Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 01:21 PM JST

PDB ID	:	4Y5W
Title	:	Transcription factor-DNA complex
Authors	:	Li, J.; Niu, F.; Ouyang, S.; Liu, Z.
Deposited on	:	2015-02-12
Resolution	:	3.10 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 (i) 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 (1)) were used in the production of this report:

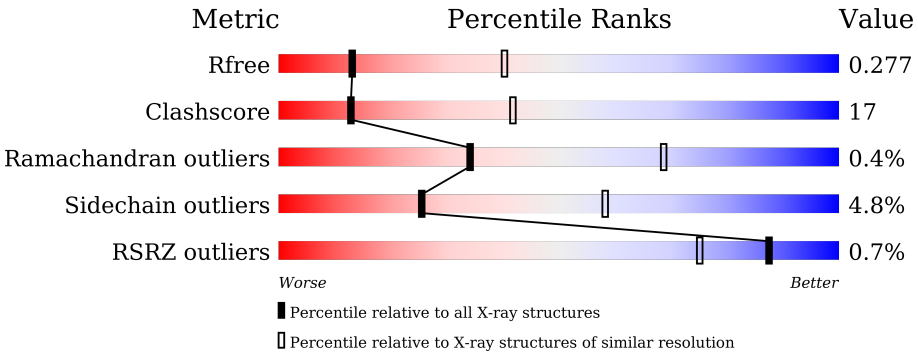
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	549	64% 19% • 13%
1	B	549	% 59% 25% • 13%
1	C	549	63% 19% • 15%
1	D	549	61% 22% • 14%
2	E	22	5% 32% 68%
2	M	22	5% 32% 59% 9%

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Mol	Chain	Length	Quality of chain
3	F	22	5% 36% 64%
3	N	22	5% 36% 64%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PTR	A	641	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17083 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 Signal transducer and activator of transcription 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	P	S	0	0	0
			3802	2421	671	693	1	16			
1	B	477	Total	C	N	O	P	S	0	1	0
			3804	2425	671	691	1	16			
1	D	472	Total	C	N	O	P	S	0	0	0
			3745	2389	656	683	1	16			
1	C	465	Total	C	N	O	P	S	0	0	0
			3697	2361	649	670	1	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	SER	-	expression tag	UNP P42226
A	111	ASN	-	expression tag	UNP P42226
A	112	ALA	-	expression tag	UNP P42226
B	110	SER	-	expression tag	UNP P42226
B	111	ASN	-	expression tag	UNP P42226
B	112	ALA	-	expression tag	UNP P42226
D	110	SER	-	expression tag	UNP P42226
D	111	ASN	-	expression tag	UNP P42226
D	112	ALA	-	expression tag	UNP P42226
C	110	SER	-	expression tag	UNP P42226
C	111	ASN	-	expression tag	UNP P42226
C	112	ALA	-	expression tag	UNP P42226

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	22	Total	C	N	O	P	0	0	0
			457	217	89	129	22			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	22	Total	C	N	O	P	0	0	0
			457	217	89	129	22			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*TP*GP*TP*CP*TP*TP*CP*CP*TP *AP*GP*GP*AP*AP*AP*TP*CP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	22	Total	C	N	O	P	0	0	0
			445	214	74	135	22			
3	N	22	Total	C	N	O	P	0	0	0
			445	214	74	135	22			

- Molecule 4 is water.

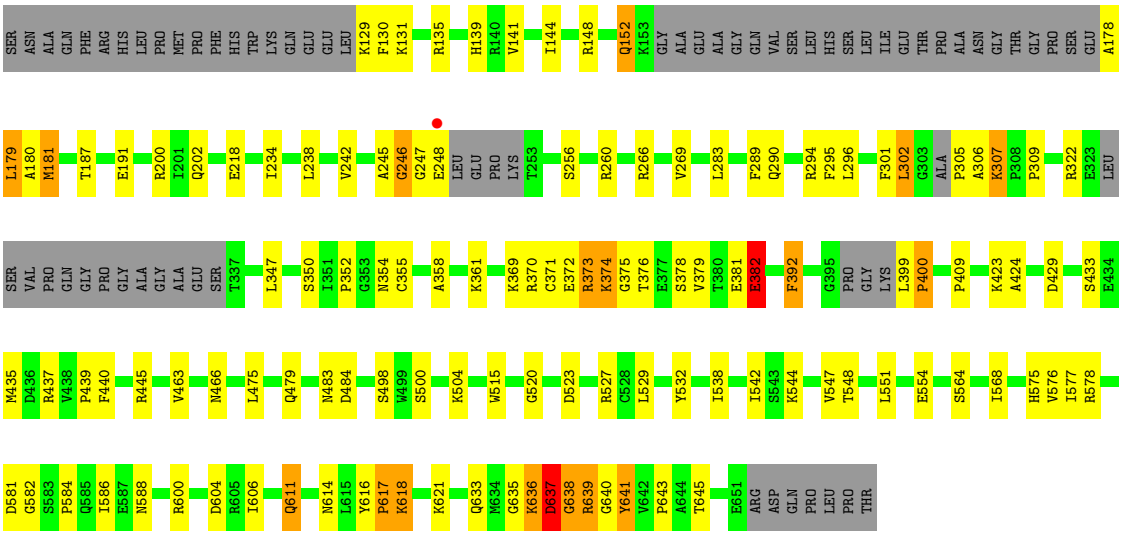
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		
4	B	54	Total	O	0	0
			54	54		
4	D	24	Total	O	0	0
			24	24		
4	F	2	Total	O	0	0
			2	2		
4	M	5	Total	O	0	0
			5	5		
4	N	2	Total	O	0	0
			2	2		
4	C	42	Total	O	0	0
			42	42		

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.

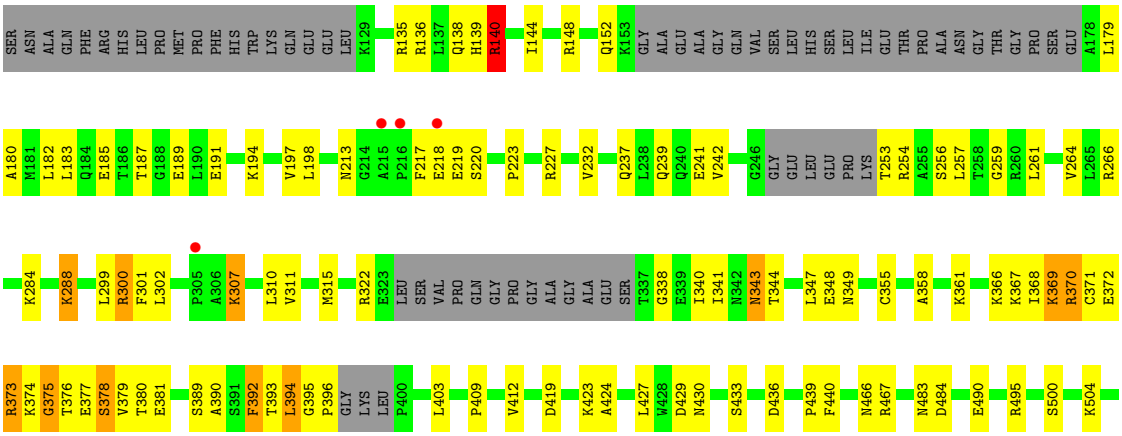
• Molecule 1: Signal transducer and activator of transcription 6

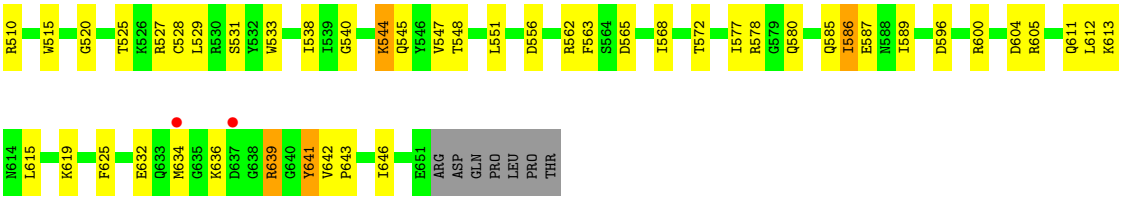
Chain A:



• Molecule 1: Signal transducer and activator of transcription 6

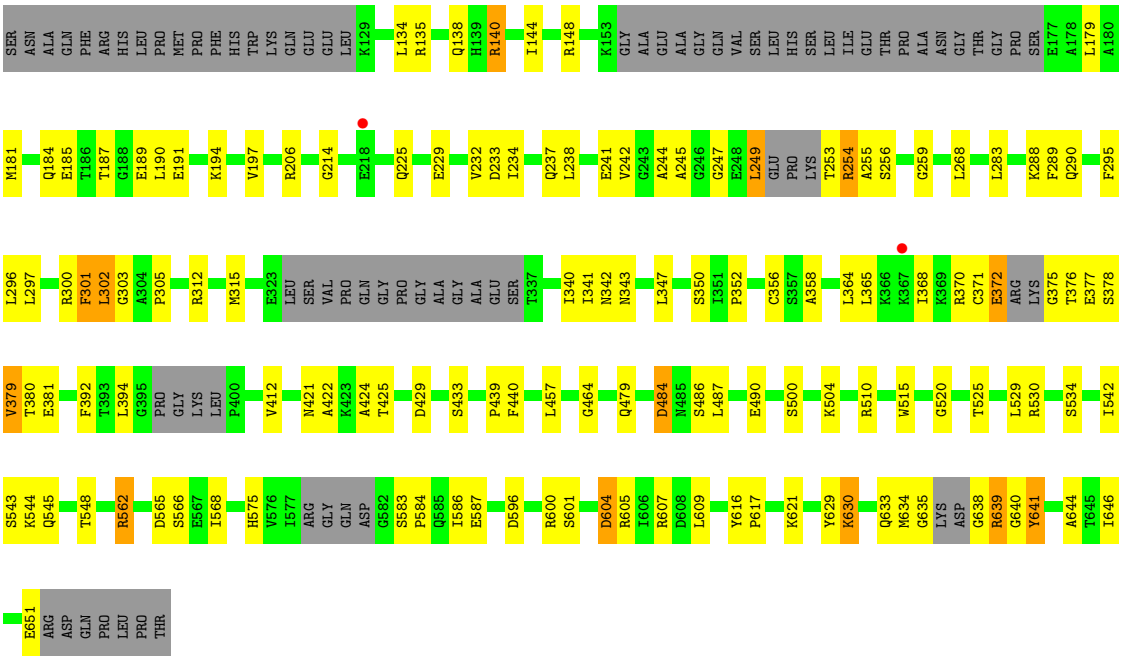
Chain B:





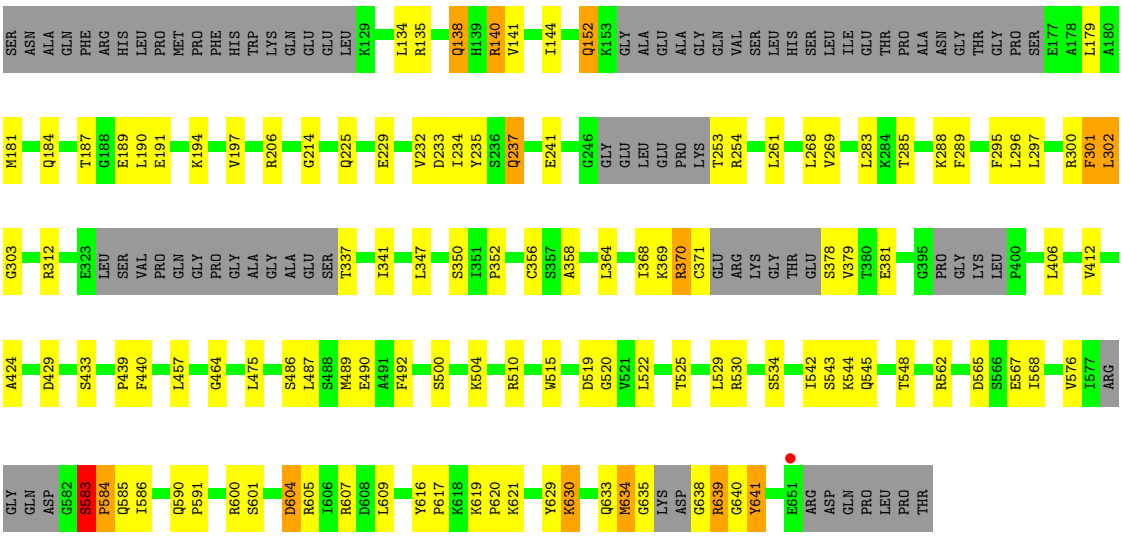
• Molecule 1: Signal transducer and activator of transcription 6

Chain D:



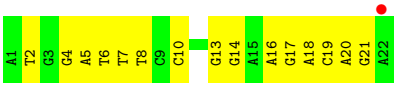
• Molecule 1: Signal transducer and activator of transcription 6

Chain C:



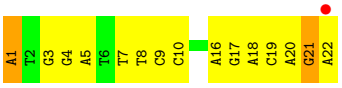
• Molecule 2: DNA (5'-D(P*AP*TP*GP*GP*AP*TP*TP*TP*CP*CP*TP*AP*GP*GP*AP*AP*GP*AP*CP*AP*A)-3')

Chain E:



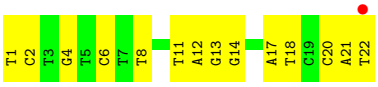
• Molecule 2: DNA (5'-D(P*AP*TP*GP*GP*AP*TP*TP*TP*CP*CP*TP*AP*GP*GP*AP*AP*GP*AP*CP*AP*A)-3')

Chain M:



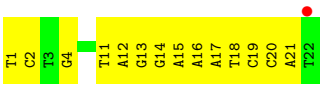
• Molecule 3: DNA (5'-D(P*TP*TP*GP*TP*CP*TP*TP*CP*CP*TP*AP*GP*GP*AP*AP*AP*TP*CP*CP*AP*T)-3')

Chain F:



• Molecule 3: DNA (5'-D(P*TP*TP*GP*TP*CP*TP*TP*CP*CP*TP*AP*GP*GP*AP*AP*AP*TP*CP*CP*AP*T)-3')

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.30Å 94.24Å 147.78Å 99.85° 101.73° 89.93°	Depositor
Resolution (Å)	38.81 – 3.10 38.81 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.5 (38.81-3.10) 85.2 (38.81-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.250 , 0.278 0.250 , 0.277	Depositor DCC
R_{free} test set	2918 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 27.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.095 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	17083	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 9.64% 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: PTR

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	0.36	2/3851 (0.1%)	0.55	3/5186 (0.1%)
1	B	0.32	1/3856 (0.0%)	0.51	2/5196 (0.0%)
1	C	0.31	1/3744 (0.0%)	0.53	2/5043 (0.0%)
1	D	0.31	1/3792 (0.0%)	0.55	2/5107 (0.0%)
2	E	0.63	0/514	1.00	0/792
2	M	0.66	0/514	1.03	2/792 (0.3%)
3	F	0.57	0/496	0.95	0/762
3	N	0.63	0/496	1.00	0/762
All	All	0.37	5/17263 (0.0%)	0.62	11/23640 (0.0%)

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	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	GLU	C-N	-5.59	1.21	1.34
1	A	617	PRO	N-CD	5.46	1.55	1.47
1	B	396	PRO	N-CD	5.27	1.55	1.47
1	C	584	PRO	N-CD	5.09	1.54	1.47
1	D	584	PRO	N-CD	5.00	1.54	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	21	DG	P-O3'-C3'	-7.83	110.31	119.70
1	A	369	LYS	O-C-N	7.52	134.73	122.70
2	M	1	DA	O5'-P-OP2	-7.18	99.24	105.70
1	C	583	SER	C-N-CD	6.08	141.16	128.40
1	D	583	SER	C-N-CD	6.04	141.08	128.40
1	A	369	LYS	CA-C-N	-5.93	104.15	117.20
1	A	375	GLY	N-CA-C	-5.71	98.82	113.10
1	B	395	GLY	C-N-CD	5.61	140.19	128.40
1	B	140	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	302	LEU	N-CA-C	5.14	124.89	111.00
1	C	302	LEU	N-CA-C	5.12	124.82	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	GLU	Peptide
1	A	638	GLY	Peptide
1	B	375	GLY	Peptide
1	C	301	PHE	Peptide
1	D	301	PHE	Peptide

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	3802	0	3882	161	1
1	B	3804	0	3884	133	1
1	C	3697	0	3778	84	0
1	D	3745	0	3815	118	0
2	E	457	0	248	22	0
2	M	457	0	248	23	3
3	F	445	0	251	31	0
3	N	445	0	251	12	0
4	A	102	0	0	16	0
4	B	54	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	42	0	0	3	0
4	D	24	0	0	1	0
4	F	2	0	0	0	0
4	M	5	0	0	2	0
4	N	2	0	0	0	0
All	All	17083	0	16357	547	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 17.

