Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2024 – 02:22 PM JST

PDB ID	:	8YRS
Title	:	Crystal structure of human RECQ1 helicase containing a flexible linker in complex with tailed duplex DNA
Authors	:	Das, T.; Das, A.K.; Ganguly, A.
Deposited on	:	2024-03-21
Resolution	:	2.43 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:

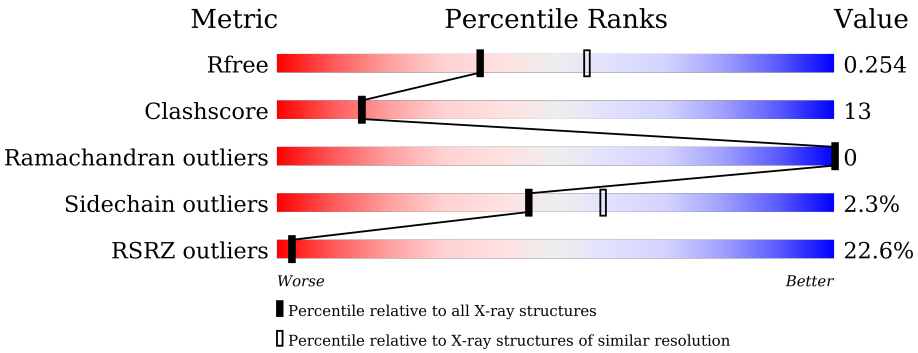
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.43 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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 <=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	599	12% 64% 23% · 12%
1	B	599	23% 64% 23% · 12%
2	C	13	15% 46% 46% 8%
2	P	13	69% 15% 77% 8%
3	D	27	56% 48% 41% 11%
3	Q	27	59% 11% 56% · 30%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9835 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 ATP-dependent DNA helicase Q1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4220	2686	720	779	35			
1	B	530	Total	C	N	O	S	0	0	0
			4216	2684	720	777	35			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP P46063
A	29	GLY	-	expression tag	UNP P46063
A	30	SER	-	expression tag	UNP P46063
A	31	SER	-	expression tag	UNP P46063
A	32	HIS	-	expression tag	UNP P46063
A	33	HIS	-	expression tag	UNP P46063
A	34	HIS	-	expression tag	UNP P46063
A	35	HIS	-	expression tag	UNP P46063
A	36	HIS	-	expression tag	UNP P46063
A	37	HIS	-	expression tag	UNP P46063
A	38	SER	-	expression tag	UNP P46063
A	39	SER	-	expression tag	UNP P46063
A	40	GLY	-	expression tag	UNP P46063
A	41	LEU	-	expression tag	UNP P46063
A	42	VAL	-	expression tag	UNP P46063
A	43	PRO	-	expression tag	UNP P46063
A	44	ARG	-	expression tag	UNP P46063
A	45	GLY	-	expression tag	UNP P46063
A	46	SER	-	expression tag	UNP P46063
A	47	HIS	-	expression tag	UNP P46063
A	48	MET	-	expression tag	UNP P46063
A	481	GLY	-	linker	UNP P46063
A	482	GLY	-	linker	UNP P46063
A	483	GLY	-	linker	UNP P46063
A	484	GLY	-	linker	UNP P46063

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Chain	Residue	Modelled	Actual	Comment	Reference
A	485	SER	-	linker	UNP P46063
A	486	GLY	-	linker	UNP P46063
A	487	GLY	-	linker	UNP P46063
A	488	GLY	-	linker	UNP P46063
A	489	GLY	-	linker	UNP P46063
A	490	SER	-	linker	UNP P46063
B	28	MET	-	initiating methionine	UNP P46063
B	29	GLY	-	expression tag	UNP P46063
B	30	SER	-	expression tag	UNP P46063
B	31	SER	-	expression tag	UNP P46063
B	32	HIS	-	expression tag	UNP P46063
B	33	HIS	-	expression tag	UNP P46063
B	34	HIS	-	expression tag	UNP P46063
B	35	HIS	-	expression tag	UNP P46063
B	36	HIS	-	expression tag	UNP P46063
B	37	HIS	-	expression tag	UNP P46063
B	38	SER	-	expression tag	UNP P46063
B	39	SER	-	expression tag	UNP P46063
B	40	GLY	-	expression tag	UNP P46063
B	41	LEU	-	expression tag	UNP P46063
B	42	VAL	-	expression tag	UNP P46063
B	43	PRO	-	expression tag	UNP P46063
B	44	ARG	-	expression tag	UNP P46063
B	45	GLY	-	expression tag	UNP P46063
B	46	SER	-	expression tag	UNP P46063
B	47	HIS	-	expression tag	UNP P46063
B	48	MET	-	expression tag	UNP P46063
B	481	GLY	-	linker	UNP P46063
B	482	GLY	-	linker	UNP P46063
B	483	GLY	-	linker	UNP P46063
B	484	GLY	-	linker	UNP P46063
B	485	SER	-	linker	UNP P46063
B	486	GLY	-	linker	UNP P46063
B	487	GLY	-	linker	UNP P46063
B	488	GLY	-	linker	UNP P46063
B	489	GLY	-	linker	UNP P46063
B	490	SER	-	linker	UNP P46063

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	13	0
			264	126	51	75	12			
2	P	13	Total	C	N	O	P	0	13	0
			264	126	51	75	12			

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	24	Total	C	N	O	P	0	24	0
			487	232	83	148	24			
3	Q	19	Total	C	N	O	P	0	19	0
			382	182	64	117	19			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

