E:32:ILE:HD12	1:E:32:ILE:H	1.84	0.43
1:G:298:SER:OG	1:G:310:THR:HG23	2.19	0.43
1:A:170:PRO:HG3	1:A:193:ILE:HD11	2.01	0.43
2:F:164:PHE:CD1	2:F:189:ILE:HG13	2.54	0.43
1:C:35:THR:HG23	1:C:77:THR:HG23	2.00	0.43
1:C:164:MET:HE2	1:C:164:MET:HB3	1.85	0.43
1:A:184:VAL:HG23	1:A:220:ILE:HD11	2.01	0.43
1:E:331:ALA:HA	1:E:354:PHE:O	2.19	0.43
1:A:56:PHE:CE2	1:A:70:GLU:HB2	2.53	0.42
1:E:293:SER:HA	1:E:317:PRO:HB3	2.01	0.42
1:C:295:GLY:HA2	1:C:318:ILE:HG13	2.01	0.42
1:G:29:MET:HE3	1:G:311:SER:CB	2.48	0.42
1:A:128:ALA:HB3	1:A:150:ASP:N	2.35	0.42
1:G:96:ASP:H	1:G:135:TRP:NE1	2.17	0.42
1:G:112:MET:CE	1:G:123:ILE:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:LYS:HG2	1:E:171:GLU:C	2.44	0.42
1:C:165:MET:HE2	1:C:165:MET:HB2	1.90	0.42
1:E:102:PHE:CE1	1:E:112:MET:HG3	2.55	0.42
1:A:174:TYR:CZ	2:B:199:SER:HB3	2.54	0.42
1:G:26:HIS:ND1	1:G:27:ASN:HB3	2.34	0.42
1:G:31:ASP:OD2	1:G:356:ARG:HG3	2.19	0.42
1:G:58:ILE:HD13	1:G:94:TRP:HZ2	1.84	0.42
1:G:88:PRO:HD2	1:G:106:CYS:HB2	2.02	0.42
1:A:48:SER:HB2	1:A:52:LEU:HD12	2.01	0.42
1:E:41:SER:HB3	1:E:335:SER:HB3	2.01	0.42
1:A:91:ASP:HB3	1:A:133:ILE:HG22	2.02	0.42
1:A:307:LYS:HE3	1:A:307:LYS:HB3	1.79	0.42
1:E:48:SER:HB2	1:E:52:LEU:CD1	2.49	0.42
1:E:307:LYS:HE3	1:E:310:THR:OG1	2.20	0.42
1:E:58:ILE:HD13	1:E:94:TRP:HZ2	1.85	0.41
1:G:78:ILE:HB	1:G:80:LYS:NZ	2.35	0.41
1:G:102:PHE:CE1	1:G:112:MET:HB2	2.55	0.41
1:G:112:MET:HB3	1:G:123:ILE:HD13	2.01	0.41
1:G:183:ALA:HB3	1:G:195:TYR:HB2	2.02	0.41
1:C:297:PHE:CZ	1:C:311:SER:HB3	2.55	0.41
1:A:104:ALA:HB1	1:A:130:VAL:HG12	2.03	0.41
1:A:365:ARG:NH2	4:A:404:HOH:O	2.54	0.41
1:C:187:THR:OG1	1:C:191:GLY:HA3	2.20	0.41
2:D:158:THR:OG1	2:D:159:GLY:N	2.53	0.41
1:E:272:ASP:HB3	2:F:187:GLN:CG	2.49	0.41
1:G:294:ASP:OD2	1:G:296:ARG:HG2	2.20	0.41
1:C:252:LYS:HD3	1:C:252:LYS:C	2.45	0.41
1:E:49:PRO:HD2	1:E:52:LEU:HD12	2.02	0.41
1:G:187:THR:OG1	1:G:191:GLY:HA3	2.21	0.41
1:G:362:LEU:HD23	1:G:362:LEU:HA	1.89	0.41
1:A:200:GLN:HE21	1:A:200:GLN:HB2	1.71	0.41
1:C:192:LEU:HD12	1:C:192:LEU:HA	1.93	0.41
1:E:324:ASN:ND2	1:E:326:ASN:OD1	2.48	0.41
1:G:31:ASP:OD1	1:G:356:ARG:HG3	2.21	0.41
1:G:216:ARG:HH21	2:H:200:LEU:HB2	1.83	0.41
1:A:190:ARG:HD2	1:A:211:LEU:O	2.21	0.41
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.83	0.41
2:B:201:GLU:OE1	2:B:201:GLU:N	2.46	0.41
1:C:145:MET:HE2	1:C:145:MET:HB3	1.87	0.41
1:E:211:LEU:HD13	1:E:235:SER:HB3	2.02	0.41
1:G:108:LYS:HG2	1:G:128:ALA:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:LEU:HG	1:G:300:TRP:HB2	2.02	0.41
1:A:256:THR:OG1	3:X:61:ASP:HB2	2.21	0.41
1:E:26:HIS:HA	1:E:315:ASP:OD1	2.20	0.41
1:C:358:ALA:C	1:C:360:GLU:N	2.75	0.40
1:E:178:VAL:HG22	1:E:183:ALA:HB2	2.03	0.40
1:E:183:ALA:HB3	1:E:195:TYR:HB2	2.03	0.40
2:B:198:LYS:NZ	2:B:206:GLU:OE2	2.42	0.40
1:E:282:HIS:HE1	1:E:284:VAL:HG13	1.86	0.40
1:A:221:PHE:HB3	1:A:281:PHE:CZ	2.57	0.40
1:C:106:CYS:SG	2:D:205:LEU:HD13	2.62	0.40
1:G:76:GLN:CG	1:G:77:THR:N	2.84	0.40
1:C:211:LEU:HD12	1:C:233:LEU:HD23	2.03	0.40
1:C:217:CYS:SG	1:C:279:ILE:HG13	2.62	0.40
1:C:261:ARG:HG2	1:C:273:ILE:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/378 (89%)	327 (98%)	8 (2%)	0	100	100
1	C	334/378 (88%)	323 (97%)	11 (3%)	0	100	100
1	E	330/378 (87%)	324 (98%)	6 (2%)	0	100	100
1	G	330/378 (87%)	326 (99%)	4 (1%)	0	100	100
2	B	47/67 (70%)	44 (94%)	2 (4%)	1 (2%)	5	20
2	D	40/67 (60%)	38 (95%)	2 (5%)	0	100	100
2	F	50/67 (75%)	48 (96%)	2 (4%)	0	100	100
2	H	42/67 (63%)	40 (95%)	2 (5%)	0	100	100
3	I	7/21 (33%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	6/21 (29%)	6 (100%)	0	0	100	100
3	K	7/21 (33%)	7 (100%)	0	0	100	100
3	X	7/21 (33%)	7 (100%)	0	0	100	100
All	All	1535/1864 (82%)	1497 (98%)	37 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	193	LYS

