Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:23 PM GMT

PDB ID	:	3TS8
Title	:	Crystal structure of a multidomain human p53 tetramer bound to the natural CDKN1A(p21) p53-response element
Authors	:	Halazonetis, T.D.; Emamzadah, S.
Deposited on	:	2011-09-12
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

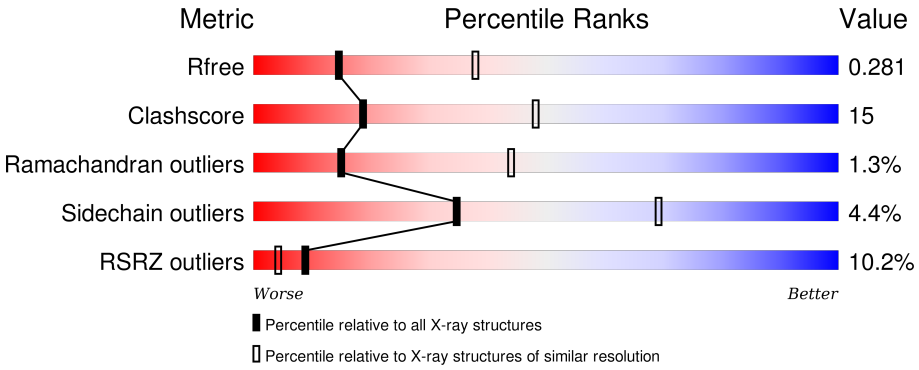
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	234	4% 75% 24%
1	B	234	26% 48% 48%
1	C	234	2% 74% 26%
1	D	234	11% 71% 27%
2	K	26	46% 50%

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Mol	Chain	Length	Quality of chain
3	L	26	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8621 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1863	1157	339	354	13			
1	B	234	Total	C	N	O	S	0	0	0
			1863	1157	339	354	13			
1	C	234	Total	C	N	O	S	0	0	0
			1863	1157	339	354	13			
1	D	234	Total	C	N	O	S	0	0	0
			1863	1157	339	354	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
A	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
A	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637
A	182	SER	CYS	ENGINEERED MUTATION	UNP P04637
A	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
A	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
A	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
A	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
A	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637
A	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
A	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
A	253	VAL	THR	ENGINEERED MUTATION	UNP P04637
A	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
A	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
A	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
A	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
A	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637
A	356	THR	GLY	ENGINEERED MUTATION	UNP P04637
B	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
B	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
B	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	CYS	ENGINEERED MUTATION	UNP P04637
B	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
B	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
B	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
B	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
B	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637
B	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
B	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
B	253	VAL	THR	ENGINEERED MUTATION	UNP P04637
B	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
B	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
B	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
B	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
B	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637
B	356	THR	GLY	ENGINEERED MUTATION	UNP P04637
C	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
C	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
C	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637
C	182	SER	CYS	ENGINEERED MUTATION	UNP P04637
C	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
C	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
C	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
C	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
C	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637
C	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
C	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
C	253	VAL	THR	ENGINEERED MUTATION	UNP P04637
C	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
C	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
C	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
C	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
C	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637
C	356	THR	GLY	ENGINEERED MUTATION	UNP P04637
D	135	VAL	CYS	ENGINEERED MUTATION	UNP P04637
D	141	VAL	CYS	ENGINEERED MUTATION	UNP P04637
D	146	TYR	TRP	ENGINEERED MUTATION	UNP P04637
D	182	SER	CYS	ENGINEERED MUTATION	UNP P04637
D	203	ALA	VAL	ENGINEERED MUTATION	UNP P04637
D	209	PRO	ARG	ENGINEERED MUTATION	UNP P04637
D	229	TYR	CYS	ENGINEERED MUTATION	UNP P04637
D	233	TYR	HIS	ENGINEERED MUTATION	UNP P04637
D	234	PHE	TYR	ENGINEERED MUTATION	UNP P04637

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Chain	Residue	Modelled	Actual	Comment	Reference
D	235	LYS	ASN	ENGINEERED MUTATION	UNP P04637
D	236	PHE	TYR	ENGINEERED MUTATION	UNP P04637
D	253	VAL	THR	ENGINEERED MUTATION	UNP P04637
D	268	ASP	ASN	ENGINEERED MUTATION	UNP P04637
D	322	THR	PRO	ENGINEERED MUTATION	UNP P04637
D	323	MET	LEU	ENGINEERED MUTATION	UNP P04637
D	340	GLN	MET	ENGINEERED MUTATION	UNP P04637
D	344	ARG	LEU	ENGINEERED MUTATION	UNP P04637
D	356	THR	GLY	ENGINEERED MUTATION	UNP P04637

- Molecule 2 is a DNA chain called CDKN1A(p21) sense strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	26	Total	C	N	O	P	0	0	0
			534	255	105	149	25			

- Molecule 3 is a DNA chain called CDKN1A(p21) anti-sense strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	26	Total	C	N	O	P	0	0	0
			526	254	88	159	25			