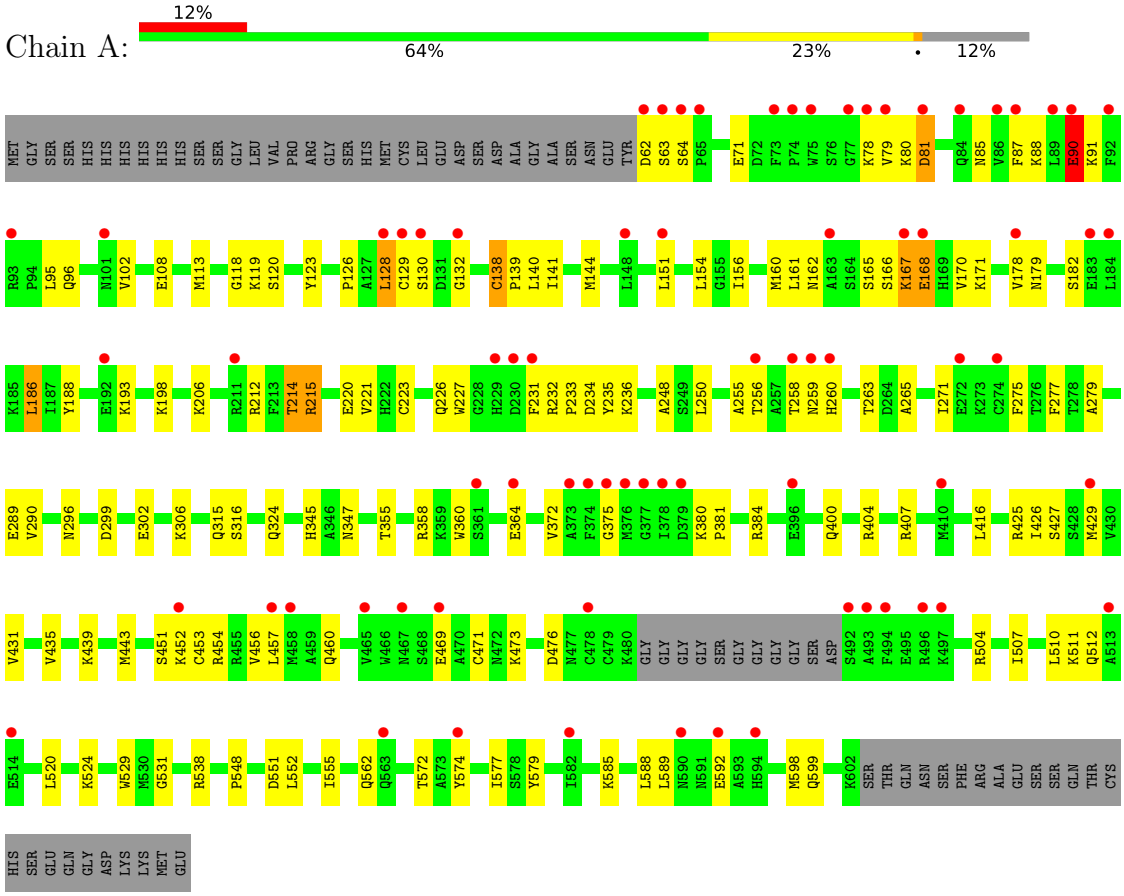
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

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.

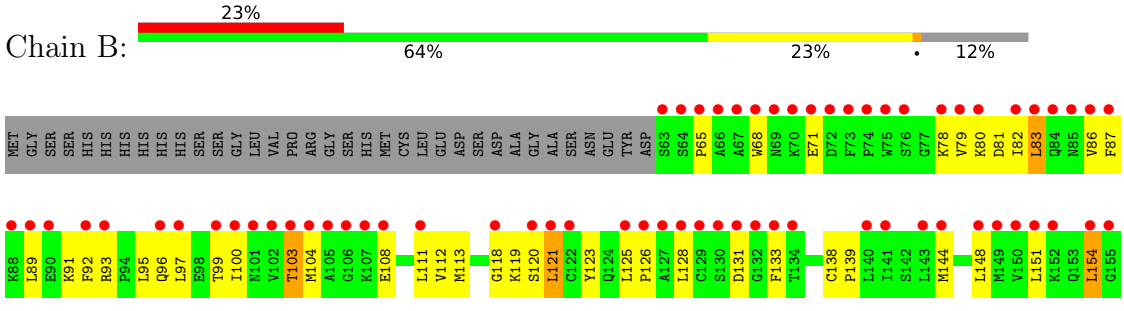
• Molecule 1: ATP-dependent DNA helicase Q1

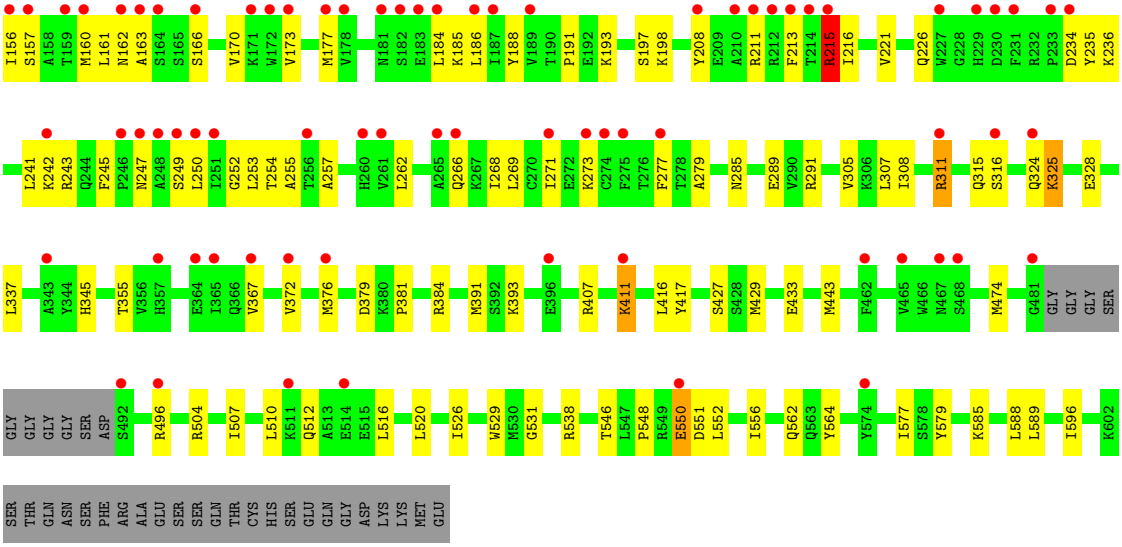
Chain A:



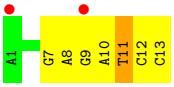
• Molecule 1: ATP-dependent DNA helicase Q1

Chain B:

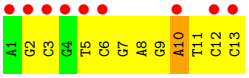




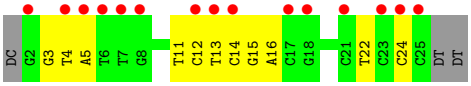
• Molecule 2: DNA (5'-D(*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*CP*C)-3')



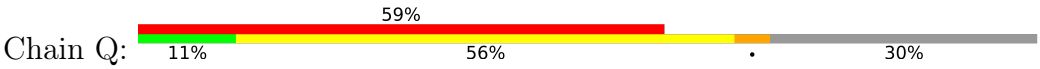
• Molecule 2: DNA (5'-D(*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*CP*C)-3')

