Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:49 AM GMT

PDB ID	:	2O8E
Title	:	human MutSalpha (MSH2/MSH6) bound to a G T mispair, with ADP bound to MSH2 only
Authors	:	Warren, J.J.; Pohlhaus, T.J.; Changela, A.; Modrich, P.L.; Beese, L.S.
Deposited on	:	2006-12-12
Resolution	:	3.30 Å(reported)

The following versions of software and data (see references (i)) 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
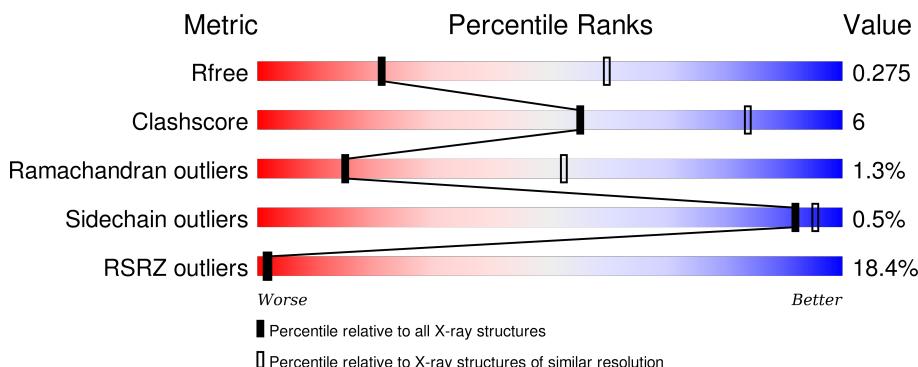
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
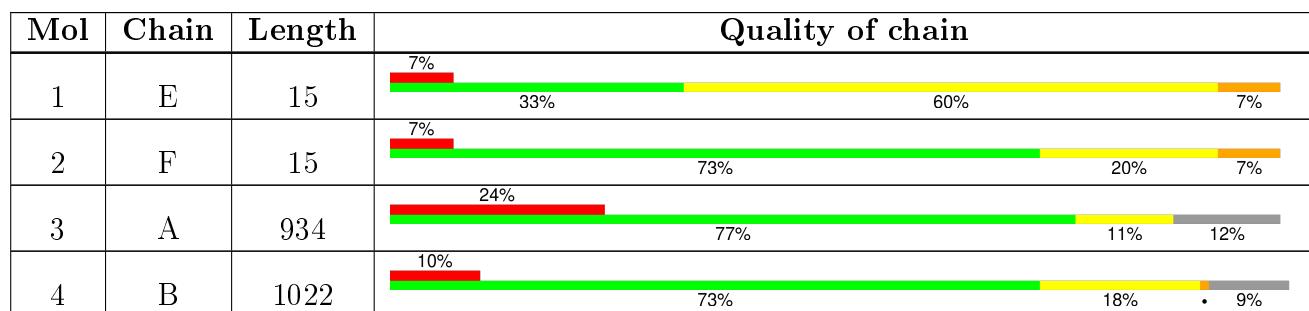
The reported resolution of this entry is 3.30 Å.

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	Percentile Ranks	Value
Rfree		0.275
Clashscore		6
Ramachandran outliers		1.3%
Sidechain outliers		0.5%
RSRZ outliers		18.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	E	15	7% / 33% 60% 7%
2	F	15	7% / 73% 20% 7%
3	A	934	24% / 77% 11% 12%
4	B	1022	10% / 73% 18% · 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14587 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 DNA chain called 5'-D(*GP*AP*AP*CP*CP*GP*CP*GP*GP*GP*CP*TP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total 310	C 146	N 64	O 86	P 14	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total 300	C 144	N 51	O 91	P 14	0	0	0

- Molecule 3 is a protein called DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	824	Total 6474	C 4105	N 1102	O 1233	S 34	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	PHE	ENGINEERED	UNP P43246

- Molecule 4 is a protein called DNA mismatch repair protein MSH6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	935	Total 7465	C 4736	N 1281	O 1397	S 51	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	MET	-	INITIATING METHIONINE	UNP P52701
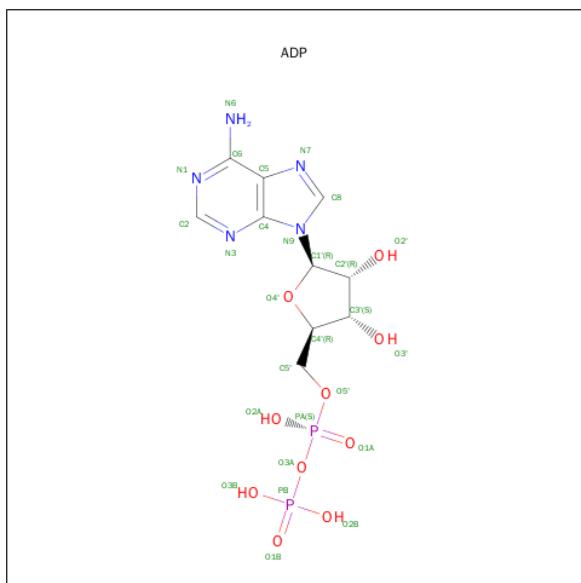
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Chain	Residue	Modelled	Actual	Comment	Reference
B	340	GLY	-	CLONING ARTIFACT	UNP P52701