All (547) 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)
3:F:13:DG:H2"	3:F:14:DG:C8	1.30	1.61
3:F:13:DG:H2"	3:F:14:DG:N7	1.26	1.48
1:A:302:LEU:HD22	1:A:306:ALA:CB	1.54	1.36
1:A:302:LEU:CD2	1:A:306:ALA:HB3	1.56	1.34
1:A:302:LEU:CG	1:A:306:ALA:HB3	1.59	1.33
3:F:13:DG:C2'	3:F:14:DG:N7	1.92	1.33
1:A:381:GLU:OE1	1:A:504:LYS:HE2	1.34	1.25
1:B:301:PHE:CD2	1:B:392:PHE:HE2	1.53	1.24
1:A:374:LYS:N	4:A:701:HOH:O	1.69	1.21
1:A:374:LYS:HD2	2:M:21:DG:OP1	1.40	1.20
3:F:13:DG:C2'	3:F:14:DG:C8	2.25	1.18
1:C:378:SER:HA	1:C:381:GLU:OE1	1.43	1.17
2:M:21:DG:H2"	2:M:22:DA:OP2	1.35	1.13
1:D:249:LEU:HB2	1:D:253:THR:CB	1.81	1.11
1:B:301:PHE:CD2	1:B:392:PHE:CE2	2.39	1.10
1:A:637:ASP:HB2	1:A:641:PTR:N	1.68	1.08
1:A:381:GLU:OE1	1:A:504:LYS:CE	2.02	1.07
1:A:637:ASP:OD1	1:A:640:GLY:HA2	1.55	1.06
1:B:381:GLU:OE2	1:B:504:LYS:HE3	1.53	1.06
1:A:302:LEU:CD1	1:A:306:ALA:HB3	1.86	1.05
1:A:637:ASP:HB2	1:A:641:PTR:H	0.88	1.03
1:A:527:ARG:NH2	4:A:702:HOH:O	1.89	1.02
1:A:302:LEU:HD22	1:A:306:ALA:HB3	1.17	1.01
1:A:637:ASP:CB	1:A:641:PTR:H	1.74	1.00
1:A:307:LYS:H	1:A:307:LYS:HD2	1.26	0.99
1:D:255:ALA:O	1:D:259:GLY:N	1.95	0.98
2:M:21:DG:C2'	2:M:22:DA:OP2	2.13	0.97
1:B:373:ARG:NH1	4:B:701:HOH:O	1.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD22	1:A:306:ALA:HB1	1.43	0.95
1:B:636:LYS:HE2	1:D:651:GLU:C	1.87	0.94
1:B:373:ARG:O	1:B:373:ARG:NE	2.03	0.91
1:A:374:LYS:CD	2:M:21:DG:OP1	2.20	0.90
1:A:637:ASP:OD1	1:A:639:ARG:N	2.04	0.90
1:D:372:GLU:N	1:D:372:GLU:OE2	2.04	0.90
3:F:13:DG:C5	3:F:14:DG:O6	2.25	0.90
1:B:373:ARG:H	1:B:373:ARG:HE	1.19	0.90
1:D:370:ARG:HH11	1:D:370:ARG:HG3	1.36	0.90
1:A:302:LEU:HD13	1:A:306:ALA:N	1.88	0.89
1:A:374:LYS:CB	4:A:798:HOH:O	2.20	0.88
1:A:302:LEU:HD13	1:A:306:ALA:CB	2.03	0.88
1:A:616:TYR:CD1	1:A:617:PRO:HA	2.08	0.88
1:A:302:LEU:CG	1:A:306:ALA:CB	2.51	0.85
1:A:637:ASP:CB	1:A:641:PTR:O	2.24	0.85
1:B:374:LYS:HB2	1:B:375:GLY:O	1.75	0.85
1:A:302:LEU:HD13	1:A:306:ALA:HB3	1.56	0.83
1:A:373:ARG:HD2	1:A:373:ARG:O	1.77	0.83
1:D:148:ARG:HD2	1:D:244:ALA:HB3	1.60	0.83
1:B:301:PHE:HB2	1:B:392:PHE:HZ	1.43	0.82
1:C:190:LEU:HD13	1:C:234:ILE:HD11	1.60	0.82
1:D:134:LEU:HG	1:D:138:GLN:HE21	1.44	0.82
1:A:302:LEU:HD13	1:A:306:ALA:H	1.43	0.82
3:F:13:DG:H2"	3:F:14:DG:H8	1.35	0.82
1:A:302:LEU:CD1	1:A:305:PRO:HG2	2.10	0.82
1:A:614:ASN:OD1	1:A:618:LYS:O	1.96	0.82
1:B:540:GLY:O	1:B:563:PHE:CD2	2.33	0.81
1:C:134:LEU:HG	1:C:138:GLN:HE21	1.45	0.81
1:B:301:PHE:HD2	1:B:392:PHE:CE2	1.94	0.81
1:A:638:GLY:H	1:A:639:ARG:HG2	1.43	0.80
1:A:302:LEU:CB	1:A:306:ALA:HB3	2.10	0.80
1:A:578:ARG:HG2	1:A:584:PRO:HB3	1.63	0.79
2:E:10:DC:H5	3:F:13:DG:H1	1.31	0.79
2:M:8:DT:OP2	4:M:101:HOH:O	2.00	0.79
1:A:302:LEU:CB	1:A:306:ALA:CB	2.61	0.78
1:D:190:LEU:HD13	1:D:234:ILE:HD11	1.65	0.78
1:A:135:ARG:O	1:A:139:HIS:ND1	2.15	0.78
3:F:13:DG:H2'	3:F:14:DG:N7	1.99	0.77
1:A:378:SER:HB2	1:A:381:GLU:HG3	1.67	0.77
1:A:637:ASP:HB2	1:A:641:PTR:O	1.84	0.77
1:D:379:VAL:HG22	2:E:6:DT:P	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:O	1:A:382:GLU:HG3	1.84	0.76
2:E:19:DC:H5	3:F:4:DG:H1	1.32	0.76
1:A:302:LEU:CD2	1:A:306:ALA:CB	2.30	0.76
3:F:13:DG:C4	3:F:14:DG:C6	2.74	0.76
1:A:636:LYS:HE3	1:A:636:LYS:N	2.01	0.75
1:A:178:ALA:N	1:A:247:GLY:O	2.20	0.75
1:D:370:ARG:NH2	1:D:412:VAL:O	2.19	0.74
3:F:13:DG:C4	3:F:14:DG:O6	2.41	0.74
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.52	0.74
1:C:634:MET:SD	1:C:635:GLY:N	2.61	0.74
1:B:374:LYS:HB2	1:B:375:GLY:C	2.07	0.74
1:D:378:SER:H	1:D:381:GLU:HG3	1.51	0.74
1:B:525:THR:HA	1:B:529:LEU:HB2	1.71	0.73
1:A:500:SER:HA	1:A:504:LYS:HB2	1.71	0.72
1:A:302:LEU:HD12	1:A:305:PRO:HG2	1.71	0.72
1:A:637:ASP:CG	1:A:640:GLY:HA2	2.09	0.72
1:A:374:LYS:HB3	4:A:798:HOH:O	1.85	0.72
1:B:500:SER:HA	1:B:504:LYS:HB2	1.71	0.72
1:B:135:ARG:O	1:B:139:HIS:ND1	2.20	0.72
1:B:636:LYS:O	1:B:643:PRO:HD3	1.90	0.71
2:M:19:DC:H5	3:N:4:DG:H1	1.38	0.71
1:A:638:GLY:H	1:A:639:ARG:CG	2.02	0.71
1:B:301:PHE:HB2	1:B:392:PHE:CZ	2.24	0.71
1:B:379:VAL:HG13	3:F:6:DC:OP1	1.91	0.71
1:A:381:GLU:CD	1:A:504:LYS:HE2	2.12	0.70
1:A:576:VAL:HG12	1:A:586:ILE:HG22	1.73	0.70
1:A:307:LYS:H	1:A:307:LYS:CD	1.98	0.70
1:A:302:LEU:HB3	1:A:306:ALA:CB	2.19	0.70
3:F:13:DG:C2	3:F:14:DG:C6	2.78	0.70
1:B:373:ARG:HE	1:B:373:ARG:N	1.89	0.70
2:M:9:DC:H5	3:N:14:DG:H1	1.40	0.70
1:B:375:GLY:H	1:B:377:GLU:H	1.37	0.70
1:A:296:LEU:O	4:A:703:HOH:O	2.10	0.69
1:D:370:ARG:HD2	1:D:379:VAL:HG12	1.74	0.69
1:B:213:ASN:HD21	1:B:427:LEU:HA	1.57	0.69
1:D:380:THR:HG21	1:D:421:ASN:HB3	1.73	0.69
1:C:576:VAL:HG23	1:C:585:GLN:O	1.93	0.69
1:A:429:ASP:O	1:A:433:SER:OG	2.09	0.68
1:B:527:ARG:NH2	4:B:706:HOH:O	2.25	0.68
1:A:381:GLU:OE1	1:A:504:LYS:NZ	2.27	0.68
1:A:639:ARG:HG3	1:A:641:PTR:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:GLY:O	1:D:376:THR:OG1	2.12	0.68
1:A:638:GLY:N	1:A:639:ARG:HG2	2.08	0.67
1:B:636:LYS:O	1:B:642:VAL:HA	1.94	0.67
1:B:394:LEU:HD12	1:B:394:LEU:C	2.14	0.67
1:D:376:THR:O	4:D:701:HOH:O	2.13	0.67
1:D:601:SER:OG	1:D:604:ASP:OD1	2.12	0.67
1:B:220:SER:O	4:B:702:HOH:O	2.13	0.67
3:F:13:DG:N3	3:F:14:DG:C6	2.63	0.67
1:B:390:ALA:O	1:B:403:LEU:N	2.27	0.66
2:M:10:DC:H5	3:N:13:DG:H1	1.42	0.66
1:A:483:ASN:O	1:B:466:ASN:ND2	2.29	0.66
1:B:375:GLY:N	1:B:377:GLU:H	1.94	0.66
1:B:540:GLY:O	1:B:563:PHE:HD2	1.76	0.66
1:D:500:SER:HA	1:D:504:LYS:HB2	1.77	0.66
1:B:213:ASN:HD21	1:B:427:LEU:HD12	1.61	0.65
1:C:356:CYS:SG	4:C:708:HOH:O	2.54	0.65
1:B:217:PHE:HB3	1:B:219:GLU:HG2	1.79	0.65
1:D:424:ALA:HB2	1:D:515:TRP:CD1	2.31	0.65
2:E:19:DC:H2"	2:E:20:DA:O4'	1.97	0.65
1:C:424:ALA:HB2	1:C:515:TRP:CD1	2.32	0.64
1:D:370:ARG:HG3	1:D:370:ARG:NH1	2.10	0.64
1:A:141:VAL:HA	1:A:144:ILE:HD12	1.79	0.63
1:B:140:ARG:HD3	1:B:182:LEU:HD11	1.80	0.63
1:B:600:ARG:NH1	1:B:604:ASP:HB3	2.13	0.63
1:B:429:ASP:O	1:B:433:SER:OG	2.16	0.63
1:A:374:LYS:O	1:A:374:LYS:NZ	2.29	0.63
1:A:641:PTR:O2P	1:A:641:PTR:HE2	1.98	0.62
1:A:374:LYS:HE2	4:A:755:HOH:O	1.99	0.62