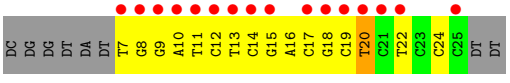


• Molecule 3: DNA (27-MER)



• Molecule 3: DNA (27-MER)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.32Å 96.57Å 96.81Å 90.00° 106.88° 90.00°	Depositor
Resolution (Å)	46.64 – 2.43 46.64 – 2.43	Depositor EDS
% Data completeness (in resolution range)	64.9 (46.64-2.43) 59.5 (46.64-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.237 , 0.257 0.238 , 0.254	Depositor DCC
R_{free} test set	33792 reflections (5.59%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9835	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.42	1/4304 (0.0%)	0.75	15/5804 (0.3%)
1	B	0.43	2/4300 (0.0%)	0.79	9/5798 (0.2%)
2	C	0.73	0/296	1.01	1/455 (0.2%)
2	P	1.05	1/296 (0.3%)	1.14	0/455
3	D	1.02	5/543 (0.9%)	1.34	7/835 (0.8%)
3	Q	0.92	0/425	1.29	4/652 (0.6%)
All	All	0.54	9/10164 (0.1%)	0.87	36/13999 (0.3%)

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	A	0	1
1	B	0	3
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4[A]	DT	C1'-N1	10.70	1.63	1.49
3	D	4[A]	DT	N1-C6	7.75	1.43	1.38
3	D	4[A]	DT	N1-C2	5.82	1.42	1.38
3	D	3[A]	DG	N9-C8	5.45	1.41	1.37
2	P	10[B]	DA	N9-C4	5.24	1.41	1.37
3	D	3[A]	DG	N9-C4	5.18	1.42	1.38
1	A	167	LYS	CB-CG	-5.16	1.38	1.52
1	B	103	THR	CB-CG2	-5.03	1.35	1.52
1	B	550	GLU	CD-OE1	-5.01	1.20	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4[A]	DT	C6-N1-C2	-14.04	114.28	121.30
3	D	3[A]	DG	C8-N9-C4	-12.23	101.51	106.40
1	B	97	LEU	CA-CB-CG	10.13	138.60	115.30
1	A	457	LEU	CB-CG-CD2	-9.10	95.53	111.00
1	B	411	LYS	CA-CB-CG	-9.08	93.42	113.40
3	D	5[A]	DA	O4'-C4'-C3'	-8.67	100.80	106.00
1	A	592	GLU	N-CA-CB	8.10	125.18	110.60
1	A	81	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	81	ASP	CB-CG-OD1	-7.38	111.65	118.30
1	B	215	ARG	CB-CG-CD	-7.24	92.78	111.60
1	A	452	LYS	CB-CG-CD	-7.19	92.90	111.60
3	Q	20[B]	DT	O4'-C1'-N1	6.73	112.71	108.00
1	A	469	GLU	CA-CB-CG	6.67	128.08	113.40
1	A	452	LYS	CA-CB-CG	6.56	127.84	113.40
1	A	168	GLU	CA-CB-CG	-6.50	99.09	113.40
1	B	215	ARG	CG-CD-NE	6.34	125.11	111.80
1	A	167	LYS	CA-CB-CG	6.12	126.86	113.40
1	B	121	LEU	CB-CG-CD2	-6.10	100.62	111.00
3	D	3[A]	DG	N9-C4-C5	6.10	107.84	105.40
1	A	592	GLU	CA-CB-CG	6.07	126.76	113.40
1	B	103	THR	OG1-CB-CG2	-6.06	96.06	110.00
1	A	81	ASP	N-CA-CB	5.86	121.15	110.60
1	A	128	LEU	CB-CG-CD1	-5.85	101.05	111.00
3	D	5[A]	DA	O4'-C1'-N9	5.79	112.06	108.00
3	Q	20[B]	DT	OP1-P-O3'	5.69	117.73	105.20
1	A	81	ASP	CB-CA-C	-5.63	99.13	110.40
3	D	4[A]	DT	C5-C6-N1	5.60	127.06	123.70
2	C	11[A]	DT	O4'-C1'-N1	5.50	111.85	108.00
1	A	90	GLU	CB-CA-C	-5.49	99.41	110.40
3	Q	20[B]	DT	C1'-O4'-C4'	-5.35	104.75	110.10
3	D	3[A]	DG	N7-C8-N9	5.28	115.74	113.10
1	B	83	LEU	CA-CB-CG	-5.25	103.22	115.30
1	A	90	GLU	CA-CB-CG	5.24	124.92	113.40
1	B	91	LYS	CB-CA-C	-5.10	100.21	110.40
1	B	325	LYS	N-CA-CB	5.04	119.67	110.60
3	Q	20[B]	DT	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	GLU	Sidechain
1	B	215	ARG	Sidechain
1	B	311	ARG	Sidechain
1	B	328	GLU	Sidechain