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

- Molecule 6 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	10	Total 10	O 10	0	0
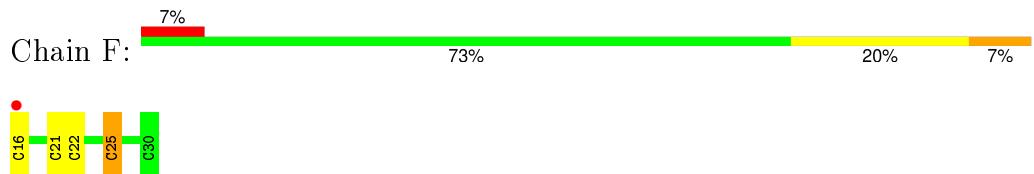
3 Residue-property plots ⓘ

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.
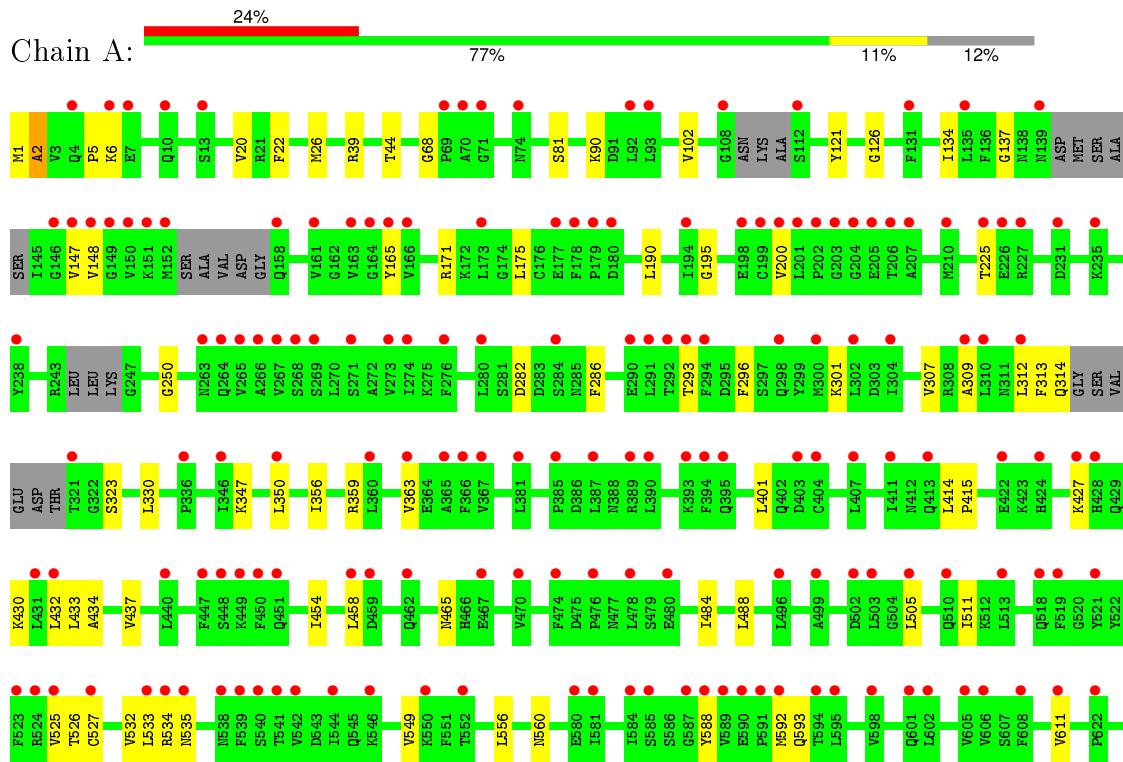
- Molecule 1: 5'-D(*GP*AP*AP*CP*CP*GP*CP*GP*GP*GP*CP*TP*AP*GP*G)-3'
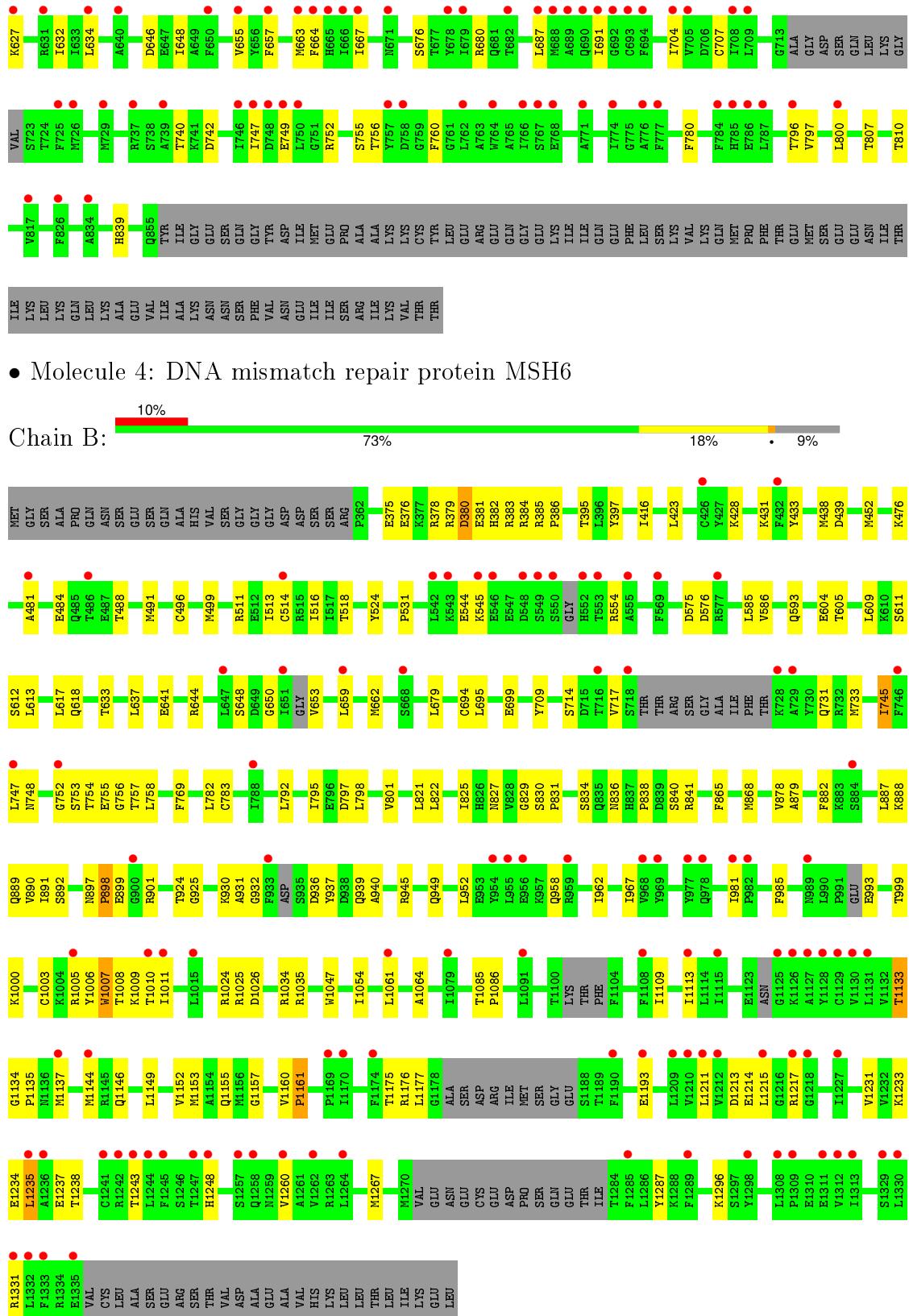
- Molecule 2: 5'-D(*CP*CP*TP*AP*GP*CP*CP*TP*GP*CP*GP*GP*TP*TP*C)-3'