1:B:424:ALA:HB2	1:B:515:TRP:CD1	2.34	0.62
1:D:638:GLY:N	1:D:641:PTR:O	2.32	0.62
1:A:302:LEU:HD13	1:A:306:ALA:CA	2.30	0.61
3:F:13:DG:C6	3:F:14:DG:O6	2.52	0.61
1:D:380:THR:HG22	1:D:380:THR:O	2.00	0.61
1:C:548:THR:HG22	1:C:586:ILE:HD11	1.81	0.61
1:A:370:ARG:NE	1:A:379:VAL:CG2	2.64	0.61
1:A:641:PTR:O1P	1:C:562:ARG:NH2	2.33	0.61
1:D:380:THR:HG23	1:D:422:ALA:HA	1.82	0.61
1:A:376:THR:O	1:A:376:THR:HG22	2.01	0.61
1:B:144:ILE:HG22	1:B:241:GLU:HG2	1.83	0.61
1:A:463:VAL:O	4:A:704:HOH:O	2.17	0.60
1:D:378:SER:N	1:D:381:GLU:HG3	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:O	1:B:259:GLY:N	2.34	0.60
1:B:307:LYS:H	1:B:307:LYS:HD2	1.66	0.60
1:B:381:GLU:OE2	1:B:504:LYS:CE	2.41	0.60
1:A:616:TYR:CG	1:A:617:PRO:HA	2.37	0.60
1:A:639:ARG:NH1	1:C:567:GLU:OE1	2.34	0.60
1:D:368:ILE:HG23	1:D:368:ILE:O	2.02	0.60
1:A:374:LYS:HB3	4:A:715:HOH:O	2.00	0.59
1:A:636:LYS:HE3	1:A:636:LYS:CA	2.30	0.59
1:D:135:ARG:NE	1:D:138:GLN:OE1	2.36	0.59
1:C:140:ARG:NH2	1:C:189:GLU:OE2	2.30	0.59
1:C:500:SER:HA	1:C:504:LYS:HB2	1.84	0.59
1:B:376:THR:HG23	1:B:376:THR:O	2.01	0.59
1:A:633:GLN:NE2	1:A:645:THR:OG1	2.36	0.59
1:A:374:LYS:CE	2:M:21:DG:OP1	2.50	0.59
1:C:601:SER:OG	1:C:604:ASP:OD1	2.15	0.59
1:B:409:PRO:HG3	1:B:440:PHE:CD1	2.38	0.59
1:A:307:LYS:HD2	1:A:307:LYS:N	2.09	0.58
1:B:311:VAL:HG12	1:B:390:ALA:CB	2.33	0.58
1:B:375:GLY:H	1:B:377:GLU:N	2.00	0.58
1:A:409:PRO:HG3	1:A:440:PHE:CD1	2.38	0.58
1:A:374:LYS:CA	4:A:701:HOH:O	2.36	0.58
1:C:350:SER:OG	1:C:352:PRO:O	2.21	0.58
1:D:548:THR:HG22	1:D:586:ILE:HD11	1.84	0.58
1:D:350:SER:OG	1:D:352:PRO:O	2.21	0.57
1:A:302:LEU:CD1	1:A:306:ALA:H	2.14	0.57
1:B:646:ILE:HD11	1:D:646:ILE:HB	1.86	0.57
1:A:424:ALA:HB2	1:A:515:TRP:CD1	2.40	0.57
1:A:374:LYS:HE3	2:M:21:DG:OP1	2.03	0.57
1:D:380:THR:HG21	1:D:421:ASN:CB	2.34	0.57
1:B:315:MET:HB2	1:B:340:ILE:HD11	1.87	0.57
1:D:370:ARG:NH1	2:E:7:DT:OP2	2.38	0.57
1:C:370:ARG:NH2	1:C:412:VAL:O	2.34	0.57
1:B:179:LEU:N	1:B:180:ALA:HB3	2.19	0.57
1:B:538:ILE:HG22	1:B:540:GLY:N	2.20	0.57
1:B:341:ILE:HD11	1:B:366:LYS:HD3	1.87	0.57
1:D:249:LEU:HD13	1:D:253:THR:CB	2.35	0.57
1:D:347:LEU:HA	1:D:358:ALA:HB2	1.87	0.57
1:D:600:ARG:HG2	1:D:605:ARG:HG3	1.86	0.57
1:A:551:LEU:HB3	1:A:576:VAL:CG1	2.35	0.56
1:A:551:LEU:HB3	1:A:576:VAL:HG11	1.86	0.56
1:D:378:SER:HB3	1:D:381:GLU:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:ASP:OD1	1:D:604:ASP:N	2.36	0.56
1:C:544:LYS:O	1:C:548:THR:HG23	2.05	0.56
1:C:607:ARG:HB2	1:C:629:TYR:CZ	2.40	0.56
1:C:600:ARG:HG2	1:C:605:ARG:HG3	1.86	0.56
1:C:337:THR:N	1:C:369:LYS:HB2	2.21	0.56
1:B:343:ASN:OD1	1:B:343:ASN:N	2.39	0.56
1:B:374:LYS:N	1:B:375:GLY:HA2	2.21	0.56
4:M:101:HOH:O	1:C:285:THR:HG21	2.05	0.56
1:D:545:GLN:O	1:D:548:THR:OG1	2.19	0.56
1:C:545:GLN:O	1:C:548:THR:OG1	2.19	0.56
1:D:234:ILE:HA	1:D:237:GLN:HE21	1.72	0.55
1:B:213:ASN:ND2	1:B:427:LEU:HA	2.21	0.55
1:D:232:VAL:HG23	1:D:268:LEU:HD23	1.88	0.55
1:D:429:ASP:O	1:D:433:SER:OG	2.18	0.55
1:C:429:ASP:O	1:C:433:SER:OG	2.18	0.55
1:A:354:ASN:OD1	4:A:705:HOH:O	2.18	0.55
1:A:637:ASP:CA	1:A:641:PTR:O	2.55	0.55
1:C:135:ARG:NE	1:C:138:GLN:OE1	2.39	0.55
1:D:544:LYS:O	1:D:548:THR:HG23	2.06	0.55
1:B:232:VAL:HG21	1:B:300:ARG:HG2	1.89	0.54
3:N:13:DG:H2"	3:N:14:DG:C8	2.42	0.54
1:A:179:LEU:HA	1:A:180:ALA:HB3	1.88	0.54
1:A:371:CYS:SG	1:A:372:GLU:HB2	2.47	0.54
1:A:635:GLY:HA2	1:A:643:PRO:HD2	1.89	0.54
1:B:288:LYS:HE2	1:B:361:LYS:O	2.07	0.54
1:D:229:GLU:HG2	1:D:300:ARG:HG2	1.89	0.54
1:B:311:VAL:HG12	1:B:390:ALA:HB2	1.88	0.54
1:D:206:ARG:NH1	1:D:433:SER:O	2.40	0.54
3:N:1:DT:H1'	3:N:2:DC:H5'	1.89	0.54
1:A:200:ARG:NH2	4:A:727:HOH:O	2.41	0.54
1:A:542:ILE:HG12	1:A:547:VAL:HG23	1.90	0.54
1:D:380:THR:CG2	1:D:422:ALA:HA	2.37	0.54
1:D:392:PHE:CE2	1:D:394:LEU:HB2	2.42	0.54
1:D:464:GLY:O	1:D:530:ARG:NE	2.32	0.54
2:M:7:DT:H2"	2:M:8:DT:O2	2.08	0.54
1:B:393:THR:HG22	1:B:393:THR:O	2.07	0.54
1:D:607:ARG:HB2	1:D:629:TYR:CZ	2.42	0.54
1:B:639:ARG:HG2	1:B:639:ARG:HH21	1.73	0.54
1:D:378:SER:HB3	1:D:381:GLU:HG3	1.90	0.53
1:A:639:ARG:CB	1:A:640:GLY:CA	2.86	0.53
1:C:302:LEU:N	1:C:303:GLY:HA2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:THR:HG21	1:D:421:ASN:C	2.29	0.53
2:E:7:DT:H2"	2:E:8:DT:O2	2.08	0.53
1:C:638:GLY:N	1:C:641:PTR:O	2.42	0.53
1:D:140:ARG:NH2	1:D:189:GLU:OE2	2.33	0.53
1:D:370:ARG:NH1	2:E:7:DT:P	2.82	0.53
1:C:464:GLY:O	1:C:530:ARG:NE	2.34	0.53
2:M:16:DA:H2"	2:M:17:DG:C8	2.44	0.52
1:A:638:GLY:N	1:A:639:ARG:CB	2.73	0.52
1:B:589:ILE:HD11	1:D:644:ALA:HB2	1.91	0.52
1:D:370:ARG:HH11	1:D:370:ARG:CG	2.13	0.52
2:M:20:DA:H4'	2:M:20:DA:OP1	2.09	0.52
1:A:373:ARG:O	1:A:373:ARG:NH1	2.42	0.52
1:A:639:ARG:CB	1:A:641:PTR:N	2.72	0.52
1:C:268:LEU:HG	1:C:297:LEU:HD11	1.91	0.52
1:C:510:ARG:HG3	1:C:510:ARG:HH11	1.75	0.52
1:C:179:LEU:HB3	1:C:181:MET:HB2	1.92	0.52
1:A:637:ASP:HA	1:A:641:PTR:O	2.09	0.52
1:D:379:VAL:HG22	2:E:6:DT:OP1	2.10	0.52
3:N:17:DA:H2"	3:N:18:DT:H5'	1.92	0.52
1:C:492:PHE:HZ	4:C:701:HOH:O	1.91	0.52
1:A:638:GLY:CA	1:A:639:ARG:HG2	2.39	0.52
1:C:585:GLN:HA	1:C:585:GLN:NE2	2.25	0.52
1:D:634:MET:SD	1:D:635:GLY:N	2.83	0.51
1:A:347:LEU:HA	1:A:358:ALA:HB2	1.91	0.51
1:B:641:PTR:O2P	1:D:566:SER:OG	2.28	0.51
1:C:525:THR:HA	1:C:529:LEU:HB2	1.92	0.51
1:C:229:GLU:HG2	1:C:300:ARG:HG2	1.93	0.51
2:E:20:DA:H4'	2:E:20:DA:OP1	2.11	0.51
3:F:1:DT:H2"	3:F:2:DC:H5'	1.92	0.51
3:F:13:DG:C1'	3:F:14:DG:N7	2.70	0.51
1:B:136:ARG:NH2	1:B:189:GLU:OE2	2.44	0.51
1:A:564:SER:OG	1:C:641:PTR:O1P	2.21	0.51
1:D:525:THR:HA	1:D:529:LEU:HB2	1.93	0.51
1:A:374:LYS:HB2	4:A:798:HOH:O	2.01	0.51
1:C:347:LEU:HA	1:C:358:ALA:HB2	1.92	0.50
1:B:544:LYS:O	1:B:548:THR:HG23	2.12	0.50
1:B:641:PTR:P	1:D:566:SER:HG	2.35	0.50
1:C:607:ARG:HB2	1:C:629:TYR:CE1	2.46	0.50
1:D:245:ALA:CB	1:D:254:ARG:HH12	2.24	0.50
1:D:268:LEU:HG	1:D:297:LEU:HD11	1.91	0.50
1:C:510:ARG:HH12	1:C:565:ASP:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLN:O	1:B:242:VAL:HG22	2.12	0.50