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	4220	0	4240	96	4
1	B	4216	0	4239	114	4
2	C	264	0	147	12	0
2	P	264	0	147	14	0
3	D	487	0	259	6	0
3	Q	382	0	215	24	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9835	0	9247	256	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (256) 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:103:THR:HG21	1:B:215:ARG:HH22	1.26	1.00
1:B:103:THR:HG22	1:B:215:ARG:HH12	1.28	0.97
1:B:307:LEU:CD2	1:B:311:ARG:NH1	2.36	0.89
1:A:473:LYS:O	1:A:473:LYS:HD3	1.76	0.86
3:Q:15[B]:DG:H2'	3:Q:16[B]:DA:C8	2.10	0.86
1:A:85:ASN:O	1:A:88:LYS:NZ	2.11	0.84
1:B:103:THR:CG2	1:B:215:ARG:HH22	1.93	0.82
1:A:555:ILE:HA	1:A:598:MET:HE1	1.61	0.82
1:B:216:ILE:HB	1:B:250:LEU:HD12	1.62	0.82
2:P:11[B]:DT:H2'	2:P:12[B]:DC:C6	2.18	0.79
1:B:289:GLU:OE1	1:B:291:ARG:NE	2.14	0.76
2:C:7[A]:DG:H2"	2:C:8[A]:DA:C8	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLN:NE2	1:B:118:GLY:O	2.20	0.74
1:B:71:GLU:OE2	1:B:80:LYS:NZ	2.14	0.73
1:B:108:GLU:HA	1:B:250:LEU:O	1.88	0.73
1:B:83:LEU:HD13	1:B:92:PHE:CZ	2.24	0.73
1:A:167:LYS:O	1:A:170:VAL:HG22	1.87	0.73
3:Q:8[B]:DG:H2'	3:Q:9[B]:DG:C8	2.25	0.72
1:B:103:THR:HG21	1:B:215:ARG:NH2	2.04	0.71
1:A:128:LEU:HD21	1:A:156:ILE:HD13	1.73	0.71
1:B:103:THR:HG22	1:B:215:ARG:NH1	2.05	0.70
1:A:381:PRO:HA	1:A:407:ARG:HB2	1.73	0.70
2:C:12[A]:DC:H2'	2:C:13[A]:DC:C6	2.27	0.70
1:A:431:VAL:O	1:B:243:ARG:NH2	2.20	0.69
1:B:191:PRO:HB2	1:B:234:ASP:HB3	1.74	0.69
1:B:108:GLU:HG3	1:B:250:LEU:HB3	1.75	0.69
1:B:526:ILE:HD11	1:B:556:ILE:HD12	1.75	0.69
1:B:526:ILE:CD1	1:B:556:ILE:HD12	2.24	0.67
1:B:92:PHE:CE1	1:B:121:LEU:HD21	2.31	0.66
3:Q:14[B]:DC:H2'	3:Q:15[B]:DG:C8	2.30	0.66
2:C:11[A]:DT:H2'	2:C:12[A]:DC:C6	2.32	0.65
1:B:250:LEU:HD21	1:B:269:LEU:HD23	1.78	0.65
1:B:78:LYS:O	1:B:81:ASP:OD1	2.14	0.65
2:C:10[A]:DA:H2'	2:C:11[A]:DT:C6	2.31	0.65
1:B:211:ARG:HH22	1:B:247:ASN:HD22	1.46	0.64
1:B:307:LEU:CD2	1:B:311:ARG:HH12	2.12	0.62
2:P:9[B]:DG:H2"	2:P:10[B]:DA:C8	2.35	0.62
1:B:86:VAL:HG11	1:B:128:LEU:CD1	2.30	0.62
1:A:435:VAL:O	1:A:439:LYS:HG3	1.99	0.62
3:Q:13[B]:DT:H2'	3:Q:14[B]:DC:C6	2.34	0.61
3:D:14[A]:DC:H2'	3:D:15[A]:DG:C8	2.35	0.61
1:A:113:MET:HE2	1:A:119:LYS:HG3	1.81	0.61
1:B:128:LEU:HD23	1:B:185:LYS:HG3	1.83	0.61
1:A:62:ASP:HB2	1:A:275:PHE:CD1	2.36	0.60
1:B:173:VAL:O	1:B:177:MET:HG3	2.02	0.60
1:A:562:GLN:O	1:A:585:LYS:HE2	2.02	0.60
3:Q:16[B]:DA:H2'	3:Q:17[B]:DC:C6	2.38	0.59
2:P:7[B]:DG:H2"	2:P:8[B]:DA:C8	2.37	0.59
1:B:126:PRO:HB2	1:B:215:ARG:CZ	2.33	0.58
1:B:379:ASP:OD1	1:B:379:ASP:N	2.34	0.58
2:C:11[A]:DT:H2"	2:C:12[A]:DC:O5'	2.04	0.58
1:B:507:ILE:HD12	1:B:589:LEU:HD12	1.86	0.57
1:A:577:ILE:HD11	1:A:579:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASN:O	1:B:411:LYS:HG2	2.04	0.57
1:A:144:MET:HG2	1:A:188:TYR:HB3	1.85	0.57
1:B:86:VAL:HG11	1:B:128:LEU:HD13	1.86	0.57
3:Q:12[B]:DC:H2"	3:Q:13[B]:DT:OP2	2.04	0.57
1:A:453:CYS:SG	1:A:471:CYS:HB2	2.45	0.56
1:A:531:GLY:O	1:A:538:ARG:NE	2.38	0.56
2:P:2[B]:DG:H2"	2:P:3[B]:DC:C5	2.41	0.56
1:A:226:GLN:HB3	1:B:226:GLN:HB3	1.88	0.56
1:B:307:LEU:HD23	1:B:311:ARG:NH1	2.21	0.56
3:D:11[A]:DT:H2'	3:D:12[A]:DC:C6	2.41	0.55
1:A:113:MET:HG3	1:A:279:ALA:HB2	1.87	0.55
1:B:208:TYR:CD2	1:B:245:PHE:HD1	2.23	0.55
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.88	0.55
1:B:305:VAL:HG21	1:B:337:LEU:HD23	1.88	0.55
1:B:208:TYR:HB2	1:B:213:PHE:HD2	1.71	0.55
1:B:381:PRO:HA	1:B:407:ARG:HB2	1.88	0.55
1:A:90:GLU:HB2	1:A:91:LYS:HG2	1.88	0.55
1:A:96:GLN:NE2	1:A:118:GLY:O	2.37	0.55
1:B:103:THR:CG2	1:B:215:ARG:NH2	2.67	0.55
1:A:113:MET:HG3	1:A:279:ALA:CB	2.38	0.54
1:A:139:PRO:HB2	1:A:140:LEU:HD22	1.90	0.54
1:B:100:ILE:O	1:B:104:MET:HB2	2.08	0.54
2:P:10[B]:DA:H2'	2:P:11[B]:DT:C5	2.43	0.53
1:A:167:LYS:HB3	1:A:168:GLU:OE1	2.07	0.53
3:Q:11[B]:DT:H1'	3:Q:12[B]:DC:OP2	2.07	0.53
2:P:12[B]:DC:H2"	2:P:13[B]:DC:O5'	2.07	0.53