- Molecule 3: DNA mismatch repair protein Msh2

• Molecule 4: DNA mismatch repair protein MSH6

Chain B:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	257.51Å 257.51Å 257.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 91.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-3.30) 98.4 (91.04-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.253 , 0.291 0.234 , 0.275	Depositor DCC
R_{free} test set	2219 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	91.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 151.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Outliers	0 of 43625 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	14587	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	E	0.75	0/349	1.61	12/538 (2.2%)
2	F	0.65	0/334	1.40	4/513 (0.8%)
3	A	0.32	0/6575	0.58	0/8866
4	B	0.48	1/7609 (0.0%)	0.71	1/10254 (0.0%)
All	All	0.43	1/14867 (0.0%)	0.72	17/20171 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	993	GLU	CD-OE2	6.76	1.33	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	14	DG	O4'-C1'-N9	7.45	113.21	108.00
1	E	1	DG	O4'-C1'-N9	6.80	112.76	108.00
1	E	1	DG	P-O3'-C3'	6.52	127.52	119.70
1	E	4	DC	P-O3'-C3'	6.43	127.42	119.70
4	B	756	GLY	N-CA-C	-6.16	97.70	113.10
1	E	4	DC	O4'-C1'-N1	6.14	112.30	108.00
1	E	14	DG	O4'-C1'-C2'	-5.94	101.15	105.90
1	E	8	DG	O4'-C1'-N9	-5.88	103.89	108.00
1	E	1	DG	C3'-C2'-C1'	-5.72	95.63	102.50
1	E	13	DA	P-O3'-C3'	5.68	126.52	119.70
2	F	21	DC	P-O3'-C3'	5.63	126.46	119.70
2	F	21	DC	O4'-C4'-C3'	-5.63	102.25	104.50
1	E	11	DC	C1'-O4'-C4'	-5.55	104.55	110.10
2	F	16	DC	O4'-C1'-N1	5.38	111.77	108.00
1	E	14	DG	C3'-C2'-C1'	-5.37	96.06	102.50
1	E	12	DT	N3-C4-O4	5.30	123.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	25	DC	O4'-C1'-C2'	-5.05	101.86	105.90

There are no chirality outliers.

There are no planarity outliers.

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	E	310	0	168	4	0
2	F	300	0	171	2	0
3	A	6474	0	6500	62	0
4	B	7465	0	7444	120	0
5	A	1	0	0	0	0
6	A	27	0	12	0	0
7	B	10	0	0	1	0
All	All	14587	0	14295	182	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 6.