1:B:378:SER:CB	1:B:381:GLU:HG3	2.42	0.50
1:D:510:ARG:HG3	1:D:510:ARG:HH11	1.77	0.50
1:A:606:ILE:HG22	1:A:621:LYS:HD2	1.93	0.50
1:B:538:ILE:O	4:B:703:HOH:O	2.20	0.50
1:B:556:ASP:HB2	1:B:578:ARG:HB2	1.94	0.50
1:A:638:GLY:N	1:A:639:ARG:HB2	2.27	0.50
1:A:639:ARG:HB3	1:A:640:GLY:C	2.32	0.50
1:A:639:ARG:HB3	1:A:641:PTR:HD2	1.93	0.50
1:B:419:ASP:O	1:B:423:LYS:HG3	2.11	0.50
1:B:390:ALA:O	1:B:403:LEU:HB2	2.11	0.50
1:D:607:ARG:HB2	1:D:629:TYR:CE1	2.47	0.50
1:A:245:ALA:O	1:A:248:GLU:HB3	2.12	0.50
1:A:290:GLN:HG2	1:A:361:LYS:HA	1.92	0.50
1:A:639:ARG:HB2	1:A:641:PTR:N	2.26	0.50
1:D:370:ARG:NH1	1:D:370:ARG:CG	2.73	0.50
1:A:639:ARG:CG	1:A:641:PTR:HB3	2.40	0.49
1:D:249:LEU:CB	1:D:253:THR:CB	2.73	0.49
1:C:206:ARG:NH1	1:C:433:SER:O	2.45	0.49
1:A:538:ILE:O	4:A:706:HOH:O	2.20	0.49
1:B:367:LYS:NZ	3:F:8:DT:OP1	2.45	0.49
1:A:302:LEU:CB	1:A:306:ALA:HB2	2.42	0.49
1:B:218:GLU:HB3	1:B:219:GLU:HA	1.93	0.49
1:C:530:ARG:NH1	1:C:534:SER:OG	2.46	0.49
1:A:238:LEU:O	1:A:242:VAL:HG23	2.11	0.49
1:B:577:ILE:HD11	1:B:587:GLU:OE1	2.13	0.49
1:D:179:LEU:HD23	1:D:181:MET:HB2	1.95	0.49
1:D:144:ILE:HG22	1:D:241:GLU:HG2	1.94	0.49
1:A:523:ASP:O	1:A:527:ARG:HG3	2.13	0.49
1:D:302:LEU:N	1:D:303:GLY:HA2	2.27	0.49
1:C:233:ASP:O	1:C:237:GLN:HG2	2.12	0.49
1:B:611:GLN:O	1:B:613:LYS:HG2	2.12	0.49
1:D:370:ARG:HG3	2:E:7:DT:OP1	2.13	0.49
1:A:439:PRO:HA	1:A:440:PHE:HA	1.50	0.49
1:D:254:ARG:O	1:D:256:SER:N	2.41	0.49
1:D:542:ILE:HG22	1:D:543:SER:O	2.13	0.49
1:A:636:LYS:CA	1:A:636:LYS:CE	2.91	0.48
1:C:542:ILE:HG22	1:C:543:SER:O	2.13	0.48
1:B:347:LEU:HA	1:B:358:ALA:HB2	1.95	0.48
1:C:475:LEU:HD13	1:C:489:MET:HA	1.94	0.48
1:C:609:LEU:O	1:C:621:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:O	1:A:238:LEU:HD23	2.12	0.48
1:D:379:VAL:CG2	2:E:6:DT:P	2.98	0.48
2:M:4:DG:H1	3:N:19:DC:H42	1.60	0.48
1:C:144:ILE:HG22	1:C:241:GLU:HG2	1.95	0.48
1:A:370:ARG:CZ	1:A:379:VAL:HG22	2.42	0.48
1:A:638:GLY:HA3	1:A:639:ARG:HG2	1.94	0.48
1:B:375:GLY:N	1:B:377:GLU:N	2.60	0.48
1:A:445:ARG:HD2	1:A:498:SER:HB3	1.95	0.48
1:B:510:ARG:HH11	1:B:510:ARG:HG3	1.79	0.48
3:F:13:DG:N3	3:F:14:DG:C5	2.82	0.48
1:C:232:VAL:HG23	1:C:268:LEU:HD23	1.95	0.48
1:B:183:LEU:HB3	1:B:257:LEU:HD11	1.95	0.48
1:B:596:ASP:O	1:B:605:ARG:NH2	2.35	0.48
2:M:19:DC:H2"	2:M:20:DA:O4'	2.14	0.48
1:C:510:ARG:NH1	1:C:565:ASP:O	2.47	0.48
1:A:256:SER:O	1:A:260:ARG:HG3	2.14	0.48
1:A:269:VAL:HG13	1:A:295:PHE:HZ	1.78	0.48
1:D:225:GLN:HB2	1:D:296:LEU:HD22	1.95	0.47
1:B:187:THR:O	1:B:191:GLU:HG3	2.14	0.47
1:D:305:PRO:HD3	1:D:394:LEU:HD21	1.95	0.47
1:B:148:ARG:NE	1:B:241:GLU:OE1	2.40	0.47
1:D:283:LEU:HD11	1:D:289:PHE:CD1	2.50	0.47
1:D:380:THR:O	1:D:425:THR:OG1	2.29	0.47
1:C:604:ASP:OD1	1:C:604:ASP:N	2.44	0.47
1:A:202:GLN:HG2	1:A:435:MET:HG2	1.95	0.47
1:B:544:LYS:HA	1:B:547:VAL:HB	1.97	0.47
1:D:179:LEU:HB3	1:D:181:MET:HB2	1.96	0.47
1:C:368:ILE:HD12	1:C:369:LYS:H	1.80	0.47
1:B:217:PHE:CB	1:B:219:GLU:HG2	2.44	0.47
1:D:479:GLN:HB2	1:D:484:ASP:O	2.15	0.47
1:C:439:PRO:HA	1:C:440:PHE:HA	1.50	0.47
1:C:542:ILE:O	1:C:562:ARG:HD2	2.15	0.47
1:C:638:GLY:HA2	1:C:639:ARG:HA	1.65	0.47
1:A:374:LYS:HG2	4:A:798:HOH:O	2.14	0.47
1:B:368:ILE:HD12	1:B:369:LYS:H	1.80	0.47
1:C:605:ARG:O	1:C:609:LEU:HD12	2.15	0.47
1:B:551:LEU:HB3	1:B:586:ILE:HD11	1.96	0.46
1:C:341:ILE:CG1	1:C:364:LEU:HB3	2.45	0.46
1:A:181:MET:HE2	1:A:181:MET:HB2	1.79	0.46
1:A:639:ARG:CB	1:A:640:GLY:HA2	2.45	0.46
1:B:299:LEU:HG	1:B:349:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:16:DA:H2"	2:E:17:DG:C8	2.50	0.46
1:B:194:LYS:O	1:B:197:VAL:HG12	2.15	0.46
3:F:1:DT:H1'	3:F:2:DC:H5'	1.97	0.46
1:C:152:GLN:O	1:C:152:GLN:HG2	2.16	0.46
1:B:615:LEU:N	1:B:619:LYS:O	2.47	0.46
1:C:486:SER:N	4:C:701:HOH:O	2.19	0.46
1:A:350:SER:OG	1:A:352:PRO:O	2.29	0.46
1:B:194:LYS:O	1:B:198:LEU:HD13	2.15	0.46
1:A:373:ARG:HD2	1:A:373:ARG:C	2.28	0.46
1:D:301:PHE:C	1:D:303:GLY:HA2	2.36	0.46
2:E:18:DA:H2"	2:E:19:DC:O2	2.16	0.46
1:B:436:ASP:OD1	1:B:436:ASP:N	2.48	0.46
3:F:17:DA:H2"	3:F:18:DT:H5'	1.98	0.46
2:M:7:DT:H72	2:M:8:DT:H71	1.97	0.46
1:B:302:LEU:HD21	1:B:392:PHE:HE1	1.79	0.46
1:D:530:ARG:NH1	1:D:534:SER:OG	2.49	0.46
3:F:11:DT:H2"	3:F:12:DA:N7	2.31	0.46
1:C:225:GLN:HB2	1:C:296:LEU:HD22	1.97	0.46
1:D:341:ILE:CG1	1:D:364:LEU:HB3	2.46	0.46
1:A:423:LYS:NZ	4:A:723:HOH:O	2.49	0.46
1:A:639:ARG:HB3	1:A:641:PTR:N	2.31	0.46
1:B:223:PRO:O	1:B:227:ARG:HG3	2.16	0.46
3:F:20:DC:H2"	3:F:21:DA:C8	2.51	0.46
3:N:14:DG:H2"	3:N:15:DA:O5'	2.16	0.46
1:C:544:LYS:HD3	1:C:562:ARG:NH2	2.31	0.46
1:A:581:ASP:N	1:A:582:GLY:HA2	2.31	0.45
1:D:214:GLY:O	1:D:457:LEU:HB3	2.16	0.45
3:N:11:DT:H2"	3:N:12:DA:N7	2.31	0.45
1:C:187:THR:O	1:C:191:GLU:HG3	2.15	0.45
1:A:309:PRO:HG3	1:A:392:PHE:HE1	1.81	0.45
1:D:605:ARG:O	1:D:609:LEU:HD12	2.16	0.45
1:B:545:GLN:O	1:B:548:THR:OG1	2.22	0.45
1:D:562:ARG:NH1	1:D:565:ASP:OD2	2.50	0.45
1:A:307:LYS:HB3	1:A:307:LYS:HE3	1.75	0.45
1:B:379:VAL:HG11	3:F:6:DC:H5"	1.97	0.45
2:E:4:DG:H2"	2:E:5:DA:O5'	2.16	0.45
1:B:572:THR:HG23	1:B:589:ILE:O	2.16	0.45
1:C:235:TYR:HE1	1:C:261:LEU:HB3	1.82	0.45
1:A:529:LEU:HA	1:A:532:TYR:CD1	2.52	0.45
1:D:187:THR:O	1:D:191:GLU:HG3	2.16	0.45
1:C:519:ASP:HA	1:C:522:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:ARG:HA	1:C:640:GLY:HA2	1.55	0.45
1:B:379:VAL:HG23	1:B:380:THR:N	2.32	0.45
1:B:510:ARG:HH12	1:B:565:ASP:HB3	1.81	0.44
1:A:309:PRO:HG3	1:A:392:PHE:CE1	2.51	0.44
1:A:373:ARG:O	1:A:374:LYS:HD3	2.17	0.44
1:A:637:ASP:HB2	1:A:641:PTR:C	2.47	0.44
1:B:253:THR:O	1:B:253:THR:OG1	2.35	0.44
1:B:373:ARG:CD	1:B:377:GLU:HB3	2.47	0.44
3:F:21:DA:H3'	3:F:22:DT:H4'	1.99	0.44
1:C:630:LYS:HA	1:C:630:LYS:HZ3	1.83	0.44
1:A:302:LEU:HD13	1:A:305:PRO:HG2	1.97	0.44
1:A:484:ASP:OD1	1:B:467:ARG:NH2	2.50	0.44
1:B:355:CYS:SG	4:B:711:HOH:O	2.61	0.44
1:D:630:LYS:HA	1:D:630:LYS:HZ3	1.82	0.44
3:F:1:DT:C2'	3:F:2:DC:H5'	2.48	0.44
1:D:596:ASP:O	1:D:605:ARG:NH2	2.37	0.44
1:C:194:LYS:O	1:C:197:VAL:HG12	2.17	0.44
