Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 AM GMT

PDB ID	:	3CVG
Title	:	Crystal structure of a periplasmic putative metal binding protein
Authors	:	Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-04-18
Resolution	:	1.97 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 ⓘ symbol.

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

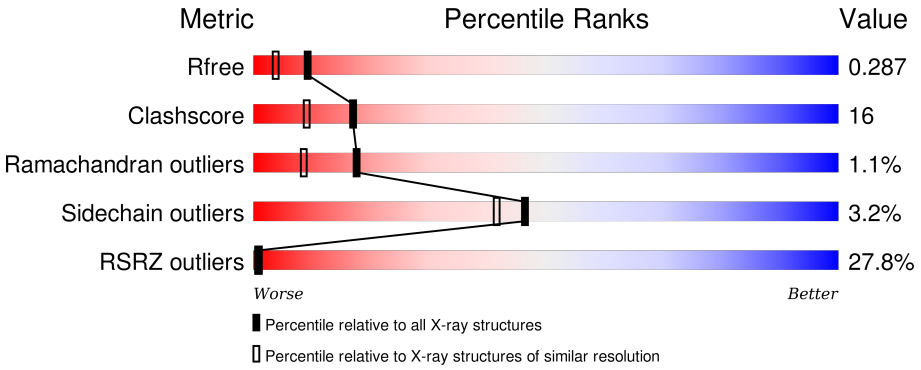
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	294	15% 72% 19% • 8%
1	B	294	28% 66% 24% • 8%
1	C	294	19% 45% 24% • 30%
1	D	294	33% 61% 28% •• 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8486 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 Putative metal binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	Se	0	0	0
			2113	1356	353	399	5			
1	B	270	Total	C	N	O	Se	0	0	0
			2113	1356	353	399	5			
1	C	207	Total	C	N	O	Se	0	0	0
			1640	1055	276	304	5			
1	D	268	Total	C	N	O	Se	0	0	0
			2096	1347	351	393	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MSE	-	EXPRESSION TAG	UNP Q1DXA6
A	20	SER	-	EXPRESSION TAG	UNP Q1DXA6
A	21	LEU	-	EXPRESSION TAG	UNP Q1DXA6
A	305	GLU	-	EXPRESSION TAG	UNP Q1DXA6
A	306	GLY	-	EXPRESSION TAG	UNP Q1DXA6
A	307	HIS	-	EXPRESSION TAG	UNP Q1DXA6
A	308	HIS	-	EXPRESSION TAG	UNP Q1DXA6
A	309	HIS	-	EXPRESSION TAG	UNP Q1DXA6
A	310	HIS	-	EXPRESSION TAG	UNP Q1DXA6
A	311	HIS	-	EXPRESSION TAG	UNP Q1DXA6
A	312	HIS	-	EXPRESSION TAG	UNP Q1DXA6
B	19	MSE	-	EXPRESSION TAG	UNP Q1DXA6
B	20	SER	-	EXPRESSION TAG	UNP Q1DXA6
B	21	LEU	-	EXPRESSION TAG	UNP Q1DXA6
B	305	GLU	-	EXPRESSION TAG	UNP Q1DXA6
B	306	GLY	-	EXPRESSION TAG	UNP Q1DXA6
B	307	HIS	-	EXPRESSION TAG	UNP Q1DXA6
B	308	HIS	-	EXPRESSION TAG	UNP Q1DXA6
B	309	HIS	-	EXPRESSION TAG	UNP Q1DXA6
B	310	HIS	-	EXPRESSION TAG	UNP Q1DXA6
B	311	HIS	-	EXPRESSION TAG	UNP Q1DXA6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	312	HIS	-	EXPRESSION TAG	UNP Q1DXA6
C	19	MSE	-	EXPRESSION TAG	UNP Q1DXA6
C	20	SER	-	EXPRESSION TAG	UNP Q1DXA6
C	21	LEU	-	EXPRESSION TAG	UNP Q1DXA6
C	305	GLU	-	EXPRESSION TAG	UNP Q1DXA6
C	306	GLY	-	EXPRESSION TAG	UNP Q1DXA6
C	307	HIS	-	EXPRESSION TAG	UNP Q1DXA6
C	308	HIS	-	EXPRESSION TAG	UNP Q1DXA6
C	309	HIS	-	EXPRESSION TAG	UNP Q1DXA6
C	310	HIS	-	EXPRESSION TAG	UNP Q1DXA6
C	311	HIS	-	EXPRESSION TAG	UNP Q1DXA6
C	312	HIS	-	EXPRESSION TAG	UNP Q1DXA6
D	19	MSE	-	EXPRESSION TAG	UNP Q1DXA6
D	20	SER	-	EXPRESSION TAG	UNP Q1DXA6
D	21	LEU	-	EXPRESSION TAG	UNP Q1DXA6
D	305	GLU	-	EXPRESSION TAG	UNP Q1DXA6
D	306	GLY	-	EXPRESSION TAG	UNP Q1DXA6
D	307	HIS	-	EXPRESSION TAG	UNP Q1DXA6
D	308	HIS	-	EXPRESSION TAG	UNP Q1DXA6
D	309	HIS	-	EXPRESSION TAG	UNP Q1DXA6
D	310	HIS	-	EXPRESSION TAG	UNP Q1DXA6
D	311	HIS	-	EXPRESSION TAG	UNP Q1DXA6
D	312	HIS	-	EXPRESSION TAG	UNP Q1DXA6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	159	Total O 159 159	0	0