All (182) 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)
4:B:1133:THR:HB	4:B:1134:GLY:HA3	1.36	1.07
4:B:554:ARG:HH22	4:B:604:GLU:HG3	1.39	0.85
4:B:1133:THR:HB	4:B:1134:GLY:CA	2.06	0.84
4:B:1133:THR:CB	4:B:1134:GLY:HA3	2.10	0.82
4:B:945:ARG:HD2	4:B:1024:ARG:HH12	1.44	0.82
4:B:868:MET:HG2	4:B:1054:ILE:HD12	1.66	0.76
4:B:380:ASP:HB3	4:B:382:HIS:H	1.51	0.75
4:B:897:ASN:HB3	4:B:901:ARG:HH21	1.53	0.73
4:B:795:ILE:HG23	4:B:1064:ALA:HA	1.72	0.71
4:B:699:GLU:HB3	4:B:827:ASN:OD1	1.90	0.71
4:B:385:ARG:HD2	4:B:386:PRO:HD2	1.73	0.70
4:B:544:GLU:OE2	4:B:605:THR:OG1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:380:ASP:HB2	4:B:384:ARG:H	1.58	0.68
4:B:897:ASN:HB3	4:B:901:ARG:NH2	2.10	0.66
3:A:525:VAL:HG12	3:A:526:THR:H	1.61	0.66
4:B:930:LYS:H	4:B:930:LYS:HD2	1.61	0.65
4:B:932:GLY:HA2	4:B:936:ASP:H	1.62	0.65
4:B:930:LYS:N	4:B:930:LYS:HD2	2.12	0.65
3:A:5:PRO:HB3	3:A:81:SER:HB3	1.78	0.65
4:B:496:CYS:HA	4:B:499:MET:HG2	1.79	0.65
4:B:1176:ARG:HE	4:B:1193:GLU:HG3	1.61	0.64
4:B:385:ARG:CD	4:B:386:PRO:HD2	2.28	0.64
3:A:430:LYS:HA	3:A:433:LEU:HB2	1.80	0.64
4:B:888:LYS:O	4:B:892:SER:OG	2.17	0.63
3:A:359:ARG:NH2	3:A:691:ILE:O	2.32	0.63
3:A:350:LEU:HB2	3:A:356:ILE:HG12	1.80	0.61
4:B:641:GLU:HB3	4:B:644:ARG:HG3	1.82	0.61
4:B:381:GLU:HB2	4:B:395:THR:HB	1.82	0.61
3:A:39:ARG:HE	3:A:44:THR:HG21	1.66	0.60
4:B:1153:MET:HB3	4:B:1160:VAL:HG12	1.84	0.60
4:B:1235:LEU:HD21	4:B:1243:THR:HG21	1.84	0.59
1:E:4:DC:H2'	1:E:5:DC:C6	2.38	0.59
4:B:936:ASP:HA	4:B:939:GLN:HB3	1.85	0.58
4:B:1176:ARG:NE	4:B:1193:GLU:HG3	2.18	0.58
4:B:898:PRO:O	4:B:899:GLU:HG3	2.03	0.58
4:B:518:THR:HG21	4:B:593:GLN:NE2	2.19	0.58
4:B:644:ARG:O	4:B:648:SER:HB3	2.04	0.57
4:B:380:ASP:O	4:B:397:TYR:HB2	2.03	0.57
4:B:798:LEU:HD13	4:B:1061:LEU:HD23	1.87	0.57
4:B:747:LEU:HA	4:B:757:THR:HG21	1.86	0.56
3:A:588:TYR:O	3:A:592:MET:HG2	2.06	0.56
3:A:505:LEU:HD12	3:A:511:ILE:HD11	1.87	0.56
4:B:733:MET:HE1	4:B:1152:VAL:HG22	1.87	0.56
4:B:484:GLU:HB2	4:B:514:CYS:SG	2.46	0.56
3:A:309:ALA:O	3:A:680:ARG:HD2	2.07	0.55
4:B:423:LEU:HD13	4:B:481:ALA:HB2	1.88	0.55
4:B:745:ILE:HD11	4:B:1152:VAL:HG21	1.88	0.55
3:A:430:LYS:C	3:A:432:LEU:H	2.10	0.55
4:B:981:ILE:HD11	4:B:985:PHE:HB2	1.87	0.55
4:B:1007:TRP:H	4:B:1011:ILE:HD12	1.72	0.55
4:B:836:ASN:O	4:B:841:ARG:NH2	2.38	0.55
4:B:585:LEU:HD12	4:B:709:TYR:CE2	2.43	0.54
3:A:414:LEU:N	3:A:415:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:380:ASP:HB2	4:B:384:ARG:N	2.24	0.53
4:B:381:GLU:HB2	4:B:395:THR:CB	2.37	0.53
3:A:634:LEU:HB2	3:A:655:VAL:HB	1.90	0.53
4:B:829:GLY:HA2	4:B:1034:ARG:HG2	1.90	0.53
3:A:664:PHE:HB3	3:A:797:VAL:HG22	1.91	0.53
4:B:868:MET:CG	4:B:1054:ILE:HD12	2.38	0.53
4:B:1025:ARG:HG3	4:B:1026:ASP:N	2.22	0.52
4:B:575:ASP:OD1	4:B:576:ASP:N	2.40	0.52
4:B:496:CYS:HA	4:B:499:MET:CG	2.39	0.52
4:B:1234:GLU:HG3	4:B:1238:THR:HB	1.92	0.51
4:B:890:VAL:HG23	4:B:891:ILE:HG23	1.92	0.51
4:B:887:LEU:O	4:B:891:ILE:HG12	2.10	0.51
1:E:7:DC:H2"	4:B:431:LYS:HD2	1.92	0.51
4:B:782:LEU:O	4:B:1155:GLN:NE2	2.40	0.51
4:B:586:VAL:HG11	4:B:613:LEU:HD11	1.93	0.51
4:B:897:ASN:O	4:B:901:ARG:NE	2.44	0.51
4:B:899:GLU:O	4:B:901:ARG:NH1	2.44	0.51
4:B:1175:THR:HG22	4:B:1211:LEU:HD12	1.93	0.51
3:A:20:VAL:HG21	3:A:68:GLY:HA2	1.93	0.51
3:A:755:SER:HA	4:B:1248:HIS:HB3	1.92	0.51
4:B:889:GLN:HA	4:B:901:ARG:HD3	1.92	0.50
4:B:609:LEU:HB3	4:B:618:GLN:HE21	1.76	0.50
4:B:633:THR:O	4:B:637:LEU:HG	2.12	0.50
4:B:488:THR:OG1	4:B:491:MET:HG3	2.12	0.50
4:B:545:LYS:HE3	4:B:679:LEU:HD21	1.93	0.50
4:B:516:ILE:HB	4:B:694:CYS:HA	1.92	0.50
4:B:1085:THR:HB	4:B:1086:PRO:HD2	1.93	0.49
4:B:949:GLN:HA	4:B:952:LEU:HB3	1.94	0.49
3:A:687:LEU:O	3:A:691:ILE:HG13	2.12	0.49
3:A:90:LYS:NZ	3:A:134:ILE:O	2.45	0.49
4:B:1109:ILE:HD12	4:B:1287:TYR:HB2	1.93	0.49
3:A:330:LEU:HA	3:A:611:VAL:HG21	1.93	0.49
3:A:511:ILE:HG12	3:A:525:VAL:HG22	1.95	0.48
2:F:22:DC:H2"	4:B:452:MET:HE3	1.95	0.48
3:A:359:ARG:O	3:A:363:VAL:HG23	2.14	0.48
3:A:740:THR:HG23	3:A:742:ASP:H	1.78	0.48
4:B:428:LYS:HD2	4:B:484:GLU:OE2	2.14	0.48
4:B:585:LEU:C	4:B:585:LEU:HD23	2.34	0.48
3:A:454:ILE:HG23	3:A:458:LEU:HD13	1.96	0.48
