WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:18 PM GMT

PDB ID	:	3THY
Title	:	Human MutSbeta complexed with an IDL of 2 bases (Loop2) and ADP
Authors	:	Yang, W.
Deposited on	:	2011-08-19
Resolution	:	2.89 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
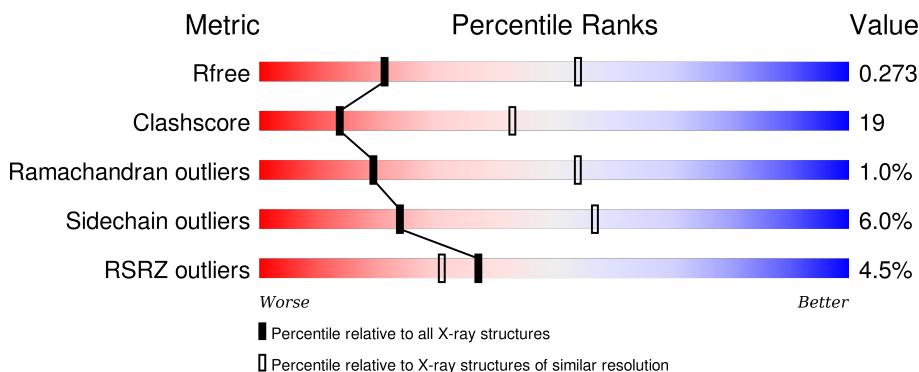
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
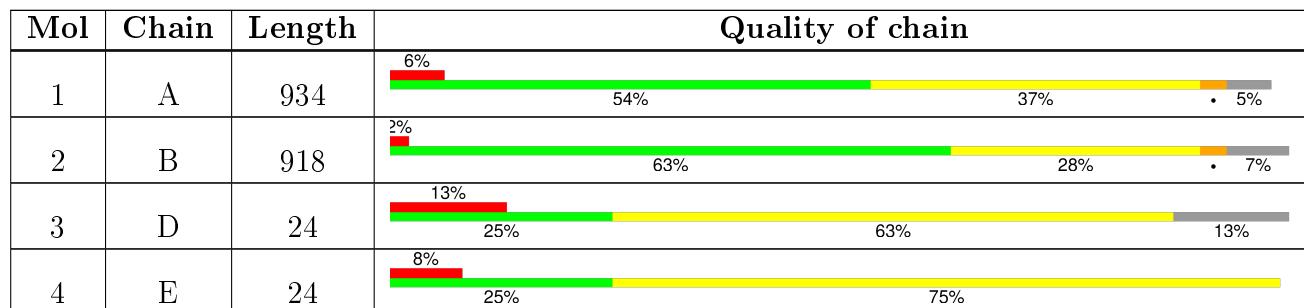
The reported resolution of this entry is 2.89 Å.

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		0.273
Clashscore		19
Ramachandran outliers		1.0%
Sidechain outliers		6.0%
RSRZ outliers		4.5%

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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	934	6% — 54% / 37% / • 5%
2	B	918	2% — 63% / 28% / • 7%
3	D	24	13% — 25% / 63% / 13%
4	E	24	8% — 25% / 75%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14678 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	883	Total	C	N	O	S	0	4	0
			6901	4383	1175	1307	36			

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	857	Total	C	N	O	S	0	5	0
			6819	4353	1164	1270	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	208	GLY	-	EXPRESSION TAG	GB 119616268
B	209	PRO	-	EXPRESSION TAG	GB 119616268
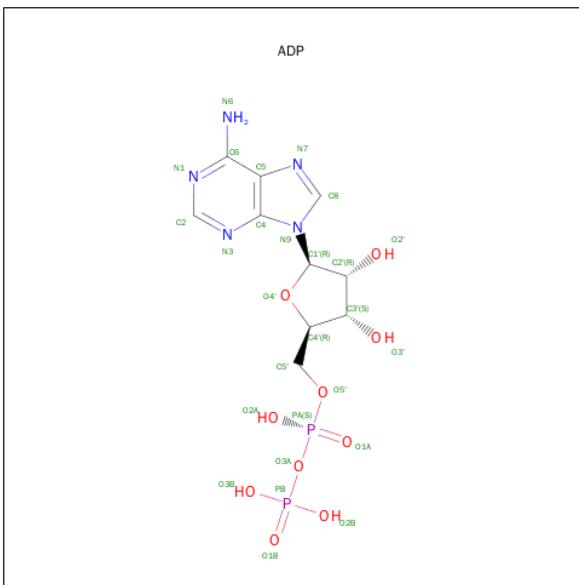
- Molecule 3 is a DNA chain called DNA Loop2 minus strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	21	Total	C	N	O	P	0	0	0
			427	205	77	125	20			