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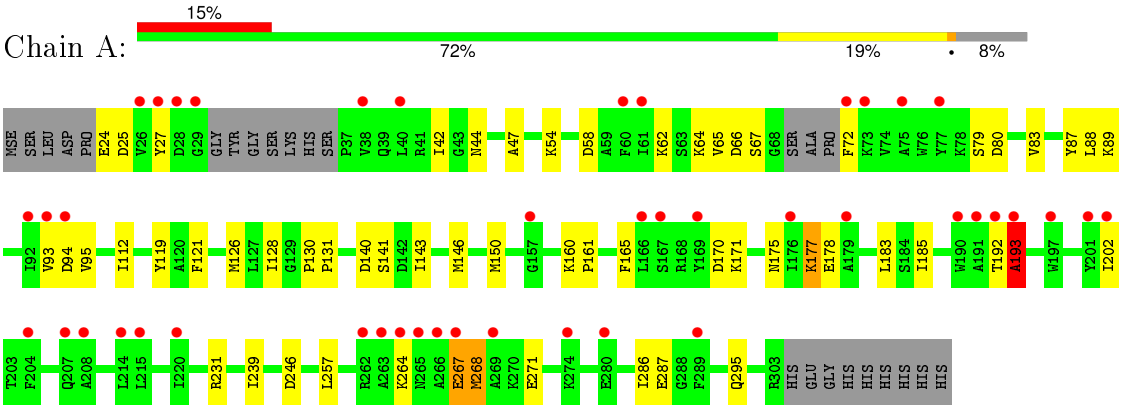
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	113	Total O 113 113	0	0
3	C	135	Total O 135 135	0	0
3	D	113	Total O 113 113	0	0

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.

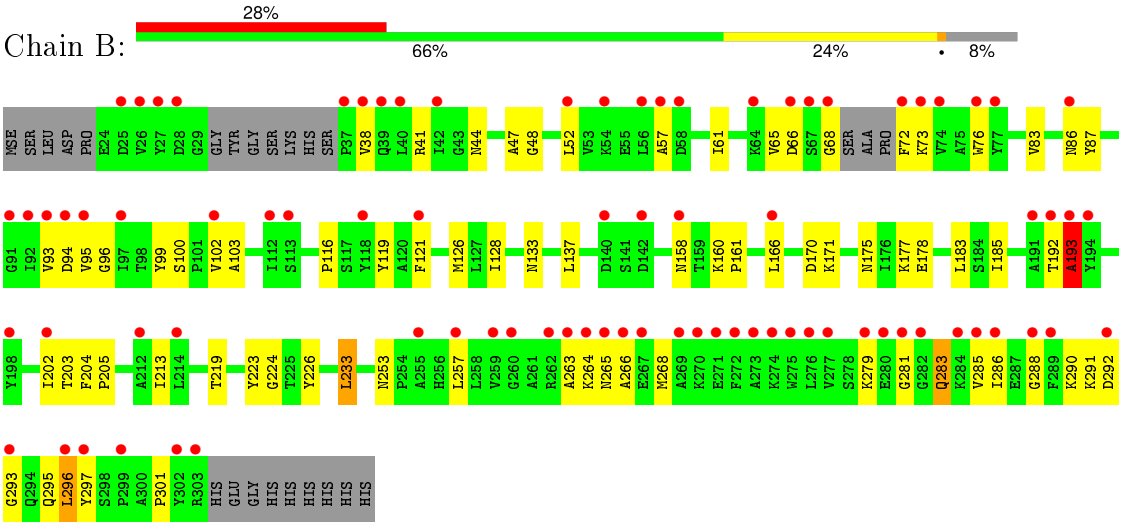
- Molecule 1: Putative metal binding protein

Chain A:



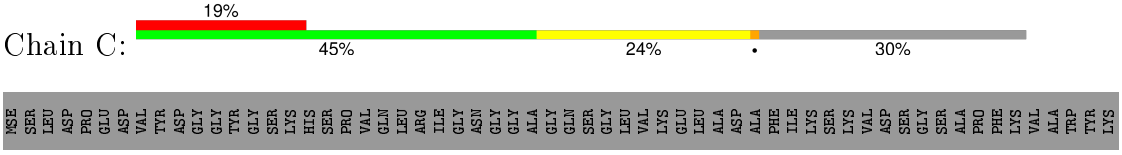
- Molecule 1: Putative metal binding protein

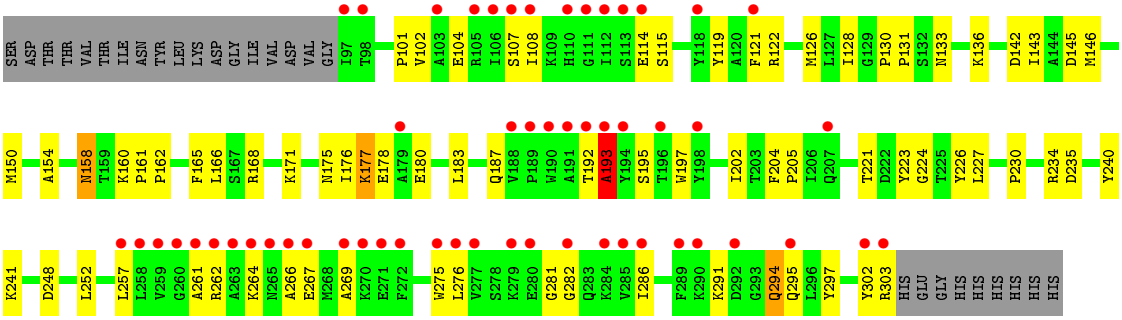
Chain B:



- Molecule 1: Putative metal binding protein

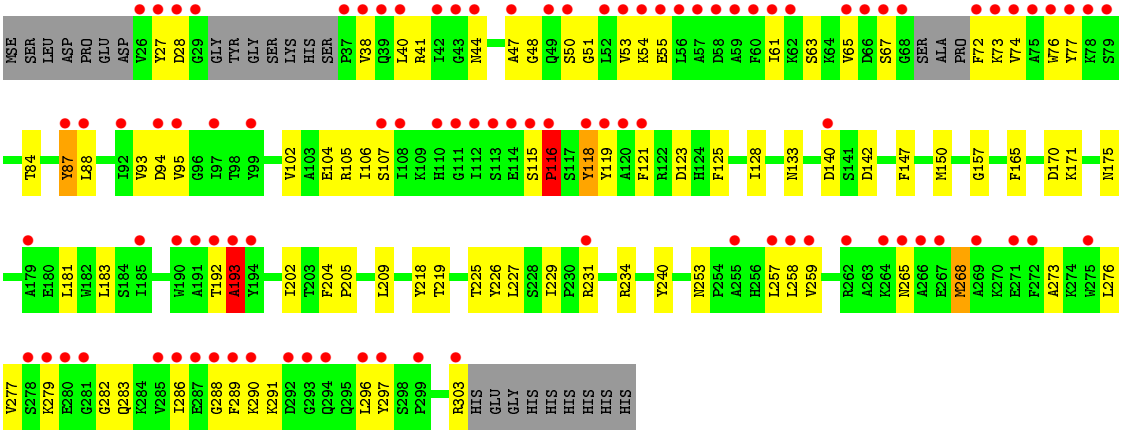
Chain C:





- Molecule 1: Putative metal binding protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	150.78Å 150.78Å 116.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.14 – 1.97 48.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.4 (44.14-1.97) 91.4 (48.49-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.289 0.258 , 0.287	Depositor DCC
R_{free} test set	2720 reflections (3.03%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 103661 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8486	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: CA

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	0/2160	0.61	1/2918 (0.0%)
1	B	0.33	0/2160	0.60	1/2918 (0.0%)
1	C	0.35	0/1681	0.62	1/2274 (0.0%)
1	D	0.33	0/2143	0.61	1/2895 (0.0%)
All	All	0.34	0/8144	0.61	4/11005 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	193	ALA	N-CA-C	-10.64	82.28	111.00
1	A	193	ALA	N-CA-C	-10.26	83.31	111.00
1	B	193	ALA	N-CA-C	-10.07	83.80	111.00
1	C	193	ALA	N-CA-C	-9.87	84.35	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2113	0	2087	59	0
1	B	2113	0	2087	72	0
1	C	1640	0	1619	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2096	0	2077	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	159	0	0	4	0
3	B	113	0	0	6	0
3	C	135	0	0	6	0
3	D	113	0	0	6	0
All	All	8486	0	7870	258	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 16.

All (258) 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:183:LEU:HD12	1:C:183:LEU:HD12	1.52	0.92
1:A:143:ILE:HA	1:A:146:MSE:HE3	1.55	0.88
1:C:136:LYS:HE3	3:C:470:HOH:O	1.76	0.85
1:D:277:VAL:HA	1:D:283:GLN:HE21	1.45	0.82
1:D:44:ASN:HD21	1:D:47:ALA:HB3	1.44	0.81
1:C:291:LYS:HD2	3:C:497:HOH:O	1.81	0.80
1:C:221:THR:HB	3:C:491:HOH:O	1.82	0.78
1:B:126:MSE:HE2	1:B:223:TYR:HA	1.65	0.78
1:A:202:ILE:HD13	1:C:192:THR:HG21	1.64	0.77
1:B:202:ILE:HD13	1:D:192:THR:HG21	1.67	0.76
1:D:118:TYR:HB2	1:D:257:LEU:HB3	1.65	0.76
1:B:160:LYS:HD2	1:B:161:PRO:HA	1.68	0.75
1:B:102:VAL:HG23	3:B:440:HOH:O	1.88	0.73
1:A:72:PHE:CE2	1:A:268:MSE:HE1	2.24	0.72
1:A:171:LYS:H	1:A:175:ASN:HD22	1.38	0.72
1:C:126:MSE:HE1	1:C:226:TYR:HB2	1.70	0.72
1:A:192:THR:HG21	1:C:202:ILE:HD13	1.70	0.71
1:C:158:ASN:H	1:C:158:ASN:HD22	1.38	0.71
1:D:44:ASN:ND2	1:D:47:ALA:HB3	2.06	0.70
1:A:171:LYS:HD2	1:C:193:ALA:HB3	1.73	0.70
1:B:171:LYS:H	1:B:175:ASN:HD22	1.39	0.70
1:A:231:ARG:HH11	1:A:231:ARG:HG2	1.55	0.70
1:A:185:ILE:HA	1:C:102:VAL:HG11	1.73	0.70
1:B:192:THR:HG21	1:D:202:ILE:HD13	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLN:HA	1:B:283:GLN:HE21	1.54	0.70
1:C:143:ILE:HD12	1:C:146:MSE:HE3	1.72	0.69
1:B:121:PHE:HB3	1:B:286:ILE:HD13	1.73	0.69
1:D:38:VAL:HG22	1:D:73:LYS:HB2	1.72	0.69
1:D:77:TYR:CD2	1:D:93:VAL:HG12	2.28	0.69
1:D:171:LYS:H	1:D:175:ASN:HD22	1.38	0.69
1:C:143:ILE:HA	1:C:146:MSE:HE3	1.73	0.68
1:C:150:MSE:HE1	1:C:165:PHE:HD1	1.58	0.68
1:C:266:ALA:HA	1:C:269:ALA:HB3	1.75	0.68
1:B:183:LEU:HD12	1:D:183:LEU:HD12	1.76	0.68
1:C:121:PHE:HB3	1:C:286:ILE:HD13	1.77	0.67
1:A:150:MSE:HE1	1:A:165:PHE:HD1	1.59	0.66
1:D:227:LEU:HD12	1:D:296:LEU:HD13	1.78	0.66
1:D:258:LEU:HG	3:D:446:HOH:O	1.96	0.65
1:A:89:LYS:HD2	1:A:112:ILE:HD11	1.77	0.65
1:D:72:PHE:CE2	1:D:268:MSE:HE1	2.33	0.64
1:C:171:LYS:H	1:C:175:ASN:HD22	1.46	0.63
1:B:295:GLN:HG3	3:B:481:HOH:O	1.98	0.63