3:A:307:VAL:HG22	3:A:312:LEU:HD12	1.97	0.47
4:B:958:GLN:O	4:B:962:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1215:LEU:HD21	4:B:1231:VAL:HG21	1.96	0.47
4:B:644:ARG:HG2	4:B:653:VAL:HG11	1.96	0.47
4:B:801:VAL:HG21	4:B:878:VAL:HG21	1.97	0.47
3:A:646:ASP:HB3	3:A:648:ILE:HG13	1.97	0.47
3:A:401:LEU:HD11	3:A:458:LEU:HD11	1.95	0.47
3:A:839:HIS:NE2	4:B:1234:GLU:OE1	2.47	0.47
4:B:1137:MET:SD	4:B:1267:MET:HG2	2.54	0.47
4:B:1176:ARG:HG3	4:B:1176:ARG:O	2.14	0.47
4:B:1233:LYS:O	4:B:1237:GLU:HB3	2.14	0.47
1:E:5:DC:H2'	1:E:6:DG:C8	2.50	0.46
3:A:756:THR:O	3:A:760:PHE:HB3	2.15	0.46
3:A:126:GLY:HA3	3:A:147:VAL:HG23	1.98	0.46
4:B:524:TYR:CE1	4:B:531:PRO:HA	2.50	0.46
3:A:556:LEU:HD23	3:A:560:ASN:HB2	1.98	0.46
4:B:1175:THR:HB	4:B:1177:LEU:HG	1.98	0.46
4:B:792:LEU:HG	4:B:1157:GLY:HA2	1.96	0.46
4:B:611:SER:OG	4:B:612:SER:N	2.45	0.46
4:B:797:ASP:HB3	4:B:882:PHE:CD1	2.51	0.46
3:A:200:VAL:HA	3:A:225:THR:O	2.16	0.46
4:B:1113:ILE:HD11	4:B:1146:GLN:HE21	1.80	0.45
3:A:667:ILE:HG12	3:A:800:LEU:HB2	1.97	0.45
4:B:754:THR:C	4:B:755:GLU:HG3	2.36	0.45
3:A:313:PHE:HZ	3:A:347:LYS:HG3	1.82	0.45
4:B:1214:GLU:OE1	4:B:1217:ARG:HD3	2.16	0.45
3:A:307:VAL:HG13	3:A:312:LEU:HB2	1.99	0.45
4:B:936:ASP:O	4:B:940:ALA:N	2.44	0.45
4:B:830:SER:HA	4:B:831:PRO:HD3	1.83	0.45
4:B:930:LYS:H	4:B:930:LYS:CD	2.27	0.44
4:B:484:GLU:O	4:B:511:ARG:HA	2.17	0.44
3:A:663:MET:HB2	3:A:796:THR:HB	2.00	0.44
3:A:22:PHE:O	3:A:26:MET:HG3	2.18	0.44
3:A:632:ILE:HB	3:A:657:PHE:HB2	1.99	0.44
3:A:175:LEU:H	3:A:293:THR:HG21	1.83	0.44
4:B:967:ILE:HG12	4:B:981:ILE:HB	1.99	0.43
3:A:532:VAL:O	3:A:533:LEU:HB2	2.18	0.43
3:A:484:ILE:O	3:A:488:LEU:HG	2.18	0.43
3:A:1:MET:O	3:A:2:ALA:HB3	2.19	0.43
3:A:427:LYS:HA	3:A:430:LYS:HB2	2.00	0.43
4:B:659:LEU:HD23	4:B:662:MET:HG3	2.01	0.43
3:A:301:LYS:HB2	3:A:707:CYS:HB3	2.01	0.43
3:A:807:THR:HB	3:A:810:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:39:ARG:HE	3:A:44:THR:CG2	2.30	0.43
4:B:838:PRO:C	4:B:840:SER:H	2.22	0.43
4:B:822:LEU:HD23	4:B:822:LEU:HA	1.88	0.43
3:A:313:PHE:CZ	3:A:347:LYS:HG3	2.54	0.43
4:B:865:PHE:CZ	4:B:1047:TRP:HB3	2.54	0.43
4:B:375:GLU:HG2	4:B:378:ARG:CZ	2.49	0.43
4:B:924:THR:HB	4:B:925:GLY:H	1.59	0.43
3:A:434:ALA:HA	3:A:437:VAL:HB	1.99	0.43
4:B:379:ARG:HD3	4:B:383:ARG:O	2.18	0.42
4:B:748:ASN:H	4:B:757:THR:HG21	1.84	0.42
4:B:879:ALA:HA	4:B:882:PHE:CD2	2.54	0.42
4:B:999:THR:OG1	4:B:1000:LYS:N	2.51	0.42
4:B:376:GLU:H	4:B:376:GLU:HG3	1.59	0.42
4:B:897:ASN:O	4:B:901:ARG:CZ	2.68	0.42
4:B:758:LEU:HD22	4:B:1149:LEU:HD22	2.02	0.42
4:B:438:MET:CG	4:B:439:ASP:H	2.33	0.42
4:B:731:GLN:HB2	4:B:783:CYS:SG	2.59	0.42
4:B:882:PHE:CE2	4:B:891:ILE:HD11	2.54	0.42
3:A:747:ILE:HB	3:A:780:PHE:HD1	1.83	0.42
4:B:769:PHE:HE1	4:B:1054:ILE:HG22	1.84	0.42
3:A:556:LEU:O	3:A:560:ASN:N	2.50	0.42
4:B:695:LEU:HD23	4:B:695:LEU:HA	1.73	0.42
3:A:313:PHE:O	3:A:314:GLN:HG3	2.19	0.42
3:A:148:VAL:HG12	3:A:165:TYR:HB3	2.02	0.42
4:B:416:ILE:HG23	4:B:513:ILE:HD11	2.01	0.42
3:A:190:LEU:HD11	3:A:296:PHE:HB2	2.01	0.42
3:A:282:ASP:HB2	3:A:286:PHE:CE2	2.54	0.41
4:B:1177:LEU:HA	4:B:1213:ASP:HB3	2.02	0.41
4:B:694:CYS:O	4:B:695:LEU:HB2	2.21	0.41
3:A:102:VAL:HB	3:A:121:TYR:HB2	2.02	0.41
4:B:428:LYS:HE3	4:B:433:TYR:CZ	2.55	0.41
4:B:378:ARG:HD3	7:B:47:HOH:O	2.19	0.41
3:A:430:LYS:HG2	3:A:433:LEU:HB2	2.02	0.41
4:B:1003:CYS:SG	4:B:1005:ARG:NH1	2.93	0.41
3:A:527:CYS:HA	3:A:549:VAL:HG23	2.02	0.41
4:B:1144:MET:O	4:B:1211:LEU:HD13	2.21	0.41
3:A:1:MET:H2	4:B:476:LYS:HG3	1.85	0.41
4:B:1008:THR:O	4:B:1010:THR:N	2.54	0.41
4:B:821:LEU:O	4:B:825:ILE:HG13	2.21	0.41
3:A:627:LYS:HA	3:A:704:ILE:HB	2.03	0.41
3:A:534:ARG:HG3	3:A:535:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:430:LYS:C	3:A:432:LEU:N	2.74	0.40
4:B:593:GLN:HG3	4:B:617:LEU:HB2	2.02	0.40
1:E:5:DC:C2'	1:E:6:DG:C8	3.04	0.40
3:A:676:SER:O	3:A:680:ARG:HG3	2.22	0.40
3:A:171:ARG:HE	3:A:593:GLN:HE22	1.68	0.40
2:F:25:DC:O5'	3:A:6:LYS:HD3	2.20	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	
3	A	810/934 (87%)	725 (90%)	78 (10%)	7 (1%)	21	60
4	B	915/1022 (90%)	813 (89%)	86 (9%)	16 (2%)	11	47
All	All	1725/1956 (88%)	1538 (89%)	164 (10%)	23 (1%)	15	52