1:C:295:PHE:O	1:C:356:CYS:HB3	2.17	0.44
1:A:639:ARG:CB	1:A:641:PTR:HB3	2.48	0.44
1:D:639:ARG:HA	1:D:640:GLY:HA2	1.51	0.44
1:C:283:LEU:HD11	1:C:289:PHE:CD1	2.52	0.44
1:B:639:ARG:HA	1:B:639:ARG:HD2	1.63	0.44
1:D:254:ARG:HD2	1:D:254:ARG:HA	1.68	0.44
1:A:575:HIS:CE1	1:A:577:ILE:HD11	2.52	0.44
1:A:611:GLN:H	1:A:611:GLN:HE21	1.65	0.44
1:B:256:SER:O	1:B:257:LEU:C	2.56	0.44
2:E:7:DT:H72	2:E:8:DT:H71	1.99	0.44
3:F:13:DG:C2	3:F:14:DG:N1	2.85	0.44
1:D:380:THR:HG23	1:D:422:ALA:CA	2.48	0.43
1:B:138:GLN:NE2	1:B:237:GLN:HE22	2.16	0.43
1:B:392:PHE:CD1	1:B:393:THR:N	2.83	0.43
1:B:185:GLU:O	1:B:189:GLU:HG3	2.18	0.43
1:D:378:SER:CA	1:D:381:GLU:HG3	2.48	0.43
1:D:609:LEU:O	1:D:621:LYS:NZ	2.51	0.43
1:C:269:VAL:HG13	1:C:295:PHE:CZ	2.53	0.43
1:C:520:GLY:HA3	1:C:568:ILE:HG23	2.01	0.43
1:A:588:ASN:HB3	1:C:641:PTR:HD1	2.00	0.43
1:D:370:ARG:NH1	2:E:7:DT:OP1	2.51	0.43
1:D:439:PRO:HA	1:D:440:PHE:HA	1.51	0.43
2:E:21:DG:N2	3:F:2:DC:C2	2.85	0.43
1:B:370:ARG:N	1:B:370:ARG:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:510:ARG:HH12	1:D:565:ASP:HB3	1.84	0.43
1:D:575:HIS:NE2	1:D:587:GLU:OE2	2.51	0.43
3:F:13:DG:C4	3:F:14:DG:C5	3.06	0.43
1:D:544:LYS:HD3	1:D:562:ARG:NH2	2.34	0.43
1:A:643:PRO:HA	1:C:590:GLN:HB2	2.01	0.43
1:D:340:ILE:HG23	1:D:343:ASN:HB3	2.01	0.43
2:M:22:DA:O4'	2:M:22:DA:OP1	2.37	0.43
2:M:18:DA:H2"	2:M:19:DC:O2	2.18	0.42
2:M:22:DA:OP1	2:M:22:DA:C4'	2.67	0.42
1:C:269:VAL:HG13	1:C:295:PHE:HZ	1.84	0.42
1:A:374:LYS:O	1:A:374:LYS:HD3	2.19	0.42
1:B:310:LEU:HD21	1:B:344:THR:HB	2.01	0.42
1:D:370:ARG:HH12	2:E:7:DT:P	2.43	0.42
1:A:544:LYS:O	1:A:548:THR:OG1	2.34	0.42
1:B:301:PHE:HD2	1:B:392:PHE:CZ	2.37	0.42
1:D:148:ARG:HD2	1:D:244:ALA:CB	2.40	0.42
1:D:295:PHE:O	1:D:356:CYS:HB3	2.19	0.42
1:A:600:ARG:CZ	1:A:604:ASP:HB3	2.50	0.42
1:D:301:PHE:O	1:D:303:GLY:HA2	2.19	0.42
2:E:5:DA:H2'	2:E:6:DT:C2	2.54	0.42
1:A:148:ARG:O	1:A:152:GLN:HG2	2.19	0.42
1:A:371:CYS:SG	1:A:372:GLU:N	2.92	0.42
3:N:20:DC:H2"	3:N:21:DA:C8	2.54	0.42
1:C:619:LYS:HA	1:C:620:PRO:HD3	1.93	0.42
1:A:638:GLY:H	1:A:639:ARG:CB	2.30	0.42
1:B:322:ARG:HE	1:B:322:ARG:HB2	1.69	0.42
1:B:520:GLY:HA3	1:B:568:ILE:HG23	2.01	0.42
1:C:237:GLN:HG2	1:C:237:GLN:H	1.63	0.42
1:A:475:LEU:O	1:A:479:GLN:HG3	2.20	0.42
1:B:254:ARG:HD3	1:B:254:ARG:HA	1.65	0.42
1:B:439:PRO:HA	1:B:440:PHE:HA	1.51	0.42
1:B:533:TRP:HZ3	1:B:540:GLY:HA3	1.84	0.42
1:D:245:ALA:HB2	1:D:254:ARG:HH12	1.85	0.42
1:B:301:PHE:CD2	1:B:392:PHE:CZ	3.00	0.42
1:B:367:LYS:HE2	1:B:367:LYS:HB2	1.91	0.42
1:B:389:SER:O	1:B:390:ALA:HB2	2.20	0.42
1:B:484:ASP:OD2	1:B:495:ARG:NH1	2.44	0.42
1:D:638:GLY:HA2	1:D:639:ARG:HA	1.59	0.42
2:E:21:DG:N2	3:F:2:DC:O2	2.53	0.42
1:A:294:ARG:NH1	4:A:711:HOH:O	2.49	0.41
1:A:578:ARG:HA	1:A:584:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:SER:HB3	1:B:381:GLU:HG3	2.02	0.41
1:D:233:ASP:O	1:D:237:GLN:HG2	2.20	0.41
2:M:7:DT:H71	3:N:16:DA:C2	2.55	0.41
1:C:301:PHE:C	1:C:303:GLY:HA2	2.40	0.41
1:A:301:PHE:HA	1:A:302:LEU:HA	1.88	0.41
1:A:302:LEU:HB3	1:A:306:ALA:HB2	2.00	0.41
1:B:368:ILE:HB	1:B:412:VAL:HG11	2.02	0.41
1:D:238:LEU:O	1:D:242:VAL:HG23	2.19	0.41
1:C:214:GLY:O	1:C:457:LEU:HB3	2.20	0.41
1:B:213:ASN:HB2	1:B:430:ASN:HB3	2.03	0.41
1:A:129:LYS:HD2	1:A:129:LYS:HA	1.86	0.41
1:A:373:ARG:O	1:A:374:LYS:HG3	2.20	0.41
1:B:148:ARG:O	1:B:152:GLN:HG2	2.20	0.41
1:B:547:VAL:HG21	1:B:562:ARG:HD2	2.01	0.41
1:A:131:LYS:O	1:A:135:ARG:HG2	2.20	0.41
1:D:245:ALA:HB2	1:D:254:ARG:NH1	2.35	0.41
1:D:288:LYS:HG3	1:D:364:LEU:HD23	2.03	0.41
1:C:590:GLN:HA	1:C:591:PRO:HD3	1.88	0.41
1:B:213:ASN:ND2	1:B:427:LEU:HD12	2.30	0.41
1:B:307:LYS:HD2	1:B:307:LYS:N	2.32	0.41
1:D:520:GLY:HA3	1:D:568:ILE:HG23	2.03	0.41
1:D:616:TYR:HA	1:D:617:PRO:HA	1.70	0.41
2:M:4:DG:H2"	2:M:5:DA:O5'	2.20	0.41
1:C:406:LEU:HD12	1:C:406:LEU:HA	1.85	0.41
1:A:246:GLY:HA2	1:A:247:GLY:HA2	1.88	0.41
1:A:399:LEU:HB2	1:A:400:PRO:HD3	2.03	0.41
1:A:187:THR:O	1:A:191:GLU:HG3	2.20	0.41
1:A:322:ARG:HE	1:A:322:ARG:HB2	1.67	0.41
1:B:611:GLN:HG2	1:B:612:LEU:N	2.36	0.41
1:D:194:LYS:O	1:D:197:VAL:HG12	2.21	0.41
2:M:8:DT:H1'	2:M:9:DC:H5'	2.03	0.41
1:A:520:GLY:HA3	1:A:568:ILE:HG23	2.03	0.41
1:B:138:GLN:HE22	1:B:237:GLN:HE22	1.69	0.41
1:B:261:LEU:O	1:B:264:VAL:HB	2.20	0.41
1:B:368:ILE:HD12	1:B:369:LYS:N	2.36	0.41
1:B:374:LYS:CB	1:B:375:GLY:C	2.85	0.41
1:B:556:ASP:OD1	1:B:578:ARG:N	2.44	0.41
1:D:341:ILE:HD12	1:D:342:ASN:ND2	2.36	0.41
1:D:510:ARG:NH1	1:D:565:ASP:O	2.53	0.41
2:M:3:DG:H2"	2:M:4:DG:C8	2.56	0.41
1:C:288:LYS:HG3	1:C:364:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD11	1:A:289:PHE:CD1	2.56	0.41
1:A:637:ASP:CG	1:A:640:GLY:CA	2.84	0.41
1:B:615:LEU:HD22	1:B:625:PHE:CE2	2.56	0.41
2:E:2:DT:H73	3:F:21:DA:N1	2.36	0.41
2:E:13:DG:H2"	2:E:14:DG:C8	2.55	0.41
1:C:370:ARG:O	1:C:371:CYS:SG	2.77	0.41
1:C:600:ARG:NH1	1:C:604:ASP:HB2	2.36	0.41
1:A:370:ARG:NE	1:A:379:VAL:HG21	2.37	0.40
1:A:409:PRO:HG2	1:A:437:ARG:HH22	1.86	0.40
1:B:538:ILE:HG22	1:B:540:GLY:CA	2.51	0.40
1:D:305:PRO:HG3	1:D:394:LEU:HD21	2.02	0.40
1:D:315:MET:HE3	1:D:365:LEU:HD13	2.02	0.40
1:B:374:LYS:HD3	1:B:374:LYS:HA	1.88	0.40
1:D:140:ARG:HH12	1:D:185:GLU:HG2	1.86	0.40
1:C:424:ALA:HB2	1:C:515:TRP:NE1	2.35	0.40
1:D:479:GLN:CB	1:D:484:ASP:O	2.69	0.40
1:A:370:ARG:NE	1:A:379:VAL:HG22	2.36	0.40
1:A:577:ILE:O	1:A:584:PRO:HA	2.22	0.40
1:D:148:ARG:NE	1:D:241:GLU:OE1	2.49	0.40
3:N:1:DT:OP2	3:N:1:DT:H6	2.03	0.40
1:C:300:ARG:HD3	1:C:300:ARG:HA	1.71	0.40
1:C:616:TYR:HA	1:C:617:PRO:HA	1.74	0.40
1:B:301:PHE:CE2	1:B:392:PHE:HE2	2.22	0.40
1:D:184:GLN:OE1	1:D:184:GLN:N	2.50	0.40
1:D:341:ILE:HG13	1:D:364:LEU:HB3	2.04	0.40
1:C:138:GLN:O	1:C:141:VAL:HB	2.21	0.40
1:C:184:GLN:OE1	1:C:184:GLN:N	2.48	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)
2:M:1:DA:OP2	2:M:22:DA:OP2[1_655]	1.50	0.70
2:M:1:DA:OP2	2:M:22:DA:P[1_655]	2.08	0.12
1:A:466:ASN:ND2	1:B:483:ASN:O[1_655]	2.13	0.07
2:M:1:DA:P	2:M:22:DA:OP2[1_655]	2.18	0.02