1:B:263:ALA:HA	3:B:487:HOH:O	1.97	0.63
1:B:296:LEU:HG	1:B:297:TYR:CE1	2.34	0.62
1:A:80:ASP:OD1	1:A:83:VAL:HG23	1.99	0.62
1:D:288:GLY:O	1:D:290:LYS:HG3	1.99	0.62
1:C:146:MSE:HE1	1:C:241:LYS:CG	2.30	0.61
1:A:177:LYS:HA	1:A:177:LYS:HE3	1.82	0.61
1:D:28:ASP:O	1:D:61:ILE:HG21	2.00	0.61
1:D:303:ARG:HD3	3:D:461:HOH:O	1.99	0.61
1:C:158:ASN:H	1:C:158:ASN:ND2	1.99	0.61
1:C:224:GLY:HA2	3:C:497:HOH:O	2.01	0.60
1:B:95:VAL:HB	1:B:257:LEU:HD11	1.83	0.60
1:B:296:LEU:HD12	1:B:297:TYR:N	2.16	0.60
1:A:121:PHE:HB3	1:A:286:ILE:HD13	1.83	0.60
1:D:28:ASP:OD1	1:D:73:LYS:HG2	2.00	0.60
1:C:294:GLN:HG2	3:C:446:HOH:O	2.01	0.60
1:C:276:LEU:HD12	1:C:282:GLY:HA3	1.83	0.59
1:A:79:SER:HB2	1:A:83:VAL:HB	1.83	0.59
1:B:183:LEU:HD12	1:D:183:LEU:CD1	2.32	0.59
1:A:72:PHE:CZ	1:A:268:MSE:HE1	2.38	0.59
1:A:140:ASP:HB2	3:A:532:HOH:O	2.02	0.59
1:B:44:ASN:ND2	1:B:47:ALA:HB3	2.18	0.58
1:C:146:MSE:HE1	1:C:241:LYS:HG2	1.84	0.58
1:D:282:GLY:O	1:D:286:ILE:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HB	1:A:257:LEU:HD11	1.86	0.58
1:D:48:GLY:HA3	1:D:76:TRP:CZ2	2.37	0.58
1:D:63:SER:O	1:D:67:SER:HB3	2.04	0.58
1:A:44:ASN:ND2	1:A:47:ALA:HB3	2.19	0.58
1:B:171:LYS:HD2	1:D:193:ALA:HB3	1.86	0.57
1:D:128:ILE:C	1:D:128:ILE:HD12	2.24	0.57
1:C:235:ASP:HB3	3:C:496:HOH:O	2.04	0.57
1:C:158:ASN:ND2	1:C:158:ASN:N	2.52	0.57
1:D:150:MSE:HE1	1:D:165:PHE:HD1	1.68	0.57
1:A:231:ARG:NH1	1:A:231:ARG:HG2	2.20	0.57
1:B:290:LYS:HG2	1:B:295:GLN:HA	1.87	0.56
1:A:246:ASP:HB3	3:A:444:HOH:O	2.05	0.56
1:D:55:GLU:HG2	3:D:431:HOH:O	2.06	0.56
1:B:183:LEU:CD1	1:D:183:LEU:HD12	2.35	0.56
1:B:213:ILE:HG21	1:B:233:LEU:HD22	1.87	0.56
1:B:192:THR:O	1:B:193:ALA:CB	2.54	0.56
1:A:72:PHE:CD2	1:A:268:MSE:HE1	2.41	0.56
1:C:158:ASN:N	1:C:158:ASN:HD22	2.00	0.56
1:B:38:VAL:HG22	1:B:73:LYS:HB2	1.87	0.56
1:C:143:ILE:HA	1:C:146:MSE:CE	2.35	0.55
1:B:52:LEU:HD22	1:B:297:TYR:CD1	2.41	0.55
1:D:88:LEU:HD23	1:D:93:VAL:HG23	1.88	0.55
1:B:263:ALA:O	1:B:266:ALA:HB2	2.07	0.54
1:B:203:THR:HB	3:B:502:HOH:O	2.07	0.54
1:B:292:ASP:OD2	1:B:293:GLY:N	2.41	0.53
1:C:223:TYR:CE2	1:C:227:LEU:HD11	2.43	0.53
1:D:227:LEU:HB3	1:D:291:LYS:HG2	1.89	0.53
1:A:65:VAL:C	1:A:67:SER:N	2.62	0.53
1:D:257:LEU:CD2	1:D:273:ALA:HA	2.38	0.53
1:D:27:TYR:HE1	1:D:53:VAL:HG12	1.74	0.53
1:C:176:ILE:O	1:C:180:GLU:HG3	2.09	0.53
1:D:289:PHE:HB3	3:D:458:HOH:O	2.08	0.53
1:D:171:LYS:H	1:D:175:ASN:ND2	2.07	0.52
1:D:72:PHE:CD2	1:D:268:MSE:HE1	2.45	0.52
1:A:58:ASP:O	1:A:62:LYS:HB2	2.09	0.52
1:C:108:ILE:HG23	1:C:115:SER:HB2	1.92	0.52
1:C:101:PRO:O	1:C:104:GLU:HB2	2.10	0.52
1:D:40:LEU:HD11	1:D:95:VAL:HG22	1.92	0.52
1:A:44:ASN:HD21	1:A:47:ALA:HB3	1.75	0.52
1:D:303:ARG:HG2	1:D:303:ARG:HH11	1.75	0.51
1:C:108:ILE:CG2	1:C:115:SER:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:PHE:HB3	1:D:286:ILE:HD13	1.93	0.51
1:D:95:VAL:HG12	1:D:259:VAL:HG22	1.93	0.51
1:B:185:ILE:HA	1:D:102:VAL:HG21	1.93	0.51
1:D:61:ILE:HD11	1:D:74:VAL:HG23	1.91	0.51
1:B:292:ASP:CG	1:B:293:GLY:H	2.13	0.51
1:A:64:LYS:HE2	1:A:64:LYS:HA	1.93	0.51
1:A:27:TYR:CD2	1:A:54:LYS:HG3	2.46	0.51
1:D:171:LYS:N	1:D:175:ASN:HD22	2.06	0.51
1:D:54:LYS:HB3	3:D:431:HOH:O	2.11	0.51
1:C:142:ASP:OD2	1:C:145:ASP:HB2	2.11	0.51
1:C:126:MSE:CE	1:C:226:TYR:HB2	2.39	0.50
1:B:192:THR:O	1:B:193:ALA:HB3	2.11	0.50
1:D:226:TYR:O	1:D:229:ILE:HG12	2.11	0.50
1:A:89:LYS:HD2	1:A:112:ILE:CD1	2.40	0.50