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	753	SER
3	A	749	GLU
4	B	650	GLY
4	B	834	SER
4	B	931	ALA
4	B	1009	LYS
4	B	1161	PRO
4	B	714	SER
4	B	752	GLY
4	B	1296	LYS
3	A	137	GLY
4	B	745	ILE

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Mol	Chain	Res	Type
3	A	2	ALA
3	A	465	ASN
4	B	898	PRO
4	B	1133	THR
3	A	323	SER
4	B	1135	PRO
4	B	1331	ARG
3	A	250	GLY
4	B	717	VAL
4	B	1260	VAL
3	A	195	GLY

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	
3	A	707/807 (88%)	706 (100%)	1 (0%)	95	98
4	B	821/899 (91%)	814 (99%)	7 (1%)	84	92
All	All	1528/1706 (90%)	1520 (100%)	8 (0%)	92	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	752	ARG
4	B	380	ASP
4	B	937	TYR
4	B	1006	TYR
4	B	1007	TRP
4	B	1035	ARG
4	B	1161	PRO
4	B	1235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\#|Z| > 2$
6	ADP	A	936	5	22,29,29	1.01	1 (4%)	27,45,45	1.95	4 (14%)

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
6	ADP	A	936	5	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	936	ADP	C5-C4	3.06	1.47	1.40

All (4) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	936	ADP	N3-C2-N1	-7.24	123.35	128.89
6	A	936	ADP	PA-O3A-PB	-3.47	121.04	132.67
6	A	936	ADP	C4-C5-N7	-3.15	106.58	109.48
6	A	936	ADP	C2'-C1'-N9	-2.42	110.59	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	E	15/15 (100%)	0.46	1 (6%)	21	17	93, 101, 115, 116	0
2	F	15/15 (100%)	0.67	1 (6%)	21	17	90, 100, 119, 123	0
3	A	824/934 (88%)	1.37	224 (27%)	1	1	95, 103, 108, 113	0
4	B	935/1022 (91%)	0.83	103 (11%)	7	6	37, 102, 116, 122	0
All	All	1789/1986 (90%)	1.07	329 (18%)	2	1	37, 103, 114, 123	0