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	295/327 (90%)	290 (98%)	5 (2%)	53	83
1	C	294/327 (90%)	282 (96%)	12 (4%)	27	62
1	E	292/327 (89%)	282 (97%)	10 (3%)	32	68
1	G	292/327 (89%)	280 (96%)	12 (4%)	27	62
2	B	47/61 (77%)	46 (98%)	1 (2%)	47	79
2	D	40/61 (66%)	38 (95%)	2 (5%)	22	54
2	F	49/61 (80%)	48 (98%)	1 (2%)	48	80
2	H	42/61 (69%)	39 (93%)	3 (7%)	13	39
3	I	9/21 (43%)	8 (89%)	1 (11%)	6	20
3	J	8/21 (38%)	8 (100%)	0	100	100
3	K	9/21 (43%)	8 (89%)	1 (11%)	6	20
3	X	9/21 (43%)	9 (100%)	0	100	100
All	All	1386/1636 (85%)	1338 (96%)	48 (4%)	32	67

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	86	THR
1	A	161	SER
1	A	184	VAL
1	A	324	ASN
2	B	171	ASP
1	C	37	SER
1	C	61	SER
1	C	64	ASN
1	C	67	ARG
1	C	71	VAL
1	C	72	GLN
1	C	77	THR
1	C	194	VAL
1	C	268	SER
1	C	302	LYS
1	C	314	LEU
1	C	328	ASN
2	D	161	THR
2	D	212	ARG
1	E	30	LYS
1	E	41	SER
1	E	105	SER
1	E	148	SER
1	E	200	GLN
1	E	268	SER
1	E	284	VAL
1	E	293	SER
1	E	340	LYS
1	E	360	GLU
2	F	180	THR
1	G	76	GLN
1	G	92	VAL
1	G	109	THR
1	G	121	ILE
1	G	148	SER
1	G	159	ARG
1	G	166	VAL
1	G	171	GLU
1	G	217	CYS
1	G	218	VAL
1	G	318	ILE
1	G	334	SER

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Mol	Chain	Res	Type
2	H	161	THR
2	H	168	THR
2	H	180	THR
3	I	55	GLU
3	K	55	GLU

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

Mol	Chain	Res	Type
1	A	55	ASN
1	A	134	HIS
1	A	140	ASN
1	A	271	GLN
1	A	282	HIS
1	C	83	GLN
1	C	214	GLN
1	C	285	HIS
1	E	83	GLN
1	E	118	ASN
1	E	196	GLN
1	E	342	HIS
1	G	83	GLN
1	G	328	ASN
1	G	357	ASN
3	X	56	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 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	339/378 (89%)	-0.52	0 100 100	35, 50, 80, 123	0
1	C	337/378 (89%)	-0.18	3 (0%) 81 74	32, 77, 116, 151	1 (0%)
1	E	336/378 (88%)	-0.34	2 (0%) 85 80	42, 66, 102, 138	0
1	G	336/378 (88%)	-0.07	2 (0%) 85 80	47, 81, 117, 154	0
2	B	51/67 (76%)	-0.31	1 (1%) 65 56	44, 60, 102, 133	0
2	D	44/67 (65%)	-0.19	0 100 100	58, 84, 98, 116	0
2	F	54/67 (80%)	-0.33	0 100 100	49, 64, 96, 106	0
2	H	46/67 (68%)	0.55	1 (2%) 62 52	77, 113, 171, 180	0
3	I	9/21 (42%)	-0.07	0 100 100	82, 93, 138, 144	0
3	J	8/21 (38%)	-0.14	0 100 100	60, 68, 99, 112	0
3	K	9/21 (42%)	0.10	0 100 100	81, 88, 128, 129	0
3	X	9/21 (42%)	0.23	0 100 100	60, 73, 111, 126	0
All	All	1578/1864 (84%)	-0.25	9 (0%) 85 80	32, 69, 116, 180	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	SER	2.8
1	E	268	SER	2.8
2	B	173	MET	2.7
1	G	36	SER	2.6
1	C	269	ALA	2.6
1	G	26	HIS	2.5
2	H	183	SER	2.2
1	C	206[A]	ARG	2.1
1	E	198	GLU	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.