1:B:279:LYS:H	1:B:279:LYS:HD2	1.77	0.50
1:D:88:LEU:CD2	1:D:93:VAL:HG23	2.40	0.50
1:B:48:GLY:HA3	1:B:76:TRP:CZ2	2.46	0.50
1:A:267:GLU:O	1:A:271:GLU:HG2	2.11	0.50
1:A:192:THR:O	1:A:193:ALA:CB	2.59	0.50
1:A:171:LYS:H	1:A:175:ASN:ND2	2.06	0.50
1:B:291:LYS:O	1:B:292:ASP:HB3	2.10	0.50
1:C:262:ARG:HH11	1:C:262:ARG:HA	1.76	0.50
1:C:262:ARG:NH1	1:C:262:ARG:HA	2.27	0.50
1:B:126:MSE:CE	1:B:223:TYR:HA	2.41	0.50
1:C:150:MSE:HE1	1:C:165:PHE:CD1	2.42	0.50
1:A:193:ALA:HB3	1:C:171:LYS:HD2	1.93	0.49
1:D:125:PHE:CE2	1:D:253:ASN:HB2	2.47	0.49
1:B:116:PRO:HG2	3:B:486:HOH:O	2.12	0.49
1:A:183:LEU:CD1	1:C:183:LEU:HD12	2.33	0.49
1:D:231:ARG:HG2	1:D:234:ARG:CZ	2.43	0.49
1:D:61:ILE:O	1:D:65:VAL:HG23	2.13	0.49
1:B:65:VAL:HA	1:B:68:GLY:O	2.13	0.49
1:A:171:LYS:N	1:A:175:ASN:HD22	2.08	0.49
1:B:296:LEU:HG	1:B:297:TYR:CD1	2.47	0.49
1:D:105:ARG:HG2	1:D:105:ARG:HH11	1.78	0.49
1:B:87:TYR:HB3	1:B:93:VAL:HG22	1.95	0.49
1:B:41:ARG:NH2	3:B:487:HOH:O	2.46	0.48
1:D:192:THR:O	1:D:193:ALA:CB	2.61	0.48
1:D:209:LEU:HD23	1:D:225:THR:HG22	1.95	0.48
1:B:204:PHE:HB3	1:B:205:PRO:HD2	1.94	0.48
1:A:88:LEU:HD23	1:A:93:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:HA	1:B:86:ASN:HD22	1.78	0.48
1:D:41:ARG:HB3	1:D:77:TYR:HE2	1.78	0.48
1:B:126:MSE:HE2	1:B:223:TYR:CA	2.41	0.48
1:D:296:LEU:HG	1:D:297:TYR:CE1	2.48	0.48
1:D:257:LEU:HD22	1:D:276:LEU:HD23	1.96	0.47
1:A:150:MSE:HE1	1:A:165:PHE:CD1	2.46	0.47
1:B:52:LEU:HD22	1:B:297:TYR:CE1	2.49	0.47
1:B:193:ALA:HB3	1:D:171:LYS:HD2	1.95	0.47
1:C:183:LEU:HD23	1:C:187:GLN:O	2.14	0.47
1:C:160:LYS:HD2	1:C:161:PRO:HA	1.96	0.47
1:C:161:PRO:HB2	1:C:162:PRO:HD2	1.97	0.47
1:C:128:ILE:HD12	1:C:128:ILE:C	2.35	0.47
1:A:94:ASP:OD1	1:A:264:LYS:O	2.33	0.47
1:D:257:LEU:HD21	1:D:273:ALA:HA	1.97	0.47
1:C:204:PHE:HB3	1:C:205:PRO:HD2	1.96	0.47
1:C:166:LEU:HD23	1:C:166:LEU:C	2.36	0.47
1:D:204:PHE:HB3	1:D:205:PRO:HD2	1.96	0.47
1:C:133:ASN:HB2	1:C:240:TYR:OH	2.15	0.46
1:C:192:THR:O	1:C:193:ALA:CB	2.63	0.46
1:D:150:MSE:CE	1:D:218:TYR:HB2	2.45	0.46
1:B:283:GLN:HA	1:B:283:GLN:NE2	2.27	0.46
1:B:170:ASP:O	1:B:171:LYS:HB2	2.16	0.46
1:B:44:ASN:HD21	1:B:47:ALA:H	1.64	0.46
1:A:170:ASP:O	1:A:171:LYS:HB2	2.15	0.46
1:D:48:GLY:HA2	1:D:53:VAL:HB	1.98	0.46
1:A:89:LYS:HD3	3:A:505:HOH:O	2.15	0.46
1:B:57:ALA:O	1:B:61:ILE:HG13	2.16	0.45
1:C:171:LYS:N	1:C:175:ASN:HD22	2.13	0.45
1:D:102:VAL:O	1:D:106:ILE:HG13	2.16	0.45
1:B:94:ASP:OD1	1:B:264:LYS:O	2.34	0.45
1:B:100:SER:HB3	1:B:103:ALA:HB3	1.98	0.45
1:B:72:PHE:CE1	1:B:268:MSE:HE3	2.51	0.45
1:A:44:ASN:HD21	1:A:47:ALA:H	1.64	0.45
1:A:65:VAL:C	1:A:67:SER:H	2.20	0.45
1:A:62:LYS:O	1:A:66:ASP:HB2	2.17	0.45
1:B:44:ASN:HD21	1:B:47:ALA:HB3	1.81	0.45
1:C:295:GLN:HG2	1:C:297:TYR:O	2.16	0.45
1:A:177:LYS:CA	1:A:177:LYS:HE3	2.46	0.45
1:B:96:GLY:O	1:B:257:LEU:HA	2.17	0.45
1:A:24:GLU:O	1:A:25:ASP:HB2	2.16	0.45
1:C:122:ARG:HB3	1:C:252:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:HD23	1:B:166:LEU:C	2.38	0.44
1:C:130:PRO:HA	1:C:131:PRO:HD3	1.94	0.44
1:D:104:GLU:O	1:D:107:SER:HB3	2.17	0.44
1:B:204:PHE:HB3	1:B:205:PRO:CD	2.48	0.44
1:B:281:GLY:O	1:B:285:VAL:HG23	2.17	0.44
1:C:204:PHE:HB3	1:C:205:PRO:CD	2.48	0.44
1:A:160:LYS:HA	1:A:161:PRO:HA	1.86	0.44
1:C:275:TRP:O	1:C:281:GLY:HA3	2.18	0.44
1:C:264:LYS:C	1:C:266:ALA:N	2.70	0.44
1:D:204:PHE:HB3	1:D:205:PRO:CD	2.48	0.43