All (329) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	206	THR	15.0
3	A	541	THR	12.7
3	A	207	ALA	11.1
3	A	202	PRO	8.9
4	B	549	SER	8.8
3	A	693	CYS	8.6
3	A	776	ALA	7.6
3	A	692	GLY	7.6
3	A	588	TYR	7.5
3	A	534	ARG	7.4
4	B	1128	TYR	7.2
4	B	550	SER	7.0
3	A	166	VAL	6.4
3	A	708	ILE	6.4
3	A	231	ASP	6.3
3	A	292	THR	6.3
3	A	165	TYR	6.1
3	A	538	ASN	6.1
3	A	108	GLY	6.1
3	A	533	LEU	6.1
4	B	1335	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
3	A	150	VAL	5.8
3	A	394	PHE	5.7
3	A	585	SER	5.6
4	B	1298	TYR	5.5
3	A	200	VAL	5.5
3	A	587	GLY	5.4
3	A	210	MET	5.4
3	A	540	SER	5.4
3	A	432	LEU	5.3
3	A	750	LEU	5.2
3	A	395	GLN	5.1
3	A	273	VAL	5.1
3	A	664	PHE	5.1
3	A	201	LEU	5.1
4	B	1126	LYS	5.0
3	A	467	GLU	5.0
3	A	404	CYS	5.0
3	A	363	VAL	4.9
3	A	480	GLU	4.9
3	A	590	GLU	4.8
3	A	746	ILE	4.8
3	A	605	VAL	4.8
3	A	694	PHE	4.7
3	A	267	VAL	4.7
3	A	447	PHE	4.7
3	A	584	ILE	4.7
3	A	350	LEU	4.7
3	A	263	ASN	4.7
3	A	535	ASN	4.5
4	B	552	HIS	4.5
4	B	954	TYR	4.5
3	A	294	PHE	4.4
4	B	747	LEU	4.3
3	A	462	GLN	4.3
3	A	269	SER	4.3
3	A	151	LYS	4.3
3	A	304	ILE	4.3
3	A	666	ILE	4.3
3	A	7	GLU	4.3
3	A	678	TYR	4.2
4	B	1308	LEU	4.2
4	B	982	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
4	B	577	ARG	4.2
4	B	1313	ILE	4.1
4	B	1174	PHE	4.1
3	A	390	LEU	4.1
3	A	542	VAL	4.0
3	A	163	VAL	4.0
3	A	608	PHE	4.0
4	B	1218	GLY	4.0
3	A	178	PHE	3.9
3	A	527	CYS	3.9
3	A	739	ALA	3.9
3	A	152	MET	3.9
3	A	737	ARG	3.9
3	A	591	PRO	3.9
3	A	496	LEU	3.8
4	B	729	ALA	3.8
4	B	1332	LEU	3.8
3	A	785	HIS	3.8
3	A	450	PHE	3.7
4	B	981	ILE	3.7
3	A	458	LEU	3.7
4	B	1115	ILE	3.7
3	A	225	THR	3.7
3	A	284	SER	3.6
4	B	1210	VAL	3.6
3	A	365	ALA	3.6
3	A	4	GLN	3.6
3	A	173	LEU	3.6
3	A	592	MET	3.6
4	B	1129	CYS	3.6
3	A	449	LYS	3.6
3	A	667	ILE	3.6
4	B	1312	VAL	3.6
3	A	238	TYR	3.5
4	B	989	ASN	3.5
4	B	1130	VAL	3.5
4	B	1127	ALA	3.5
3	A	147	VAL	3.5
3	A	726	MET	3.5
3	A	595	LEU	3.5
3	A	149	GLY	3.5
3	A	521	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
3	A	293	THR	3.5
3	A	768	GLU	3.5
4	B	1010	THR	3.5
3	A	199	CYS	3.5
3	A	148	VAL	3.4
3	A	519	PHE	3.4
3	A	663	MET	3.4
3	A	235	LYS	3.4
4	B	542	LEU	3.4
3	A	459	ASP	3.4
3	A	478	LEU	3.4
3	A	70	ALA	3.4
4	B	1131	LEU	3.3
3	A	539	PHE	3.3
3	A	387	LEU	3.3
3	A	431	LEU	3.3
3	A	158	GLN	3.3
3	A	226	GLU	3.3
3	A	524	ARG	3.3
3	A	650	PHE	3.3
3	A	393	LYS	3.3
3	A	276	PHE	3.3
4	B	1311	GLU	3.2
3	A	787	LEU	3.2
3	A	671	ASN	3.2
4	B	716	THR	3.2
3	A	194	ILE	3.2
3	A	411	ILE	3.2
3	A	366	PHE	3.2
3	A	164	GLY	3.2
3	A	440	LEU	3.2
3	A	291	LEU	3.2
4	B	1212	VAL	3.1
3	A	704	ILE	3.1
4	B	1257	SER	3.1
3	A	139	ASN	3.1
4	B	1309	PRO	3.1
3	A	689	ALA	3.1
4	B	959	ARG	3.1
3	A	767	SER	3.1
4	B	546	GLU	3.1
3	A	204	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	6	LYS	3.0
3	A	227	ARG	3.0
3	A	525	VAL	3.0
4	B	553	THR	3.0
3	A	428	HIS	3.0
4	B	718	SER	2.9
3	A	631	ARG	2.9
3	A	784	PHE	2.9
4	B	933	PHE	2.9
3	A	550	LYS	2.9
3	A	290	GLU	2.9
4	B	1005	ARG	2.9
3	A	640	ALA	2.9
4	B	1243	THR	2.9
3	A	589	VAL	2.9
3	A	346	ILE	2.9
4	B	1331	ARG	2.9
3	A	360	LEU	2.9
3	A	205	GLU	2.9
3	A	266	ALA	2.9
4	B	1329	SER	2.9
3	A	71	GLY	2.9
4	B	651	ILE	2.8