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	C	46	Total	O	0	0
			46	46		

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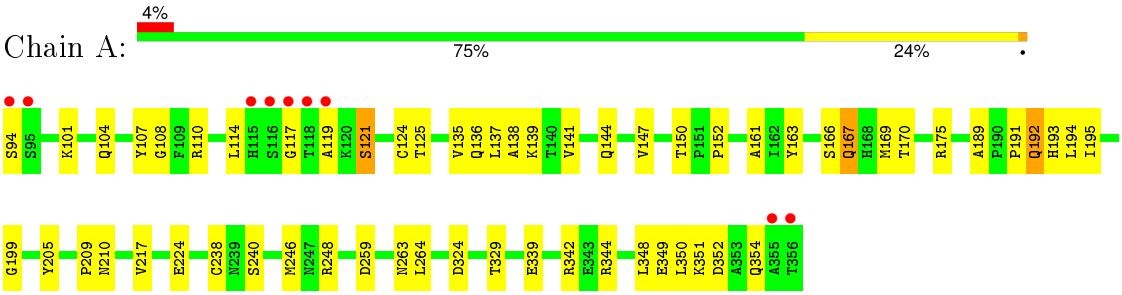
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	28	Total O 28 28	0	0
5	K	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

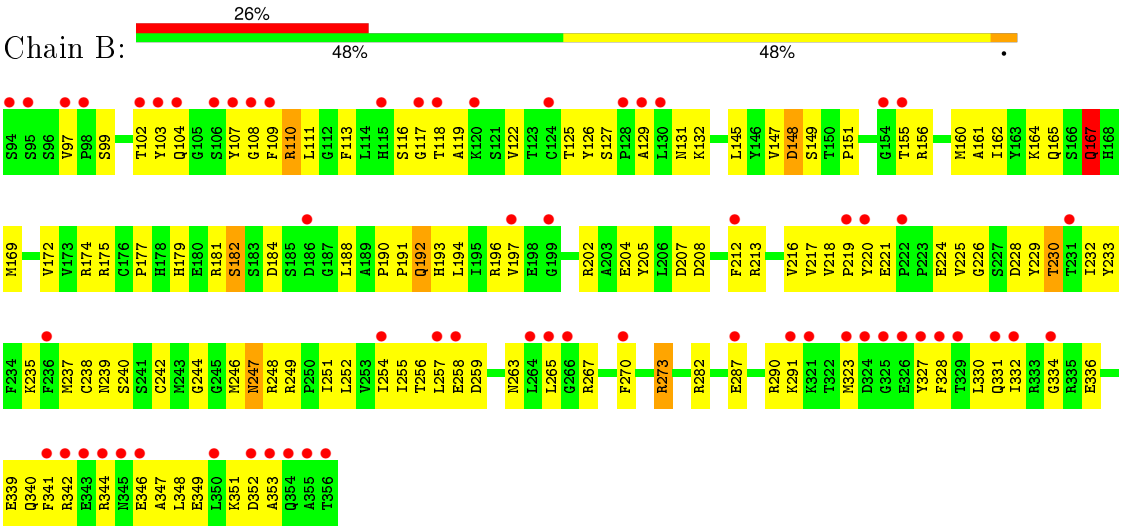
- Molecule 1: Cellular tumor antigen p53

Chain A:



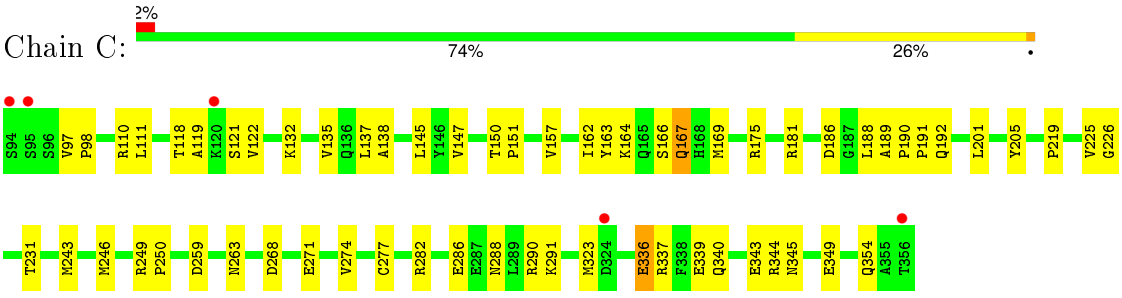
- Molecule 1: Cellular tumor antigen p53

Chain B:



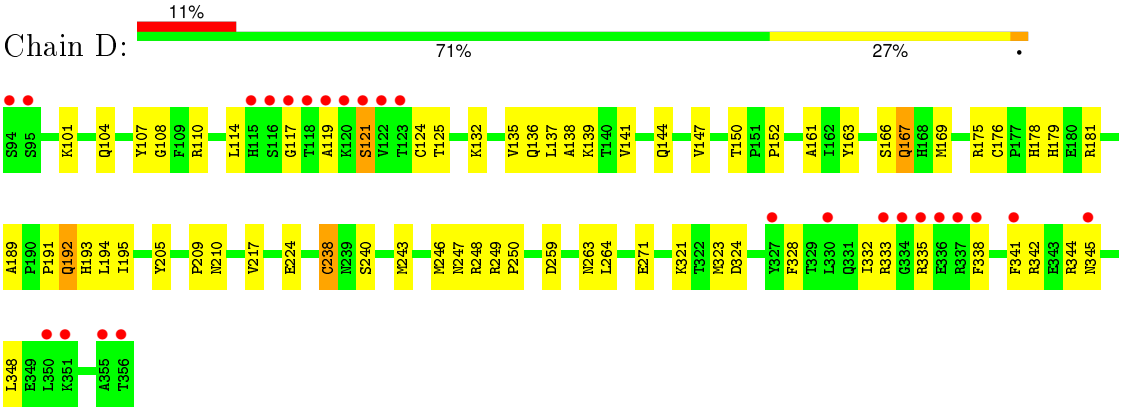
- Molecule 1: Cellular tumor antigen p53

Chain C:



• Molecule 1: Cellular tumor antigen p53

Chain D:



• Molecule 2: CDKN1A(p21) sense strand

Chain K:

• Molecule 3: CDKN1A(p21) anti-sense strand

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.81Å 169.20Å 55.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 52.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 91.9 (52.36-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.283 0.235 , 0.281	Depositor DCC
R_{free} test set	1780 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.1	EDS
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 35704 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8621	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.34	0/1903	0.55	0/2571
1	B	0.30	0/1903	0.48	0/2571
1	C	0.38	0/1903	0.59	0/2571
1	D	0.35	0/1903	0.54	0/2571
2	K	0.40	0/601	0.76	0/926
3	L	0.36	0/587	0.74	0/904
All	All	0.35	0/8800	0.58	0/12114

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
2	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	14	DC	Sidechain

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	1863	0	1822	43	0
1	B	1863	0	1822	107	0
1	C	1863	0	1822	42	0
1	D	1863	0	1822	52	0
2	K	534	0	293	13	0
3	L	526	0	298	19	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	28	0	0	2	0
5	C	46	0	0	2	0
5	D	28	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
All	All	8621	0	7879	252	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 15.