2:C:12[A]:DC:H2'	2:C:13[A]:DC:C5	2.44	0.53
1:A:139:PRO:HG2	1:A:220:GLU:HG3	1.91	0.53
1:B:99:THR:HG21	1:B:111:LEU:HD13	1.90	0.53
1:B:139:PRO:HG3	1:B:235:TYR:OH	2.09	0.53
2:P:10[B]:DA:H2'	2:P:11[B]:DT:C6	2.43	0.53
1:A:372:VAL:HG23	3:Q:24[B]:DC:H5'	1.90	0.52
2:P:6[B]:DC:H2"	2:P:7[B]:DG:C8	2.44	0.52
2:P:7[B]:DG:H2"	2:P:8[B]:DA:H8	1.74	0.52
1:B:161:LEU:HD13	1:B:173:VAL:HG21	1.90	0.52
1:B:315:GLN:HB3	1:B:384:ARG:HG3	1.91	0.52
1:B:307:LEU:HD21	1:B:311:ARG:NH1	2.23	0.51
1:A:62:ASP:HB2	1:A:275:PHE:HD1	1.75	0.51
1:B:95:LEU:HD13	1:B:277:PHE:HB3	1.93	0.51
1:A:113:MET:O	1:A:255:ALA:HA	2.10	0.51
1:B:83:LEU:HD22	1:B:92:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:MET:HE1	1:B:126:PRO:HA	1.93	0.51
1:B:148:LEU:HD11	1:B:160:MET:HB3	1.92	0.51
1:A:425:ARG:HD2	3:Q:22[B]:DT:OP1	2.11	0.51
1:B:92:PHE:HZ	1:B:125:LEU:HD13	1.76	0.51
1:B:108:GLU:OE2	1:B:249:SER:HA	2.11	0.51
2:P:5[B]:DT:H2"	2:P:6[B]:DC:C6	2.46	0.51
1:A:315:GLN:HB3	1:A:384:ARG:HG3	1.92	0.50
1:B:151:LEU:HD23	1:B:156:ILE:HD12	1.92	0.50
1:B:548:PRO:HB2	1:B:550:GLU:OE1	2.10	0.50
1:B:562:GLN:O	1:B:585:LYS:HE2	2.11	0.50
1:A:520:LEU:HD22	1:A:524:LYS:HB3	1.93	0.50
1:B:128:LEU:HD23	1:B:185:LYS:HE2	1.93	0.50
1:A:144:MET:CE	1:A:160:MET:HG3	2.41	0.50
1:B:273:LYS:O	1:B:273:LYS:HG3	2.11	0.50
2:C:9[A]:DG:H2"	2:C:10[A]:DA:H8	1.77	0.50
1:A:507:ILE:O	1:A:511:LYS:HG3	2.12	0.50
1:B:100:ILE:HD13	1:B:125:LEU:HD22	1.93	0.50
2:P:11[B]:DT:H2"	2:P:12[B]:DC:O5'	2.10	0.50
1:A:574:TYR:HB2	3:Q:20[B]:DT:C6	2.46	0.50
1:B:128:LEU:CD2	1:B:185:LYS:HG3	2.42	0.50
1:B:429:MET:HG3	3:D:22[A]:DT:H2'	1.94	0.49
1:B:113:MET:O	1:B:255:ALA:HA	2.13	0.49
1:B:133:PHE:CZ	1:B:213:PHE:HB2	2.47	0.49
1:B:307:LEU:HD22	1:B:311:ARG:NH1	2.25	0.49
1:A:289:GLU:HG3	1:A:476:ASP:HB3	1.95	0.49
1:A:360:TRP:CH2	1:A:380:LYS:HD3	2.47	0.49
1:A:179:ASN:HB3	1:A:182:SER:HB2	1.94	0.49
1:A:144:MET:HE2	1:A:160:MET:HG3	1.94	0.49
1:B:510:LEU:HD23	1:B:520:LEU:HD12	1.93	0.49
1:A:504:ARG:NH1	1:A:589:LEU:O	2.45	0.49
1:B:372:VAL:HG23	3:D:24[A]:DC:H5'	1.95	0.49
1:A:233:PRO:O	1:A:236:LYS:HG2	2.12	0.48
1:B:577:ILE:HD11	1:B:579:TYR:CZ	2.48	0.48
2:C:7[A]:DG:H2"	2:C:8[A]:DA:N7	2.28	0.48
1:B:504:ARG:NH1	1:B:589:LEU:O	2.34	0.48
2:C:9[A]:DG:H2"	2:C:10[A]:DA:C8	2.48	0.48
1:A:577:ILE:HD11	1:A:579:TYR:OH	2.14	0.48
1:B:266:GLN:HG3	1:B:271:ILE:HG23	1.95	0.48
2:P:11[B]:DT:H2'	2:P:12[B]:DC:C5	2.47	0.48
1:B:529:TRP:CZ3	1:B:552:LEU:HB3	2.48	0.48
1:A:161:LEU:HD23	1:A:193:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:O	1:A:171:LYS:HD3	2.14	0.48
1:B:108:GLU:HG3	1:B:250:LEU:CB	2.42	0.48
1:B:393:LYS:NZ	1:B:433:GLU:OE2	2.44	0.48
3:Q:10[B]:DA:H8	3:Q:10[B]:DA:O5'	1.96	0.48
3:Q:12[B]:DC:OP1	3:Q:12[B]:DC:H6	1.96	0.48
1:A:95:LEU:HD13	1:A:277:PHE:HB3	1.96	0.48
1:B:307:LEU:HD21	1:B:311:ARG:HH12	1.77	0.48
1:B:577:ILE:HD11	1:B:579:TYR:OH	2.13	0.48
1:A:130:SER:OG	1:A:215:ARG:NH1	2.44	0.48
3:Q:12[B]:DC:OP1	3:Q:12[B]:DC:H2'	2.14	0.48
3:Q:15[B]:DG:H2'	3:Q:16[B]:DA:N7	2.29	0.47
1:A:141:ILE:HG12	1:A:162:ASN:HD22	1.79	0.47
1:B:411:LYS:HD3	1:B:474:MET:CE	2.44	0.47
1:A:78:LYS:O	1:A:79:VAL:C	2.51	0.47
1:A:140:LEU:HD21	1:A:232:ARG:NH2	2.29	0.47
1:A:451:SER:HB3	1:A:599:GLN:OE1	2.14	0.47
1:B:154:LEU:O	1:B:154:LEU:HD13	2.13	0.47
1:B:112:VAL:HG22	1:B:254:THR:HG23	1.95	0.47
1:B:308:ILE:HD13	1:B:367:VAL:HG21	1.97	0.47
1:B:126:PRO:HB2	1:B:215:ARG:NH2	2.30	0.47
3:Q:16[B]:DA:H2'	3:Q:17[B]:DC:N1	2.29	0.47
3:Q:17[B]:DC:H1'	3:Q:18[B]:DG:N7	2.30	0.47
1:B:120:SER:HA	1:B:123:TYR:CE2	2.51	0.47
3:Q:7[B]:DT:H2'	3:Q:7[B]:DT:OP1	2.15	0.47
1:A:87:PHE:CD1	1:A:154:LEU:HD21	2.50	0.46
1:A:572:THR:OG1	3:Q:20[B]:DT:O4	2.20	0.46
1:A:102:VAL:CG1	1:A:275:PHE:HD2	2.29	0.46
1:A:296:ASN:HB3	1:A:299:ASP:HB2	1.96	0.46
1:A:416:LEU:HD11	1:A:443:MET:CE	2.45	0.46
3:Q:8[B]:DG:O5'	3:Q:8[B]:DG:H8	1.98	0.46
1:B:411:LYS:HD3	1:B:474:MET:HE1	1.98	0.46
3:Q:12[B]:DC:H2"	3:Q:13[B]:DT:H72	1.96	0.46