- Molecule 4 is a DNA chain called DNA Loop2 plus strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	24	Total	C	N	O	P	0	0	0
			489	234	90	142	23			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0
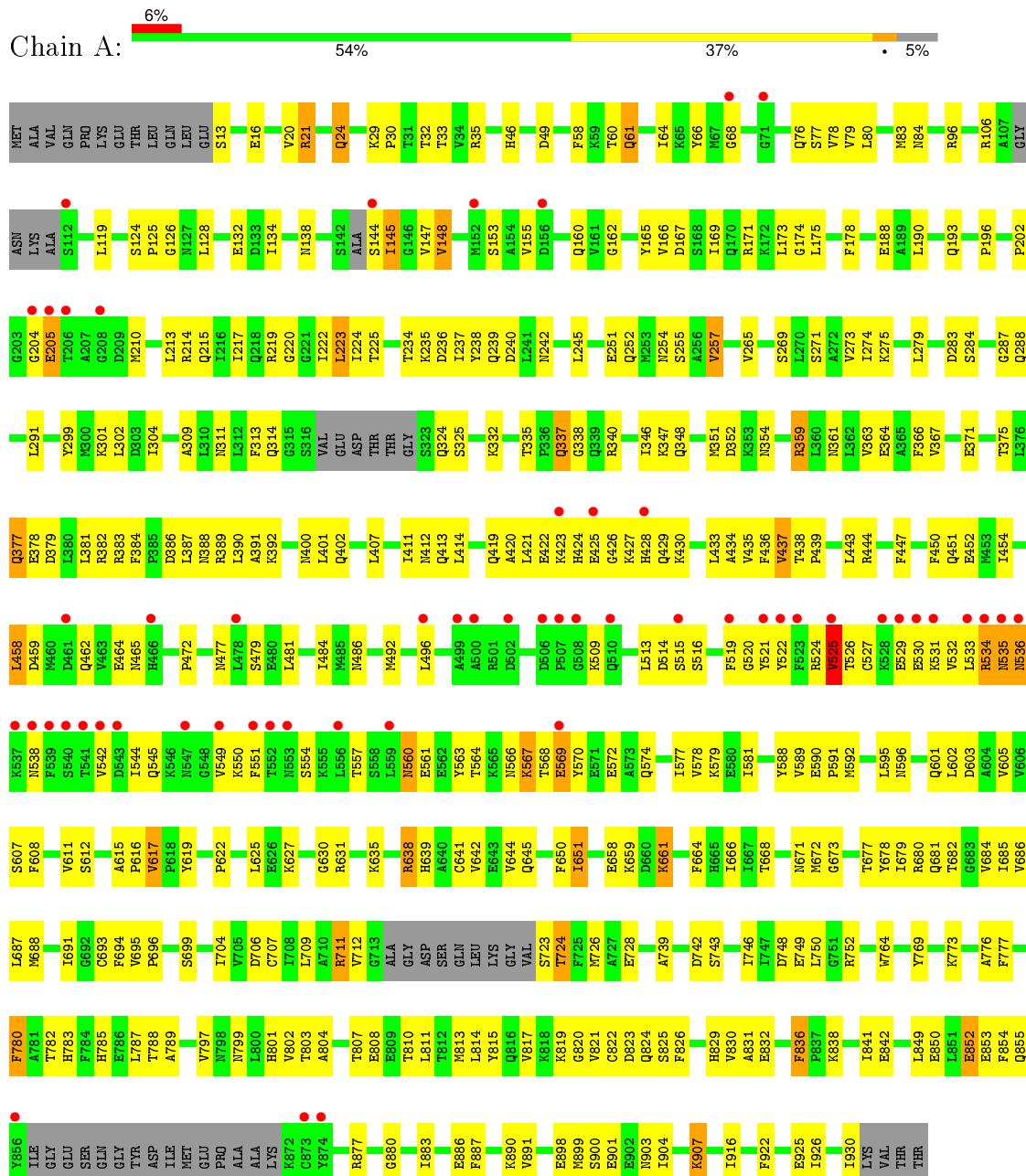
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	7	7	7	0	0
6	B	8	Total 8	O 8	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: DNA mismatch repair protein Msh2