All (252) 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:A:167:GLN:HE21	1:A:167:GLN:H	1.08	0.99
1:C:167:GLN:HE21	1:C:167:GLN:H	1.08	0.96
1:A:192:GLN:H	1:A:192:GLN:HE21	1.15	0.94
1:D:167:GLN:HE21	1:D:167:GLN:H	1.08	0.93
1:C:166:SER:HA	1:C:169:MET:HG3	1.51	0.92
1:B:132:LYS:HE2	1:B:273:ARG:HB2	1.50	0.92
1:D:192:GLN:HE21	1:D:192:GLN:H	1.16	0.87
1:C:167:GLN:NE2	1:C:167:GLN:H	1.73	0.86
1:C:167:GLN:N	1:C:167:GLN:HE21	1.76	0.83
1:B:104:GLN:HB3	1:B:108:GLY:HA2	1.62	0.82
1:B:256:THR:HG22	1:B:267:ARG:HA	1.62	0.81
1:B:111:LEU:HD11	1:B:255:ILE:HG21	1.62	0.80
1:D:192:GLN:NE2	1:D:192:GLN:H	1.80	0.80
1:D:167:GLN:HE21	1:D:167:GLN:N	1.80	0.80
1:D:167:GLN:NE2	1:D:167:GLN:H	1.79	0.79
1:A:167:GLN:NE2	1:A:167:GLN:H	1.80	0.78
1:A:192:GLN:NE2	1:A:192:GLN:H	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLN:N	1:D:192:GLN:HE21	1.82	0.77
3:L:31:DA:H2"	3:L:32:DC:H5"	1.64	0.77
1:A:167:GLN:N	1:A:167:GLN:HE21	1.80	0.77
1:A:344:ARG:HG2	1:C:344:ARG:HH22	1.49	0.77
1:B:208:ASP:HB3	1:B:213:ARG:H	1.51	0.76
1:B:97:VAL:HG21	1:B:169:MET:HB3	1.68	0.76
1:A:192:GLN:N	1:A:192:GLN:HE21	1.82	0.75
3:L:33:DA:H2"	3:L:34:DT:H5'	1.67	0.75
1:C:118:THR:HG22	1:C:282:ARG:HD3	1.67	0.75
1:B:145:LEU:HD22	1:B:230:THR:HB	1.68	0.73
1:B:147:VAL:HG21	1:B:151:PRO:HD3	1.71	0.71
1:B:110:ARG:NH1	1:B:147:VAL:HA	2.07	0.69
1:A:124:CYS:HB3	1:A:135:VAL:HG23	1.76	0.68
1:B:348:LEU:HD23	1:B:351:LYS:HD2	1.76	0.67
1:D:166:SER:HA	1:D:169:MET:HG3	1.76	0.67
1:A:166:SER:HA	1:A:169:MET:HG3	1.77	0.67
1:D:124:CYS:HB3	1:D:135:VAL:HG23	1.76	0.65
3:L:31:DA:C2'	3:L:32:DC:H5"	2.25	0.65
1:B:334:GLY:HA2	1:D:324:ASP:HB3	1.79	0.64
1:A:348:LEU:HB3	1:C:337:ARG:HH11	1.61	0.64
1:B:110:ARG:HD3	1:B:110:ARG:N	2.13	0.63
1:B:224:GLU:HG2	1:B:225:VAL:H	1.63	0.63
1:B:339:GLU:HA	1:B:342:ARG:HH21	1.63	0.63
1:B:328:PHE:HZ	1:D:335:ARG:HH11	1.47	0.62
1:B:164:LYS:HB2	1:B:252:LEU:HD13	1.81	0.62
1:B:107:TYR:HB2	1:B:265:LEU:HD21	1.81	0.61
1:B:197:VAL:HA	1:B:233:TYR:O	2.00	0.61
1:C:137:LEU:HD12	1:C:138:ALA:N	2.14	0.61
1:B:156:ARG:HG3	1:B:258:GLU:HG3	1.84	0.60
3:L:37:DT:H2"	3:L:38:DG:C8	2.37	0.59
1:C:181:ARG:HH22	1:D:181:ARG:HH21	1.51	0.59
2:K:3:DA:H61	3:L:50:DT:H3	1.49	0.59
2:K:3:DA:N6	3:L:50:DT:H3	2.02	0.58
1:D:135:VAL:HG22	1:D:136:GLN:N	2.19	0.57
1:B:127:SER:HB2	1:B:282:ARG:HE	1.70	0.56
1:A:344:ARG:NE	1:C:344:ARG:HH12	2.03	0.56
1:B:118:THR:HG22	1:B:282:ARG:HD3	1.86	0.56
1:A:329:THR:HG23	5:C:93:HOH:O	2.05	0.56
1:A:163:TYR:OH	1:A:246:MET:HA	2.06	0.56
1:C:164:LYS:HE3	1:C:271:GLU:OE1	2.06	0.56
1:A:135:VAL:HG22	1:A:136:GLN:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:30:DA:H2"	3:L:31:DA:H5'	1.88	0.55
1:B:172:VAL:HB	1:B:174:ARG:HH12	1.72	0.55
1:A:107:TYR:HB3	1:A:147:VAL:CG2	2.37	0.55
2:K:4:DG:H1	3:L:49:DC:H42	1.55	0.55
1:D:107:TYR:HB3	1:D:147:VAL:CG2	2.37	0.54
1:A:152:PRO:HG2	5:A:358:HOH:O	2.06	0.54
1:D:163:TYR:OH	1:D:246:MET:HA	2.08	0.54
1:C:288:ASN:HA	1:C:291:LYS:HE3	1.90	0.54
1:B:196:ARG:HE	1:B:237:MET:HG3	1.73	0.54
1:B:172:VAL:HB	1:B:174:ARG:NH1	2.23	0.53
1:B:256:THR:CG2	1:B:267:ARG:HD3	2.38	0.53
1:A:137:LEU:HD12	1:A:138:ALA:N	2.23	0.53
1:B:204:GLU:O	1:B:216:VAL:HA	2.07	0.53