1:B:65:PRO:HA	1:B:68:TRP:HD1	1.80	0.46
1:B:531:GLY:O	1:B:538:ARG:NE	2.49	0.46
1:B:126:PRO:HB2	1:B:215:ARG:NE	2.31	0.46
1:B:166:SER:O	1:B:170:VAL:HG23	2.15	0.46
1:A:250:LEU:HD22	1:A:271:ILE:HD11	1.98	0.46
1:A:221:VAL:HG22	1:A:265:ALA:HB1	1.98	0.46
1:B:78:LYS:HA	1:B:81:ASP:OD1	2.16	0.46
1:A:108:GLU:HA	1:A:250:LEU:O	2.16	0.45
1:A:206:LYS:HD3	1:A:206:LYS:HA	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:HE2	1:B:119:LYS:HG3	1.96	0.45
1:A:71:GLU:OE2	1:A:80:LYS:HD2	2.15	0.45
1:A:151:LEU:HD11	1:A:186:LEU:HD13	1.97	0.45
1:A:290:VAL:HB	1:A:454:ARG:NH2	2.31	0.45
1:A:426:ILE:O	1:A:429:MET:HB3	2.16	0.45
1:B:242:LYS:HE3	1:B:242:LYS:HB3	1.54	0.45
2:C:9[A]:DG:N2	3:D:13[A]:DT:O2	2.49	0.45
1:A:63:SER:O	1:A:64:SER:OG	2.33	0.45
1:A:95:LEU:HA	1:A:95:LEU:HD23	1.64	0.45
1:B:236:LYS:HA	1:B:268:ILE:HG23	1.98	0.45
1:B:87:PHE:O	1:B:89:LEU:HD12	2.17	0.45
1:A:80:LYS:O	1:A:81:ASP:C	2.56	0.44
1:A:324:GLN:NE2	1:A:347:ASN:HB2	2.32	0.44
1:B:79:VAL:O	1:B:82:ILE:HG22	2.17	0.44
1:B:123:TYR:CD2	1:B:253:LEU:HD11	2.52	0.44
1:B:162:ASN:OD1	1:B:163:ALA:N	2.48	0.44
1:B:391:MET:HB2	1:B:391:MET:HE3	1.78	0.44
1:A:193:LYS:HD2	1:A:193:LYS:HA	1.58	0.44
2:P:8[B]:DA:H1'	2:P:9[B]:DG:H5'	1.99	0.44
3:D:15[A]:DG:H2'	3:D:16[A]:DA:C8	2.53	0.44
1:B:193:LYS:O	1:B:197:SER:HB3	2.18	0.43
3:Q:12[B]:DC:OP1	3:Q:12[B]:DC:C6	2.71	0.43
1:B:307:LEU:HD23	1:B:307:LEU:HA	1.74	0.43
2:C:10[A]:DA:H2'	2:C:11[A]:DT:H71	2.00	0.43
1:A:119:LYS:HB2	1:A:119:LYS:HE2	1.78	0.43
1:A:132:GLY:HA3	1:A:212:ARG:O	2.18	0.43
1:B:157:SER:OG	1:B:184:LEU:HA	2.18	0.43
1:A:102:VAL:HG11	1:A:275:PHE:HD2	1.84	0.43
1:A:139:PRO:HG3	1:A:235:TYR:OH	2.19	0.43
1:A:120:SER:HA	1:A:123:TYR:CE2	2.54	0.43
1:A:510:LEU:HD23	1:A:520:LEU:HD12	2.01	0.43
1:B:96:GLN:O	1:B:100:ILE:HG13	2.19	0.43
1:B:307:LEU:CD2	1:B:311:ARG:HH11	2.27	0.43
1:A:162:ASN:OD1	1:A:165:SER:OG	2.23	0.43
1:A:439:LYS:HG3	1:A:439:LYS:H	1.56	0.43
1:A:529:TRP:CZ3	1:A:552:LEU:HB3	2.54	0.43
1:B:113:MET:HG3	1:B:279:ALA:CB	2.48	0.43
1:B:92:PHE:CE1	1:B:121:LEU:CD2	3.02	0.43
1:B:324:GLN:HG2	1:B:345:HIS:HB2	1.99	0.43
1:A:258:THR:HG22	1:A:259:ASN:N	2.34	0.43
1:A:126:PRO:HA	1:A:129:CYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ALA:HB1	1:B:262:LEU:HD13	2.01	0.42
2:P:12[B]:DC:H4'	2:P:13[B]:DC:OP1	2.19	0.42
1:A:585:LYS:O	1:A:588:LEU:HB2	2.20	0.42
1:B:216:ILE:HG21	1:B:241:LEU:HD13	2.01	0.42
2:C:12[A]:DC:H2"	2:C:13[A]:DC:O5'	2.17	0.42
1:A:223:CYS:O	1:A:231:PHE:HD1	2.02	0.42
3:Q:9[B]:DG:H2"	3:Q:10[B]:DA:N7	2.35	0.42
1:A:302:GLU:O	1:A:306:LYS:HG3	2.20	0.42
1:A:456:VAL:O	1:A:460:GLN:HG3	2.20	0.42
1:B:221:VAL:HG11	1:B:252:GLY:HA3	2.01	0.42
1:A:507:ILE:HG22	1:A:511:LYS:HE3	2.02	0.42
1:B:266:GLN:CG	1:B:271:ILE:HG23	2.50	0.42
1:A:324:GLN:HG2	1:A:345:HIS:HB2	2.02	0.41
1:A:355:THR:HG23	1:A:358:ARG:NH2	2.34	0.41
1:A:214:THR:O	1:A:248:ALA:HA	2.20	0.41
1:A:585:LYS:HB3	1:A:585:LYS:HE3	1.89	0.41
1:B:548:PRO:HD2	1:B:551:ASP:OD2	2.20	0.41
1:A:548:PRO:HD2	1:A:551:ASP:OD2	2.20	0.41
1:A:108:GLU:HG2	1:A:271:ILE:HG12	2.02	0.41
1:A:375:GLY:HA2	1:A:404:ARG:NH1	2.35	0.41
1:A:574:TYR:HD2	3:Q:20[B]:DT:C7	2.34	0.41
1:B:144:MET:SD	1:B:188:TYR:HB3	2.61	0.41
1:A:198:LYS:HA	1:A:198:LYS:HD3	1.85	0.41
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.94	0.41
1:B:416:LEU:HD11	1:B:443:MET:CE	2.51	0.41
1:A:227:TRP:CD1	1:A:260:HIS:CE1	3.09	0.41
1:A:512:GLN:NE2	1:A:538:ARG:O	2.47	0.41
1:B:99:THR:HG22	1:B:277:PHE:HD2	1.86	0.41
1:A:130:SER:OG	1:A:215:ARG:HD2	2.20	0.41
1:A:256:THR:HG21	1:A:400:GLN:NE2	2.35	0.41
1:B:512:GLN:HG2	1:B:516:LEU:HD11	2.03	0.41
1:B:564:TYR:CE2	1:B:596:ILE:HG12	2.56	0.41
1:B:95:LEU:O	1:B:99:THR:HG23	2.21	0.41
1:B:585:LYS:O	1:B:588:LEU:HB2	2.21	0.40
1:B:162:ASN:CG	1:B:163:ALA:N	2.75	0.40
3:Q:18[B]:DG:H2'	3:Q:19[B]:DC:C6	2.55	0.40
1:A:138:CYS:HA	1:A:139:PRO:HD3	1.97	0.40
1:A:166:SER:O	1:A:170:VAL:HG13	2.21	0.40
1:B:416:LEU:HD23	1:B:417:TYR:N	2.37	0.40