1:D:147:PHE:CE1	1:D:181:LEU:HD13	2.53	0.43
1:C:160:LYS:HA	1:C:160:LYS:HD2	1.74	0.43
1:C:257:LEU:HD23	1:C:257:LEU:C	2.38	0.43
1:B:126:MSE:HE1	1:B:226:TYR:CB	2.48	0.43
1:B:224:GLY:CA	1:B:296:LEU:HD11	2.47	0.43
1:B:279:LYS:N	1:B:279:LYS:HD2	2.33	0.43
1:B:44:ASN:HD22	1:B:48:GLY:H	1.65	0.43
1:A:64:LYS:HE2	3:A:530:HOH:O	2.19	0.43
1:B:133:ASN:HD21	1:B:137:LEU:N	2.17	0.43
1:D:227:LEU:HD13	1:D:291:LYS:HB3	2.01	0.43
1:A:62:LYS:O	1:A:66:ASP:CB	2.67	0.43
1:C:177:LYS:HA	1:C:177:LYS:HE3	2.00	0.43
1:D:94:ASP:CG	1:D:265:ASN:HD22	2.22	0.43
1:B:213:ILE:HG21	1:B:233:LEU:CD2	2.49	0.43
1:D:44:ASN:HD21	1:D:47:ALA:CB	2.25	0.43
1:A:42:ILE:HG12	1:A:95:VAL:CG2	2.49	0.42
1:A:192:THR:O	1:A:193:ALA:HB3	2.18	0.42
1:B:44:ASN:HD21	1:B:47:ALA:N	2.16	0.42
1:A:130:PRO:HA	1:A:131:PRO:HD3	1.93	0.42
1:D:133:ASN:HB2	1:D:240:TYR:OH	2.20	0.42
1:D:157:GLY:HA2	3:D:428:HOH:O	2.19	0.42
1:B:288:GLY:O	1:B:290:LYS:HG3	2.20	0.42
1:C:168:ARG:NH1	1:C:205:PRO:HG3	2.34	0.42
1:C:230:PRO:O	1:C:234:ARG:HG3	2.19	0.42
1:B:192:THR:CG2	1:D:202:ILE:HD13	2.43	0.42
1:B:224:GLY:HA2	1:B:296:LEU:HD11	2.01	0.42
1:A:126:MSE:HE3	1:A:239:ILE:HG12	2.01	0.42
1:B:160:LYS:HA	1:B:161:PRO:HA	1.92	0.42
1:B:44:ASN:ND2	1:B:48:GLY:H	2.18	0.42
1:B:99:TYR:HB3	1:B:253:ASN:OD1	2.20	0.42
1:D:118:TYR:CE1	1:D:273:ALA:HB1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:O	1:C:107:SER:HB2	2.19	0.41
1:C:154:ALA:HB1	1:C:197:TRP:CG	2.55	0.41
1:B:41:ARG:HB2	1:B:41:ARG:HE	1.73	0.41
1:D:128:ILE:HD11	1:D:219:THR:HG22	2.02	0.41
1:D:150:MSE:HE1	1:D:218:TYR:HB2	2.01	0.41
1:A:160:LYS:HA	1:A:160:LYS:HD2	1.74	0.41
1:A:192:THR:HG21	1:C:202:ILE:CD1	2.46	0.41
1:D:257:LEU:HD22	1:D:276:LEU:CD2	2.50	0.41
1:B:48:GLY:HA3	1:B:76:TRP:CE2	2.56	0.41
1:D:125:PHE:CD2	1:D:253:ASN:HB2	2.56	0.41
1:D:118:TYR:N	1:D:118:TYR:CD2	2.88	0.41
1:C:223:TYR:CZ	1:C:227:LEU:HD11	2.56	0.41
1:A:87:TYR:HB3	1:A:93:VAL:HG22	2.02	0.41
1:C:195:SER:HB3	1:C:197:TRP:CE2	2.56	0.41
1:A:128:ILE:C	1:A:128:ILE:HD12	2.41	0.41
1:C:171:LYS:H	1:C:175:ASN:ND2	2.15	0.41
1:C:257:LEU:HD23	1:C:257:LEU:O	2.21	0.41
1:C:303:ARG:HH11	1:C:303:ARG:HG3	1.84	0.41
1:D:84:THR:O	1:D:87:TYR:HB2	2.21	0.41
1:A:287:GLU:HA	1:A:295:GLN:NE2	2.35	0.41
1:C:114:GLU:HG3	1:C:261:ALA:HA	2.03	0.41
1:A:141:SER:O	1:A:146:MSE:HE2	2.21	0.41
1:A:44:ASN:HD21	1:A:47:ALA:N	2.19	0.41
1:D:170:ASP:O	1:D:171:LYS:HB2	2.22	0.40
1:A:202:ILE:CD1	1:C:192:THR:HG21	2.44	0.40
1:D:115:SER:HA	1:D:116:PRO:HA	1.76	0.40
1:D:123:ASP:HB3	1:D:253:ASN:O	2.21	0.40
1:B:128:ILE:HD12	1:B:128:ILE:C	2.42	0.40
1:B:128:ILE:HD11	1:B:219:THR:HG22	2.04	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	264/294 (90%)	256 (97%)	7 (3%)	1 (0%)	39 31
1	B	264/294 (90%)	244 (92%)	17 (6%)	3 (1%)	17 8
1	C	205/294 (70%)	191 (93%)	12 (6%)	2 (1%)	19 10
1	D	262/294 (89%)	240 (92%)	17 (6%)	5 (2%)	10 3
All	All	995/1176 (85%)	931 (94%)	53 (5%)	11 (1%)	17 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA
1	B	193	ALA
1	C	193	ALA
1	D	193	ALA
1	B	158	ASN
1	D	279	LYS
1	C	302	TYR
1	D	50	SER
1	B	301	PRO
1	D	51	GLY
1	D	116	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	222/236 (94%)	217 (98%)	5 (2%)	58 57
1	B	222/236 (94%)	214 (96%)	8 (4%)	42 36
1	C	172/236 (73%)	165 (96%)	7 (4%)	37 30
1	D	220/236 (93%)	213 (97%)	7 (3%)	46 41
All	All	836/944 (89%)	809 (97%)	27 (3%)	46 41