1:B:131:ASN:HD21	1:B:270:PHE:HA	1.74	0.53
1:B:208:ASP:CB	1:B:213:ARG:H	2.20	0.53
1:B:336:GLU:O	1:B:340:GLN:HG2	2.08	0.53
1:A:135:VAL:HG21	1:A:141:VAL:HG22	1.91	0.53
1:B:192:GLN:HG2	1:B:193:HIS:HD2	1.72	0.53
1:B:202:ARG:HB3	1:B:219:PRO:HD2	1.90	0.53
1:B:127:SER:HB2	1:B:282:ARG:NE	2.24	0.53
1:C:119:ALA:O	1:C:122:VAL:HG22	2.09	0.53
1:B:336:GLU:OE2	1:D:321:LYS:HE2	2.08	0.52
2:K:7:DA:H2"	2:K:8:DC:O5'	2.09	0.52
1:D:344:ARG:NE	1:D:348:LEU:HG	2.25	0.52
1:A:114:LEU:H	1:A:144:GLN:NE2	2.07	0.52
1:B:202:ARG:HD3	1:B:219:PRO:HG2	1.91	0.52
1:A:101:LYS:HD3	1:C:226:GLY:O	2.10	0.52
1:B:104:GLN:NE2	1:B:109:PHE:H	2.07	0.51
3:L:31:DA:H1'	3:L:32:DC:H5"	1.92	0.51
1:A:114:LEU:H	1:A:144:GLN:HE21	1.57	0.51
1:D:137:LEU:HD12	1:D:138:ALA:N	2.25	0.51
2:K:24:DG:H2"	2:K:25:DA:C8	2.45	0.51
1:D:344:ARG:HA	1:D:344:ARG:NE	2.26	0.51
1:D:259:ASP:OD2	1:D:263:ASN:HB2	2.11	0.51
1:B:116:SER:HB3	1:B:125:THR:HA	1.92	0.51
1:B:259:ASP:OD2	1:B:263:ASN:HB2	2.11	0.51
1:B:165:GLN:O	1:B:169:MET:HG3	2.11	0.51
1:D:114:LEU:H	1:D:144:GLN:NE2	2.09	0.51
1:B:177:PRO:HD3	1:B:244:GLY:O	2.10	0.50
1:C:189:ALA:HB2	1:C:205:TYR:CZ	2.46	0.50
1:B:162:ILE:HD11	1:B:254:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLY:O	1:A:121:SER:HA	2.10	0.50
1:D:104:GLN:HB3	1:D:108:GLY:HA2	1.93	0.50
1:B:194:LEU:HD12	1:B:238:CYS:HB2	1.94	0.50
1:D:117:GLY:O	1:D:121:SER:HA	2.11	0.50
2:K:14:DC:H42	3:L:39:DG:H1	1.60	0.50
1:A:107:TYR:OH	1:A:152:PRO:HD3	2.12	0.50
1:B:344:ARG:HH22	1:B:351:LYS:NZ	2.10	0.50
1:D:114:LEU:H	1:D:144:GLN:HE21	1.60	0.50
1:B:239:ASN:HB2	1:B:242:CYS:SG	2.52	0.50
1:A:259:ASP:OD2	1:A:263:ASN:HB2	2.11	0.49
1:C:98:PRO:HG2	1:C:162:ILE:HG21	1.93	0.49
1:B:160:MET:HG2	1:B:161:ALA:N	2.26	0.49
1:D:107:TYR:OH	1:D:152:PRO:HD3	2.12	0.49
1:B:202:ARG:HD3	1:B:219:PRO:CG	2.41	0.49
1:C:345:ASN:O	1:C:349:GLU:HG3	2.11	0.49
1:B:104:GLN:HE21	1:B:109:PHE:H	1.59	0.49
3:L:33:DA:H2"	3:L:34:DT:C5'	2.41	0.49
1:B:104:GLN:HB3	1:B:109:PHE:H	1.78	0.48
1:B:110:ARG:HH12	1:B:147:VAL:HA	1.76	0.48
1:A:349:GLU:HA	1:A:352:ASP:OD2	2.13	0.48
1:A:104:GLN:HB3	1:A:108:GLY:HA2	1.95	0.48
1:B:103:TYR:HB3	1:B:267:ARG:HB3	1.96	0.48
1:D:135:VAL:HG21	1:D:141:VAL:HG22	1.94	0.48
1:B:155:THR:HG23	1:B:259:ASP:HA	1.95	0.48
1:B:225:VAL:HG12	1:D:264:LEU:HD23	1.95	0.48
1:B:197:VAL:HG11	1:B:232:ILE:HD11	1.95	0.48
1:B:256:THR:HG22	1:B:267:ARG:HD3	1.96	0.47
1:C:336:GLU:O	1:C:340:GLN:HG3	2.14	0.47
1:C:219:PRO:HD2	5:C:53:HOH:O	2.14	0.47
1:D:161:ALA:HB2	1:D:195:ILE:HD11	1.96	0.47
1:B:323:MET:HA	1:B:327:TYR:OH	2.15	0.47
1:D:342:ARG:O	1:D:342:ARG:HD3	2.15	0.47
1:C:163:TYR:OH	1:C:246:MET:HA	2.15	0.47
3:L:31:DA:H2"	3:L:32:DC:C5'	2.40	0.46
1:B:172:VAL:HB	1:B:174:ARG:NH2	2.29	0.46
1:B:196:ARG:HB2	1:B:235:LYS:HB2	1.97	0.46
1:C:286:GLU:O	1:C:290:ARG:HG3	2.15	0.46
1:B:208:ASP:O	1:B:212:PHE:HA	2.15	0.46
1:B:175:ARG:CZ	1:B:237:MET:HB3	2.46	0.46
1:A:175:ARG:HD3	1:A:191:PRO:O	2.16	0.46
1:C:243:MET:HG3	1:D:178:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ASN:O	1:B:249:ARG:HG3	2.16	0.46
1:A:194:LEU:CD1	1:A:238:CYS:HB2	2.45	0.46
1:B:179:HIS:O	1:B:182:SER:HB3	2.15	0.46
1:B:190:PRO:C	1:B:192:GLN:H	2.19	0.46