All (4) 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:A:81:ASP:OD2	1:B:131:ASP:OD2[1_655]	1.81	0.39
1:A:364:GLU:CD	1:B:496:ARG:NH2[2_646]	1.91	0.29
1:A:364:GLU:OE1	1:B:496:ARG:NH2[2_646]	1.99	0.21
1:A:364:GLU:CG	1:B:496:ARG:NH2[2_646]	2.02	0.18

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	526/599 (88%)	518 (98%)	8 (2%)	0	100	100
1	B	526/599 (88%)	520 (99%)	6 (1%)	0	100	100
All	All	1052/1198 (88%)	1038 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/518 (90%)	456 (98%)	9 (2%)	52	65
1	B	464/518 (90%)	452 (97%)	12 (3%)	41	54
All	All	929/1036 (90%)	908 (98%)	21 (2%)	45	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	CYS
1	A	178	VAL
1	A	186	LEU
1	A	214	THR
1	A	215	ARG
1	A	234	ASP
1	A	263	THR
1	A	316	SER
1	A	427	SER
1	B	93	ARG
1	B	138	CYS
1	B	154	LEU
1	B	186	LEU
1	B	198	LYS
1	B	215	ARG
1	B	316	SER
1	B	325	LYS
1	B	355	THR
1	B	376	MET
1	B	427	SER
1	B	546	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	GLN
1	A	324	GLN
1	A	400	GLN
1	A	563	GLN
1	B	247	ASN
1	B	260	HIS
1	B	292	GLN
1	B	512	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	530/599 (88%)	0.93	74 (13%) 7 7	20, 52, 99, 155	0
1	B	530/599 (88%)	1.32	139 (26%) 2 2	20, 54, 129, 186	0
2	C	13/13 (100%)	1.01	2 (15%) 6 6	11, 31, 47, 51	13 (100%)
2	P	13/13 (100%)	2.76	9 (69%) 0 1	78, 92, 134, 140	13 (100%)
3	D	24/27 (88%)	2.60	15 (62%) 0 1	13, 39, 75, 83	24 (100%)
3	Q	19/27 (70%)	3.38	16 (84%) 0 0	40, 98, 137, 156	19 (100%)
All	All	1129/1278 (88%)	1.21	255 (22%) 3 3	11, 53, 117, 186	69 (6%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	1[B]	DA	8.5
1	B	92	PHE	7.5
1	B	148	LEU	7.2
1	B	215	ARG	7.2
1	B	75	TRP	7.0
3	Q	25[B]	DC	6.8
3	Q	20[B]	DT	6.5
3	D	25[A]	DC	6.5
1	B	125	LEU	6.3
1	B	156	ILE	6.0
1	A	256	THR	5.7
1	B	130	SER	5.6
3	Q	21[B]	DC	5.6
1	A	229	HIS	5.3
1	B	129	CYS	5.3
1	B	131	ASP	5.2
1	B	127	ALA	5.1
1	B	213	PHE	5.0
1	B	74	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	121	LEU	5.0
1	B	66	ALA	4.8
3	D	4[A]	DT	4.7
3	D	6[A]	DT	4.7
1	B	79	VAL	4.7
3	Q	9[B]	DG	4.7
1	B	87	PHE	4.7
1	A	376	MET	4.6
3	Q	22[B]	DT	4.6
1	B	101	ASN	4.6
1	B	128	LEU	4.5
1	B	172	TRP	4.5
1	B	229	HIS	4.5
1	B	211	ARG	4.5
1	B	132	GLY	4.4
1	B	311	ARG	4.3
1	B	83	LEU	4.2
1	B	107	LYS	4.2
1	A	429	MET	4.2
1	B	68	TRP	4.2
3	D	21[A]	DC	4.2
1	B	550	GLU	4.1
1	B	64	SER	4.1
1	B	157	SER	4.1
1	A	90	GLU	4.0
1	A	377	GLY	4.0
1	B	97	LEU	4.0
1	B	274	CYS	4.0
1	B	73	PHE	4.0
1	A	151	LEU	3.9
1	B	376	MET	3.9
1	B	151	LEU	3.9
3	Q	13[B]	DT	3.9
1	B	103	THR	3.8
3	D	7[A]	DT	3.8
1	B	162	ASN	3.8
1	B	271	ILE	3.8
1	A	130	SER	3.8
1	A	396	GLU	3.7
1	A	496	ARG	3.7
1	A	101	ASN	3.7
1	A	378	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	3.7
1	B	184	LEU	3.6
3	D	2[A]	DG	3.6
1	A	375	GLY	3.6
1	B	496	ARG	3.6
1	B	154	LEU	3.6
3	Q	10[B]	DA	3.5
1	B	144	MET	3.5
3	Q	12[B]	DC	3.5
1	A	574	TYR	3.5
1	A	211	ARG	3.5
1	A	592	GLU	3.5
1	B	275	PHE	3.5
1	B	141	ILE	3.5
1	A	87	PHE	3.4
1	B	230	ASP	3.4
2	P	2[B]	DG	3.4
1	B	133	PHE	3.4
1	B	273	LYS	3.4
1	B	183	GLU	3.4
1	B	214	THR	3.4
1	A	452	LYS	3.4
1	B	208	TYR	3.4
1	A	84	GLN	3.4
1	B	481	GLY	3.4
1	A	497	LYS	3.3