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	TYR
1	A	177	LYS
1	A	178	GLU
1	A	267	GLU
1	A	268	MSE
1	B	66	ASP
1	B	119	TYR
1	B	177	LYS
1	B	178	GLU
1	B	233	LEU
1	B	265	ASN
1	B	283	GLN
1	B	296	LEU
1	C	119	TYR
1	C	158	ASN
1	C	177	LYS
1	C	178	GLU
1	C	248	ASP
1	C	267	GLU
1	C	294	GLN
1	D	87	TYR
1	D	116	PRO
1	D	118	TYR
1	D	119	TYR
1	D	140	ASP
1	D	142	ASP
1	D	268	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	49	GLN
1	A	86	ASN
1	A	110	HIS
1	A	175	ASN
1	A	295	GLN
1	B	44	ASN
1	B	86	ASN
1	B	175	ASN
1	B	295	GLN
1	C	158	ASN
1	C	175	ASN

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Mol	Chain	Res	Type
1	C	236	GLN
1	C	265	ASN
1	D	44	ASN
1	D	49	GLN
1	D	124	HIS
1	D	175	ASN
1	D	256	HIS
1	D	265	ASN
1	D	283	GLN
1	D	295	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	265/294 (90%)	1.09	44 (16%)	2 3	15, 30, 50, 58	0
1	B	265/294 (90%)	1.63	82 (30%)	1 1	17, 39, 55, 59	0
1	C	202/294 (68%)	1.66	55 (27%)	1 1	16, 34, 57, 63	0
1	D	263/294 (89%)	1.86	96 (36%)	0 1	17, 44, 55, 60	0
All	All	995/1176 (84%)	1.55	277 (27%)	1 1	15, 36, 55, 63	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	TYR	11.2
1	C	269	ALA	9.7
1	C	266	ALA	9.6
1	B	72	PHE	9.2
1	C	272	PHE	8.7
1	B	38	VAL	8.4
1	B	26	VAL	7.4
1	D	65	VAL	7.3
1	D	257	LEU	7.3
1	A	262	ARG	7.0
1	D	53	VAL	6.8
1	C	262	ARG	6.8
1	D	72	PHE	6.8
1	B	276	LEU	6.6
1	B	302	TYR	6.4
1	B	303	ARG	6.3
1	D	76	TRP	6.3
1	D	108	ILE	6.3
1	C	261	ALA	6.2
1	D	38	VAL	6.2
1	D	61	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	37	PRO	6.1
1	D	296	LEU	6.1
1	B	118	TYR	6.1
1	B	37	PRO	5.8
1	D	66	ASP	5.8
1	B	67	SER	5.7
1	C	112	ILE	5.7
1	D	264	LYS	5.5
1	D	56	LEU	5.5
1	B	266	ALA	5.3
1	D	57	ALA	5.3
1	D	280	GLU	5.3
1	C	289	PHE	5.3
1	D	259	VAL	5.2
1	B	40	LEU	5.2
1	C	303	ARG	5.2
1	C	111	GLY	5.2
1	D	118	TYR	5.2
1	D	62	LYS	5.1
1	D	39	GLN	5.1
1	B	66	ASP	5.0
1	B	92	ILE	5.0
1	D	42	ILE	5.0
1	C	280	GLU	4.8
1	A	61	ILE	4.8
1	C	267	GLU	4.8
1	C	259	VAL	4.8
1	C	257	LEU	4.7
1	C	271	GLU	4.7
1	C	265	ASN	4.7
1	B	281	GLY	4.7
1	D	271	GLU	4.7
1	B	272	PHE	4.7
1	D	29	GLY	4.7
1	C	276	LEU	4.7
1	D	27	TYR	4.7
1	B	257	LEU	4.6
1	D	78	LYS	4.6
1	C	286	ILE	4.6
1	C	264	LYS	4.5
1	D	275	TRP	4.5
1	D	68	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	263	ALA	4.5
1	D	28	ASP	4.5
1	C	97	ILE	4.5
1	C	114	GLU	4.4
1	D	74	VAL	4.4
1	D	67	SER	4.4
1	B	74	VAL	4.3
1	A	267	GLU	4.3
1	D	113	SER	4.2
1	B	285	VAL	4.2
1	C	285	VAL	4.2
1	C	113	SER	4.2
1	D	52	LEU	4.2
1	B	140	ASP	4.2
1	D	75	ALA	4.1
1	A	280	GLU	4.1
1	B	262	ARG	4.1
1	D	95	VAL	4.1
1	B	296	LEU	4.1
1	C	108	ILE	4.1
1	A	26	VAL	4.1
1	B	273	ALA	4.0
1	D	97	ILE	4.0
1	D	267	GLU	4.0
1	B	263	ALA	4.0
1	A	27	TYR	3.9
1	D	266	ALA	3.9
1	D	59	ALA	3.9
1	B	76	TRP	3.9
1	D	281	GLY	3.8
1	D	77	TYR	3.8
1	D	87	TYR	3.8
1	B	52	LEU	3.8
1	B	93	VAL	3.8
1	D	116	PRO	3.8
1	B	280	GLU	3.7
1	B	289	PHE	3.7
1	A	269	ALA	3.7
1	A	202	ILE	3.7
1	A	93	VAL	3.7
1	D	262	ARG	3.6
1	A	40	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	28	ASP	3.6
1	C	282	GLY	3.6
1	A	263	ALA	3.6
1	D	285	VAL	3.6
1	D	193	ALA	3.5
1	D	286	ILE	3.5
1	B	73	LYS	3.5
1	B	292	ASP	3.5
1	C	258	LEU	3.5