1:B:119:ALA:O	1:B:122:VAL:HG22	2.16	0.46
1:B:129:ALA:HB2	1:B:290:ARG:HH22	1.80	0.46
1:A:107:TYR:HB3	1:A:147:VAL:HG23	1.98	0.46
1:D:107:TYR:HB3	1:D:147:VAL:HG23	1.98	0.46
1:D:323:MET:O	1:D:323:MET:HG2	2.16	0.46
1:B:107:TYR:HA	1:B:149:SER:OG	2.16	0.45
1:B:344:ARG:O	1:B:347:ALA:HB3	2.16	0.45
1:B:348:LEU:HD12	1:D:341:PHE:HZ	1.82	0.45
1:D:332:ILE:HG22	1:D:333:ARG:N	2.31	0.45
1:B:172:VAL:HB	1:B:174:ARG:HH22	1.79	0.45
1:C:150:THR:HA	1:C:151:PRO:HD3	1.80	0.45
1:B:341:PHE:HE1	1:D:345:ASN:HB2	1.81	0.45
1:B:348:LEU:HB3	1:B:352:ASP:OD2	2.17	0.45
1:D:175:ARG:HD3	1:D:191:PRO:O	2.16	0.45
1:B:346:GLU:HA	1:B:349:GLU:HG3	1.98	0.45
1:A:349:GLU:C	1:A:351:LYS:H	2.18	0.45
1:D:194:LEU:CD1	1:D:238:CYS:HB2	2.47	0.45
1:C:175:ARG:HD3	1:C:191:PRO:O	2.16	0.45
2:K:26:DG:H1	3:L:27:DC:H42	1.62	0.45
1:D:338:PHE:O	1:D:342:ARG:HB2	2.17	0.45
1:D:139:LYS:HD3	1:D:139:LYS:HA	1.84	0.45
1:B:327:TYR:HA	1:D:332:ILE:O	2.16	0.44
1:A:161:ALA:HB2	1:A:195:ILE:HD11	2.00	0.44
1:B:330:LEU:HG	1:B:332:ILE:HD11	1.99	0.44
1:C:249:ARG:HA	1:C:250:PRO:HD3	1.89	0.44
1:B:257:LEU:O	1:B:265:LEU:HB3	2.18	0.44
1:A:209:PRO:HG2	1:A:210:ASN:OD1	2.17	0.44
1:B:145:LEU:O	1:B:229:TYR:HB2	2.17	0.44
1:C:336:GLU:CD	1:C:337:ARG:H	2.21	0.44
1:A:240:SER:O	1:A:248:ARG:N	2.50	0.44
1:C:145:LEU:HD21	1:C:157:VAL:HG11	2.00	0.44
1:B:194:LEU:CD1	1:B:238:CYS:HB2	2.47	0.44
1:A:339:GLU:CD	1:A:342:ARG:HH12	2.20	0.44
2:K:16:DA:H2"	2:K:17:DA:O5'	2.17	0.44
1:A:135:VAL:HG21	1:A:141:VAL:CG2	2.47	0.44
3:L:29:DC:H2"	3:L:30:DA:C8	2.53	0.44
3:L:31:DA:C1'	3:L:32:DC:H5"	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLN:HB3	1:B:167:GLN:HE21	1.56	0.44
1:B:202:ARG:NH1	1:B:221:GLU:HG2	2.33	0.43
2:K:12:DT:H5'	2:K:12:DT:H6	1.84	0.43
1:D:166:SER:HA	1:D:169:MET:CG	2.46	0.43
1:B:151:PRO:HG2	1:B:257:LEU:HD21	1.99	0.43
1:C:186:ASP:OD2	1:C:188:LEU:HB2	2.18	0.43
1:B:197:VAL:N	1:B:205:TYR:OH	2.51	0.43
1:A:139:LYS:HA	1:A:139:LYS:HD3	1.85	0.43
1:D:209:PRO:HG2	1:D:210:ASN:OD1	2.19	0.43
1:B:331:GLN:HA	1:D:328:PHE:O	2.17	0.43
1:D:132:LYS:HD2	1:D:271:GLU:OE2	2.19	0.43
1:D:135:VAL:HG21	1:D:141:VAL:CG2	2.49	0.43
1:B:287:GLU:O	1:B:291:LYS:HB2	2.19	0.43
1:C:259:ASP:OD2	1:C:263:ASN:HB2	2.19	0.43
1:A:344:ARG:CZ	1:C:344:ARG:HH12	2.31	0.42
1:D:176:CYS:SG	1:D:179:HIS:HB2	2.59	0.42
1:B:156:ARG:HD3	1:B:217:VAL:HG11	2.01	0.42
1:C:181:ARG:HH11	1:C:181:ARG:HG3	1.84	0.42
1:B:131:ASN:ND2	1:B:270:PHE:HA	2.33	0.42
1:A:175:ARG:HD2	1:A:193:HIS:O	2.19	0.42
1:C:111:LEU:HG	1:C:268:ASP:HB3	2.01	0.42
1:B:104:GLN:HE21	1:B:108:GLY:CA	2.32	0.42
1:B:196:ARG:NE	1:B:237:MET:HG3	2.33	0.42
1:B:240:SER:O	1:B:248:ARG:HA	2.19	0.42
1:A:344:ARG:HE	1:C:344:ARG:HH12	1.66	0.42
1:B:344:ARG:HH22	1:B:351:LYS:HZ2	1.66	0.42
1:C:340:GLN:HE21	1:C:340:GLN:HB3	1.66	0.42
1:A:264:LEU:HD23	1:C:225:VAL:HB	2.01	0.42
1:A:189:ALA:HB2	1:A:205:TYR:CZ	2.55	0.42
1:B:202:ARG:HH11	1:B:219:PRO:HB2	1.84	0.42
1:A:94:SER:HB3	1:A:170:THR:O	2.20	0.42
1:D:135:VAL:HG22	1:D:136:GLN:H	1.83	0.42
2:K:17:DA:H2"	2:K:18:DC:C5'	2.50	0.42
1:C:135:VAL:O	1:C:274:VAL:HA	2.20	0.42
1:C:339:GLU:O	1:C:343:GLU:HB2	2.20	0.42
1:C:97:VAL:HG13	1:C:98:PRO:HD2	2.00	0.42