3	A	764	TRP	2.8
3	A	601	GLN	2.8
3	A	203	GLY	2.8
4	B	956	GLU	2.8
3	A	826	PHE	2.8
4	B	548	ASP	2.8
3	A	470	VAL	2.8
4	B	543	LYS	2.8
3	A	687	LEU	2.8
3	A	321	THR	2.8
3	A	552	THR	2.8
3	A	665	HIS	2.8
3	A	131	PHE	2.8
4	B	1244	LEU	2.8
4	B	788	ILE	2.8
3	A	762	LEU	2.8
4	B	1015	LEU	2.7
3	A	523	PHE	2.7
4	B	1245	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	606	VAL	2.7
3	A	427	LYS	2.7
3	A	622	PRO	2.7
4	B	978	GLN	2.7
4	B	1285	PHE	2.7
4	B	1170	ILE	2.7
3	A	13	SER	2.7
3	A	381	LEU	2.7
4	B	1209	LEU	2.7
3	A	657	PHE	2.7
4	B	1247	THR	2.7
4	B	1091	LEU	2.7
4	B	1235	LEU	2.7
3	A	777	PHE	2.6
3	A	93	LEU	2.6
3	A	611	VAL	2.6
4	B	1227	ILE	2.6
3	A	407	LEU	2.6
3	A	518	GLN	2.6
4	B	426	CYS	2.6
4	B	969	TYR	2.6
3	A	424	HIS	2.6
3	A	602	LEU	2.6
3	A	310	LEU	2.6
3	A	403	ASP	2.6
3	A	280	LEU	2.6
4	B	1125	GLY	2.6
4	B	481	ALA	2.6
3	A	367	VAL	2.6
3	A	448	SER	2.6
3	A	544	ILE	2.6
3	A	385	PRO	2.6
3	A	688	MET	2.6
3	A	817	VAL	2.6
4	B	555	ALA	2.5
3	A	634	LEU	2.5
3	A	774	ILE	2.5
4	B	1108	PHE	2.5
3	A	503	LEU	2.5
3	A	771	ALA	2.5
3	A	92	LEU	2.5
3	A	10	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	180	ASP	2.5
3	A	598	VAL	2.5
3	A	505	LEU	2.5
4	B	1248	HIS	2.5
3	A	476	PRO	2.5
3	A	264	GLN	2.5
4	B	1079	ILE	2.5
3	A	265	VAL	2.5
3	A	513	LEU	2.5
3	A	422	GLU	2.4
4	B	955	LEU	2.4
3	A	766	ILE	2.4
4	B	1211	LEU	2.4
4	B	1330	LEU	2.4
3	A	758	ASP	2.4
4	B	977	TYR	2.4
3	A	135	LEU	2.4
3	A	796	THR	2.4
3	A	302	LEU	2.4
4	B	647	LEU	2.4
4	B	1289	PHE	2.4
4	B	1011	ILE	2.4
3	A	112	SER	2.4
4	B	1262	VAL	2.4
4	B	1333	PHE	2.4
3	A	747	ILE	2.3
4	B	968	VAL	2.3
3	A	389	ARG	2.3
3	A	300	MET	2.3
3	A	580	GLU	2.3
4	B	432	PHE	2.3
4	B	752	GLY	2.3
3	A	274	ILE	2.3
3	A	725	PHE	2.3
3	A	499	ALA	2.3
3	A	800	LEU	2.3
4	B	1190	PHE	2.3
3	A	161	VAL	2.3
4	B	1193	GLU	2.3
3	A	413	GLN	2.3
4	B	900	GLY	2.3
4	B	884	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	B	1113	ILE	2.3
2	F	16	DC	2.2
3	A	748	ASP	2.2
4	B	514	CYS	2.2
4	B	1264	LEU	2.2
4	B	1260	VAL	2.2
3	A	627	LYS	2.2
3	A	298	GLN	2.2
3	A	510	GLN	2.2
4	B	1061	LEU	2.2
4	B	545	LYS	2.2
4	B	1241	CYS	2.2
3	A	705	VAL	2.2
3	A	757	TYR	2.2
4	B	1137	MET	2.2
4	B	1144	MET	2.2
3	A	679	ILE	2.2
4	B	1217	ARG	2.2
3	A	69	PRO	2.2
3	A	546	LYS	2.2
3	A	271	SER	2.2
3	A	309	ALA	2.2
3	A	834	ALA	2.2
3	A	146	GLY	2.2
1	E	15	DG	2.1
3	A	709	LEU	2.1
4	B	1215	LEU	2.1
3	A	690	GLN	2.1
4	B	1242	ARG	2.1
4	B	668	SER	2.1
4	B	728	LYS	2.1
3	A	179	PRO	2.1
3	A	268	SER	2.1
3	A	691	ILE	2.1
3	A	594	THR	2.1
4	B	486	THR	2.1
3	A	474	PHE	2.1
3	A	749	GLU	2.1
4	B	1169	PRO	2.1
4	B	1236	ALA	2.1
3	A	451	GLN	2.1
4	B	1258	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	569	PHE	2.1
3	A	729	MET	2.1
3	A	786	GLU	2.1
3	A	581	ILE	2.0
4	B	659	LEU	2.0
3	A	177	GLU	2.0
3	A	198	GLU	2.0
3	A	336	PRO	2.0
3	A	655	VAL	2.0
4	B	746	PHE	2.0
3	A	502	ASP	2.0
3	A	74	ASN	2.0
3	A	312	LEU	2.0
3	A	682	THR	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, 95th 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
6	ADP	A	936	27/27	0.93	0.20	-0.98	97,98,100,100	0
5	MG	A	935	1/1	0.91	0.29	-	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.