1	A	493	ALA	3.3
1	B	86	VAL	3.3
1	B	187	ILE	3.3
1	B	155	GLY	3.3
1	B	89	LEU	3.2
3	D	5[A]	DA	3.2
1	B	102	VAL	3.2
1	B	122	CYS	3.2
1	B	372	VAL	3.2
1	B	105	ALA	3.2
1	B	246	PRO	3.2
1	B	182	SER	3.1
1	B	248	ALA	3.1
1	B	256	THR	3.1
1	A	92	PHE	3.1
3	Q	19[B]	DC	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	274	CYS	3.1
1	B	108	GLU	3.1
1	B	84	GLN	3.1
1	B	261	VAL	3.1
2	P	13[B]	DC	3.1
1	A	469	GLU	3.1
1	B	149	MET	3.1
1	B	82	ILE	3.0
1	B	181	ASN	3.0
1	B	111	LEU	3.0
1	B	69	ASN	3.0
1	B	265	ALA	3.0
1	A	582	ILE	3.0
1	B	88	LYS	3.0
1	B	242	LYS	3.0
1	B	85	ASN	3.0
1	B	63	SER	3.0
1	B	186	LEU	3.0
1	B	231	PHE	2.9
1	A	81	ASP	2.9
1	B	212	ARG	2.9
1	B	100	ILE	2.9
1	A	467	ASN	2.9
1	A	73	PHE	2.9
1	B	396	GLU	2.9
1	A	178	VAL	2.9
1	B	67	ALA	2.9
1	B	411	LYS	2.8
1	B	99	THR	2.8
1	B	247	ASN	2.8
1	A	89	LEU	2.8
2	P	6[B]	DC	2.8
1	A	458	MET	2.8
1	A	272	GLU	2.8
1	A	374	PHE	2.8
1	B	173	VAL	2.8
1	B	210	ALA	2.8
1	B	227	TRP	2.8
1	A	129	CYS	2.8
1	B	260	HIS	2.7
1	B	266	GLN	2.7
1	A	364	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	164	SER	2.7
1	B	65	PRO	2.7
2	P	3[B]	DC	2.7
3	D	17[A]	DC	2.7
3	D	23[A]	DC	2.7
1	B	106	GLY	2.7
1	A	494	PHE	2.7
3	Q	15[B]	DG	2.7
1	A	63	SER	2.6
1	B	250	LEU	2.6
1	B	78	LYS	2.6
3	D	24[A]	DC	2.6
1	A	75	TRP	2.6
1	A	74	PRO	2.6
1	B	277	PHE	2.6
1	B	152	LYS	2.6
1	A	79	VAL	2.6
1	A	86	VAL	2.6
1	B	468	SER	2.6
1	B	492	SER	2.6
1	B	143	LEU	2.5
3	Q	18[B]	DG	2.5
1	A	64	SER	2.5
1	B	118	GLY	2.5
3	Q	14[B]	DC	2.5
1	A	457	LEU	2.5
1	B	189	VAL	2.5
1	B	465	VAL	2.5
1	A	513	ALA	2.5
1	B	163	ALA	2.5
1	B	166	SER	2.5
1	B	96	GLN	2.5
1	B	159	THR	2.5
1	B	104	MET	2.5
3	D	13[A]	DT	2.5
2	C	1[A]	DA	2.5
3	Q	8[B]	DG	2.5
1	A	492	SER	2.5
1	B	233	PRO	2.5
1	B	71	GLU	2.5
1	B	365	ILE	2.5
1	B	467	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	231	PHE	2.5
1	B	251	ILE	2.4
1	B	70	LYS	2.4
1	B	177	MET	2.4
3	Q	11[B]	DT	2.4
1	A	465	VAL	2.4
1	B	72	ASP	2.4
1	A	168	GLU	2.4
1	A	183	GLU	2.4
1	A	361	SER	2.4
1	A	132	GLY	2.4
1	A	184	LEU	2.4
1	B	462	PHE	2.4
1	B	160	MET	2.4
1	B	178	VAL	2.4
1	A	230	ASP	2.3
1	B	234	ASP	2.3
1	B	316	SER	2.3
1	A	594	HIS	2.3
1	A	379	ASP	2.3
1	B	90	GLU	2.3
3	D	18[A]	DG	2.3
1	A	148	LEU	2.3
1	B	126	PRO	2.3
1	A	192	GLU	2.3
1	A	563	GLN	2.3
1	B	324	GLN	2.3
1	A	478	CYS	2.3
1	A	167	LYS	2.3
1	B	171	LYS	2.3
1	B	367	VAL	2.3
2	P	12[B]	DC	2.3
1	A	373	ALA	2.3
1	B	343	ALA	2.3
1	A	78	LYS	2.2
1	B	80	LYS	2.2
1	B	120	SER	2.2
1	A	65	PRO	2.2
1	B	514	GLU	2.2
3	D	14[A]	DC	2.2
1	B	140	LEU	2.2
2	P	4[B]	DG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	511	LYS	2.2
1	A	128	LEU	2.2
1	B	134	THR	2.2
1	B	249	SER	2.2
1	A	260	HIS	2.2
1	B	357	HIS	2.2
1	A	259	ASN	2.1
1	A	77	GLY	2.1
1	A	62	ASP	2.1
1	B	150	VAL	2.1
1	A	514	GLU	2.1
1	B	364	GLU	2.1
2	C	9[A]	DG	2.1
3	D	12[A]	DC	2.1
3	Q	17[B]	DC	2.1
3	Q	7[B]	DT	2.1
1	B	93	ARG	2.0
1	A	258	THR	2.0
1	A	410	MET	2.0
1	A	590	ASN	2.0
1	B	574	TYR	2.0
2	P	10[B]	DA	2.0
1	B	76	SER	2.0
2	P	5[B]	DT	2.0
3	D	8[A]	DG	2.0
1	A	93	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	B	900	1/1	0.92	0.24	146,146,146,146	0
4	ZN	A	900	1/1	0.94	0.06	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.