1:B:110:ARG:O	1:B:111:LEU:HD23	2.20	0.42
1:C:137:LEU:HD12	1:C:138:ALA:H	1.82	0.42
1:B:104:GLN:HE21	1:B:104:GLN:HB3	1.58	0.41
1:B:246:MET:SD	1:B:251:ILE:HD13	2.61	0.41
1:B:107:TYR:HB3	1:B:151:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:VAL:HG21	1:B:212:PHE:O	2.20	0.41
3:L:37:DT:H2"	3:L:38:DG:N7	2.35	0.41
1:B:110:ARG:HH12	1:B:148:ASP:H	1.67	0.41
2:K:18:DC:H2"	2:K:19:DA:C8	2.55	0.41
2:K:8:DC:H2'	2:K:9:DA:C8	2.56	0.41
1:D:175:ARG:HD2	1:D:193:HIS:O	2.20	0.41
1:D:189:ALA:HB2	1:D:205:TYR:CZ	2.55	0.41
1:C:132:LYS:HD2	1:C:271:GLU:CD	2.40	0.41
1:B:160:MET:HG2	1:B:161:ALA:H	1.86	0.41
1:D:243:MET:HA	1:D:247:ASN:OD1	2.20	0.41
1:B:202:ARG:HB3	1:B:219:PRO:CD	2.51	0.41
1:C:119:ALA:C	1:C:121:SER:H	2.24	0.41
1:B:349:GLU:O	1:B:353:ALA:HB3	2.21	0.41
3:L:32:DC:H2"	3:L:33:DA:C8	2.55	0.41
1:B:99:SER:O	1:B:267:ARG:HD2	2.21	0.41
1:C:189:ALA:HA	1:C:190:PRO:HD3	1.97	0.41
3:L:33:DA:H1'	3:L:34:DT:H5"	2.01	0.40
1:B:218:VAL:HA	1:B:219:PRO:HD3	1.86	0.40
1:B:104:GLN:HB3	1:B:108:GLY:CA	2.42	0.40
2:K:19:DA:H2	3:L:34:DT:O2	2.04	0.40
1:B:344:ARG:HH22	1:B:351:LYS:HD2	1.86	0.40
1:B:246:MET:O	1:B:249:ARG:HB2	2.22	0.40
1:D:249:ARG:HA	1:D:250:PRO:HD3	1.92	0.40
1:B:226:GLY:O	1:D:101:LYS:HD3	2.21	0.40
1:B:344:ARG:NH2	1:B:351:LYS:NZ	2.69	0.40
1:B:184:ASP:HB2	1:B:196:ARG:HH22	1.86	0.40
1:B:117:GLY:C	1:B:119:ALA:H	2.24	0.40
1:A:199:GLY:N	5:A:363:HOH:O	2.55	0.40
1:B:126:TYR:CE1	1:B:131:ASN:HA	2.56	0.40
1:D:240:SER:O	1:D:248:ARG:N	2.52	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	232/234 (99%)	215 (93%)	13 (6%)	4 (2%)	11 36
1	B	232/234 (99%)	179 (77%)	47 (20%)	6 (3%)	7 22
1	C	232/234 (99%)	217 (94%)	15 (6%)	0	100 100
1	D	232/234 (99%)	212 (91%)	18 (8%)	2 (1%)	21 55
All	All	928/936 (99%)	823 (89%)	93 (10%)	12 (1%)	15 44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	354	GLN
1	B	102	THR
1	D	121	SER
1	B	182	SER
1	B	228	ASP
1	A	119	ALA
1	B	167	GLN
1	D	119	ALA
1	A	350	LEU
1	B	220	TYR
1	B	191	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	208/208 (100%)	200 (96%)	8 (4%)	40 74
1	B	208/208 (100%)	197 (95%)	11 (5%)	28 61
1	C	208/208 (100%)	198 (95%)	10 (5%)	31 66
1	D	208/208 (100%)	200 (96%)	8 (4%)	40 74
All	All	832/832 (100%)	795 (96%)	37 (4%)	35 69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	125	THR
1	A	150	THR
1	A	167	GLN
1	A	192	GLN
1	A	217	VAL
1	A	224	GLU
1	A	324	ASP
1	B	110	ARG
1	B	113	PHE
1	B	148	ASP
1	B	167	GLN
1	B	181	ARG
1	B	188	LEU
1	B	192	GLN
1	B	207	ASP
1	B	230	THR
1	B	247	ASN
1	B	273	ARG
1	C	110	ARG
1	C	147	VAL
1	C	167	GLN
1	C	192	GLN
1	C	201	LEU
1	C	231	THR
1	C	277	CYS
1	C	323	MET
1	C	336	GLU
1	C	354	GLN
1	D	110	ARG
1	D	125	THR
1	D	150	THR
1	D	167	GLN
1	D	192	GLN
1	D	217	VAL
1	D	224	GLU
1	D	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	144	GLN
1	A	167	GLN
1	A	192	GLN
1	A	288	ASN
1	A	331	GLN
1	B	104	GLN
1	B	131	ASN
1	B	144	GLN
1	B	167	GLN
1	B	192	GLN
1	B	193	HIS
1	B	214	HIS
1	B	345	ASN
1	C	104	GLN
1	C	144	GLN
1	C	167	GLN
1	C	192	GLN
1	C	340	GLN
1	D	104	GLN
1	D	144	GLN
1	D	167	GLN
1	D	192	GLN
1	D	288	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