1	C	260	GLY	3.4
1	D	303	ARG	3.4
1	C	275	TRP	3.4
1	C	103	ALA	3.4
1	B	265	ASN	3.4
1	D	60	PHE	3.4
1	D	115	SER	3.3
1	C	277	VAL	3.3
1	B	27	TYR	3.3
1	C	279	LYS	3.3
1	C	284	LYS	3.3
1	B	64	LYS	3.3
1	D	58	ASP	3.3
1	D	121	PHE	3.2
1	A	264	LYS	3.2
1	B	275	TRP	3.2
1	D	50	SER	3.2
1	D	292	ASP	3.2
1	A	72	PHE	3.2
1	D	92	ILE	3.2
1	B	267	GLU	3.2
1	C	193	ALA	3.2
1	B	68	GLY	3.1
1	C	192	THR	3.1
1	D	40	LEU	3.1
1	B	91	GLY	3.1
1	C	98	THR	3.1
1	D	120	ALA	3.1
1	D	190	TRP	3.1
1	B	282	GLY	3.0
1	B	193	ALA	3.0
1	B	25	ASP	3.0
1	B	192	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	278	SER	3.0
1	B	57	ALA	3.0
1	B	269	ALA	3.0
1	C	191	ALA	3.0
1	D	294	GLN	3.0
1	D	114	GLU	2.9
1	C	110	HIS	2.9
1	D	112	ILE	2.9
1	D	293	GLY	2.9
1	C	190	TRP	2.9
1	C	290	LYS	2.9
1	D	73	LYS	2.9
1	D	231	ARG	2.9
1	B	121	PHE	2.8
1	D	179	ALA	2.8
1	D	191	ALA	2.8
1	C	292	ASP	2.8
1	A	193	ALA	2.8
1	D	287	GLU	2.8
1	D	55	GLU	2.8
1	C	194	TYR	2.8
1	C	198	TYR	2.8
1	A	190	TRP	2.8
1	A	207	GLN	2.8
1	A	215	LEU	2.8
1	A	73	LYS	2.8
1	A	289	PHE	2.8
1	D	297	TYR	2.7
1	A	166	LEU	2.7
1	D	26	VAL	2.7
1	B	39	GLN	2.7
1	A	92	ILE	2.6
1	D	194	TYR	2.6
1	B	28	ASP	2.6
1	D	54	LYS	2.6
1	D	88	LEU	2.6
1	D	192	THR	2.6
1	B	293	GLY	2.6
1	B	113	SER	2.6
1	A	179	ALA	2.6
1	C	189	PRO	2.6
1	D	107	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	60	PHE	2.6
1	A	38	VAL	2.6
1	B	102	VAL	2.6
1	A	169	TYR	2.6
1	D	43	GLY	2.5
1	B	279	LYS	2.5
1	B	284	LYS	2.5
1	C	107	SER	2.5
1	D	49	GLN	2.5
1	D	299	PRO	2.5
1	B	54	LYS	2.5
1	B	158	ASN	2.4
1	B	259	VAL	2.4
1	B	202	ILE	2.4
1	A	266	ALA	2.4
1	D	279	LYS	2.4
1	A	75	ALA	2.4
1	C	105	ARG	2.4
1	C	106	ILE	2.4
1	D	111	GLY	2.4
1	D	269	ALA	2.4
1	D	44	ASN	2.4
1	A	167	SER	2.4
1	A	214	LEU	2.4
1	A	274	LYS	2.4
1	D	288	GLY	2.4
1	B	212	ALA	2.4
1	B	194	TYR	2.4
1	B	270	LYS	2.4
1	B	274	LYS	2.4
1	A	157	GLY	2.4
1	B	264	LYS	2.4
1	A	208	ALA	2.4
1	A	204	PHE	2.4
1	C	121	PHE	2.4
1	C	118	TYR	2.3
1	D	47	ALA	2.3
1	B	260	GLY	2.3
1	A	220	ILE	2.3
1	B	286	ILE	2.3
1	A	265	ASN	2.3
1	D	258	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	188	VAL	2.3
1	C	270	LYS	2.3
1	C	196	THR	2.3
1	D	110	HIS	2.3
1	D	79	SER	2.3
1	B	58	ASP	2.3
1	B	297	TYR	2.3
1	D	119	TYR	2.3
1	C	295	GLN	2.3
1	A	197	TRP	2.2
1	B	94	ASP	2.2
1	B	255	ALA	2.2
1	B	198	TYR	2.2
1	C	207	GLN	2.2
1	A	191	ALA	2.2
1	D	94	ASP	2.2
1	D	255	ALA	2.1
1	D	265	ASN	2.1
1	A	176	ILE	2.1
1	A	201	TYR	2.1
1	D	99	TYR	2.1
1	B	142	ASP	2.1
1	B	271	GLU	2.1
1	D	272	PHE	2.1
1	D	289	PHE	2.1
1	A	192	THR	2.1
1	B	42	ILE	2.1
1	A	94	ASP	2.1
1	B	56	LEU	2.1
1	B	299	PRO	2.1
1	B	191	ALA	2.1
1	B	277	VAL	2.1
1	A	29	GLY	2.1
1	B	97	ILE	2.1
1	B	77	TYR	2.1
1	B	166	LEU	2.1
1	B	214	LEU	2.1
1	B	95	VAL	2.1
1	D	140	ASP	2.1
1	D	185	ILE	2.0
1	B	288	GLY	2.0
1	B	86	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	112	ILE	2.0
1	A	77	TYR	2.0
1	D	290	LYS	2.0
1	C	179	ALA	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
2	CA	B	401	1/1	0.91	0.11	-3.32	49,49,49,49	0
2	CA	D	401	1/1	0.97	0.09	-	39,39,39,39	0
2	CA	A	401	1/1	0.98	0.05	-	32,32,32,32	0
2	CA	C	401	1/1	0.99	0.06	-	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.