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	465/549 (85%)	448 (96%)	14 (3%)	3 (1%)	25	59
1	B	467/549 (85%)	448 (96%)	18 (4%)	1 (0%)	47	79
1	C	448/549 (82%)	436 (97%)	10 (2%)	2 (0%)	34	69
1	D	455/549 (83%)	438 (96%)	15 (3%)	2 (0%)	34	69
All	All	1835/2196 (84%)	1770 (96%)	57 (3%)	8 (0%)	34	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLY
1	B	338	GLY
1	D	371	CYS
1	A	637	ASP
1	C	583	SER
1	D	247	GLY
1	A	400	PRO
1	C	584	PRO

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	413/469 (88%)	395 (96%)	18 (4%)	28	61
1	B	413/469 (88%)	387 (94%)	26 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	402/469 (86%)	385 (96%)	17 (4%)	30 62
1	D	406/469 (87%)	389 (96%)	17 (4%)	30 62
All	All	1634/1876 (87%)	1556 (95%)	78 (5%)	25 58

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	PHE
1	A	152	GLN
1	A	179	LEU
1	A	181	MET
1	A	266	ARG
1	A	302	LEU
1	A	307	LYS
1	A	355	CYS
1	A	373	ARG
1	A	374	LYS
1	A	382	GLU
1	A	392	PHE
1	A	554	GLU
1	A	611	GLN
1	A	618	LYS
1	A	636	LYS
1	A	637	ASP
1	A	639	ARG
1	B	140	ARG
1	B	266	ARG
1	B	284	LYS
1	B	288	LYS
1	B	300	ARG
1	B	307	LYS
1	B	343	ASN
1	B	348	GLU
1	B	369	LYS
1	B	370	ARG
1	B	371	CYS
1	B	372	GLU
1	B	373	ARG
1	B	378	SER
1	B	392	PHE
1	B	394	LEU