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	234/234 (100%)	0.11	9 (3%) 44 32	20, 40, 91, 95	0
1	B	234/234 (100%)	1.32	62 (26%) 1 0	56, 94, 95, 95	0
1	C	234/234 (100%)	-0.11	5 (2%) 67 56	14, 29, 80, 95	0
1	D	234/234 (100%)	0.33	25 (10%) 8 4	20, 40, 95, 95	0
2	K	26/26 (100%)	0.05	0 100 100	25, 47, 79, 88	0
3	L	26/26 (100%)	-0.05	0 100 100	27, 51, 79, 81	0
All	All	988/988 (100%)	0.39	101 (10%) 9 4	14, 45, 95, 95	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	THR	6.0
1	B	118	THR	5.7
1	B	350	LEU	5.7
1	D	119	ALA	5.6
1	A	119	ALA	5.5
1	B	117	GLY	5.2
1	B	102	THR	5.1
1	C	95	SER	5.0
1	B	345	ASN	5.0
1	A	356	THR	4.9
1	D	341	PHE	4.9
1	B	353	ALA	4.6
1	D	118	THR	4.6
1	B	325	GLY	4.5
1	A	95	SER	4.5
1	B	324	ASP	4.4
1	D	122	VAL	4.3
1	B	356	THR	4.2
1	B	103	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	109	PHE	4.2
1	A	116	SER	4.2
1	B	94	SER	4.2
1	D	116	SER	4.1
1	B	154	GLY	4.1
1	D	117	GLY	4.0
1	B	129	ALA	3.9
1	B	327	TYR	3.9
1	B	264	LEU	3.8
1	A	355	ALA	3.8
1	D	94	SER	3.7
1	B	323	MET	3.7
1	A	117	GLY	3.6
1	B	328	PHE	3.6
1	B	346	GLU	3.6
1	D	121	SER	3.5
1	C	120	LYS	3.5
1	D	334	GLY	3.5
1	B	321	LYS	3.5
1	B	97	VAL	3.5
1	B	95	SER	3.4
1	D	356	THR	3.3
1	B	199	GLY	3.3
1	B	354	GLN	3.3
1	B	352	ASP	3.2
1	B	219	PRO	3.1
1	C	94	SER	3.1
1	B	115	HIS	3.1
1	B	128	PRO	3.0
1	B	341	PHE	3.0
1	B	332	ILE	3.0
1	D	355	ALA	3.0
1	A	94	SER	3.0
1	A	115	HIS	3.0
1	B	108	GLY	3.0
1	B	104	GLN	2.9
1	B	326	GLU	2.9
1	B	120	LYS	2.9
1	B	254	ILE	2.9
1	B	265	LEU	2.8
1	B	258	GLU	2.8
1	B	343	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	220	TYR	2.8
1	B	155	THR	2.8
1	D	330	LEU	2.7
1	D	95	SER	2.7
1	B	98	PRO	2.7
1	B	334	GLY	2.7
1	B	186	ASP	2.6
1	D	345	ASN	2.6
1	D	337	ARG	2.6
1	D	115	HIS	2.5
1	D	350	LEU	2.5
1	B	107	TYR	2.5
1	B	266	GLY	2.5
1	B	342	ARG	2.5
1	B	355	ALA	2.4
1	B	130	LEU	2.4
1	B	329	THR	2.4
1	D	333	ARG	2.4
1	D	327	TYR	2.3
1	B	236	PHE	2.3
1	D	123	THR	2.3
1	D	335	ARG	2.3
1	B	331	GLN	2.2
1	B	257	LEU	2.2
1	D	120	LYS	2.2
1	D	351	LYS	2.2
1	B	197	VAL	2.2
1	B	270	PHE	2.2
1	D	336	GLU	2.2
1	C	356	THR	2.2
1	B	291	LYS	2.2
1	B	344	ARG	2.1
1	B	231	THR	2.1
1	D	338	PHE	2.1
1	C	324	ASP	2.1
1	B	222	PRO	2.1
1	B	287	GLU	2.1
1	B	106	SER	2.1
1	B	212	PHE	2.0
1	B	124	CYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	C	1	1/1	1.00	0.20	0.88	28,28,28,28	0
4	ZN	A	1	1/1	1.00	0.21	0.83	29,29,29,29	0
4	ZN	B	1	1/1	0.99	0.23	0.80	52,52,52,52	0
4	ZN	D	1	1/1	1.00	0.20	0.74	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.