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Mol	Chain	Res	Type
1	B	490	GLU
1	B	528	CYS
1	B	531	SER
1	B	544	LYS
1	B	580	GLN
1	B	585	GLN
1	B	586	ILE
1	B	632	GLU
1	B	634	MET
1	B	639	ARG
1	D	140	ARG
1	D	249	LEU
1	D	254	ARG
1	D	290	GLN
1	D	312	ARG
1	D	372	GLU
1	D	377	GLU
1	D	379	VAL
1	D	484	ASP
1	D	486	SER
1	D	487	LEU
1	D	490	GLU
1	D	562	ARG
1	D	604	ASP
1	D	630	LYS
1	D	633	GLN
1	D	639	ARG
1	C	138	GLN
1	C	140	ARG
1	C	152	GLN
1	C	237	GLN
1	C	253	THR
1	C	254	ARG
1	C	312	ARG
1	C	370	ARG
1	C	379	VAL
1	C	487	LEU
1	C	490	GLU
1	C	583	SER
1	C	604	ASP
1	C	630	LYS
1	C	633	GLN

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Mol	Chain	Res	Type
1	C	634	MET
1	C	639	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	611	GLN
1	B	213	ASN
1	B	237	GLN
1	B	628	HIS
1	D	237	GLN
1	D	290	GLN
1	C	585	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	D	641	1	15,16,17	1.26	1 (6%)	19,22,24	0.70	0
1	PTR	C	641	1	15,16,17	1.26	1 (6%)	19,22,24	0.64	0
1	PTR	B	641	1	15,16,17	1.28	1 (6%)	19,22,24	0.69	0
1	PTR	A	641	1	15,16,17	0.80	0	19,22,24	0.98	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	D	641	1	-	0/10/11/13	0/1/1/1
1	PTR	C	641	1	-	1/10/11/13	0/1/1/1
1	PTR	B	641	1	-	0/10/11/13	0/1/1/1
1	PTR	A	641	1	-	2/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	641	PTR	OH-CZ	-4.55	1.30	1.40
1	D	641	PTR	OH-CZ	-4.42	1.30	1.40
1	C	641	PTR	OH-CZ	-4.39	1.30	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	641	PTR	CB-CA-C	-2.01	107.70	111.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	641	PTR	C-CA-CB-CG
1	C	641	PTR	O-C-CA-CB
1	A	641	PTR	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	641	PTR	1	0
1	C	641	PTR	3	0
1	B	641	PTR	2	0
1	A	641	PTR	17	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	477/549 (86%)	-0.16	1 (0%)	95	90	25, 55, 102, 137	0
1	B	476/549 (86%)	-0.09	6 (1%)	77	59	23, 56, 105, 140	0
1	C	464/549 (84%)	-0.09	1 (0%)	95	90	43, 72, 114, 146	0
1	D	471/549 (85%)	-0.16	2 (0%)	92	84	46, 72, 112, 148	0
2	E	22/22 (100%)	-0.25	1 (4%)	33	16	74, 86, 103, 142	0
2	M	22/22 (100%)	-0.37	1 (4%)	33	16	74, 86, 111, 144	0
3	F	22/22 (100%)	-0.36	1 (4%)	33	16	48, 89, 114, 129	0
3	N	22/22 (100%)	-0.36	1 (4%)	33	16	50, 90, 114, 155	0
All	All	1976/2284 (86%)	-0.14	14 (0%)	87	75	23, 66, 110, 155	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	22	DA	4.5
3	N	22	DT	4.3
1	B	305	PRO	3.9
1	B	215	ALA	3.1
1	C	651	GLU	3.1
1	D	218	GLU	2.7
1	B	216	PRO	2.6
1	B	634	MET	2.6
3	F	22	DT	2.5
1	B	637	ASP	2.4
1	D	367	LYS	2.3
2	M	22	DA	2.3
1	B	218	GLU	2.3
1	A	248	GLU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PTR	A	641	16/17	0.82	0.26	70,75,78,85	0
1	PTR	B	641	16/17	0.88	0.19	65,68,75,77	0
1	PTR	D	641	16/17	0.96	0.20	45,50,52,52	0
1	PTR	C	641	16/17	0.97	0.18	43,46,49,49	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.