• Molecule 2: DNA mismatch repair protein Msh3

Chain B:

• Molecule 3: DNA Loop2 minus strand

Chain D:

• Molecule 4: DNA Loop2 plus strand

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.27Å 91.11Å 95.63Å 67.82° 86.98° 73.35°	Depositor
Resolution (Å)	44.19 – 2.89 44.19 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.3 (44.19-2.89) 80.4 (44.19-2.89)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.194 , 0.274 0.191 , 0.273	Depositor DCC
R_{free} test set	1123 reflections (2.82%)	DCC
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 39869 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14678	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: 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	A	0.25	0/7022	0.41	0/9473
2	B	0.26	0/6957	0.41	0/9401
3	D	0.46	0/478	1.02	0/736
4	E	0.44	0/548	1.00	0/844
All	All	0.27	0/15005	0.48	0/20454

There are no bond length outliers.

There are no bond angle outliers.

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	A	6901	0	6867	299	0
2	B	6819	0	6878	216	0
3	D	427	0	239	21	0
4	E	489	0	272	25	0
5	A	27	0	12	1	0
6	A	7	0	0	1	0
6	B	8	0	0	0	0
All	All	14678	0	14268	536	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 19.

All (536) 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:711:ARG:HG3	1:A:711:ARG:HH21	1.01	1.13
1:A:711:ARG:HG3	1:A:711:ARG:NH2	1.82	0.87
1:A:534:ARG:HB2	1:A:534:ARG:HH21	1.39	0.85
3:D:11:DA:H2"	3:D:12:DA:O5'	1.77	0.83
4:E:28:DA:H2"	4:E:29:DT:H5'	1.59	0.83
4:E:26:DT:H2"	4:E:27:DC:H5'	1.62	0.82
1:A:425:GLU:HA	1:A:430:LYS:HG2	1.61	0.81
2:B:387:ALA:HB1	2:B:614:ARG:HD2	1.62	0.81
2:B:531:THR:HA	2:B:534:ARG:NH1	1.98	0.79
1:A:61:GLN:HG3	1:A:64:ILE:HD12	1.66	0.78
2:B:1004:PRO:O	2:B:1007:GLU:HG2	1.85	0.76
2:B:691:THR:HA	2:B:794:CYS:SG	2.25	0.76
1:A:128:LEU:HD13	1:A:134:ILE:HG22	1.67	0.76
1:A:706:ASP:HB2	1:A:742:ASP:HB2	1.67	0.76
2:B:439:VAL:HG12	2:B:440:GLN:H	1.49	0.76
1:A:711:ARG:HH21	1:A:711:ARG:CG	1.91	0.74
2:B:246:LYS:NZ	4:E:35:DG:H1'	2.02	0.74
1:A:590:GLU:HB3	1:A:591:PRO:HD3	1.71	0.73
2:B:985:LEU:HD23	2:B:1008:LEU:HD12	1.71	0.73
1:A:525:VAL:HG21	1:A:529:GLU:HG2	1.69	0.72
2:B:851:LYS:HG3	2:B:917:GLU:HG2	1.71	0.72
1:A:414:LEU:HD23	1:A:444:ARG:HD3	1.71	0.71
3:D:14:DC:H5"	3:D:15:DC:C5	2.25	0.71
1:A:301:LYS:HB2	1:A:707:CYS:HB3	1.71	0.71
2:B:529:ASN:OD1	2:B:531:THR:HB	1.89	0.71
1:A:532:VAL:HG12	1:A:535:ASN:HD22	1.56	0.70
2:B:439:VAL:HG12	2:B:440:GLN:N	2.06	0.70
3:D:21:DA:H2"	3:D:22:DT:H5"	1.72	0.70
3:D:13:DG:H2"	3:D:14:DC:O5'	1.92	0.69
2:B:233:GLN:HG3	2:B:234:HIS:CD2	2.28	0.68
1:A:20:VAL:HG21	1:A:68:GLY:HA2	1.74	0.67
2:B:858:ILE:HG23	2:B:862:LEU:HD12	1.77	0.67
2:B:447:GLU:HG2	2:B:500:TYR:CE1	2.29	0.67
2:B:569:LYS:O	2:B:573:GLN:HG2	1.93	0.67
1:A:242:ASN:HD21	1:A:255:SER:H	1.41	0.67
1:A:391:ALA:HB2	1:A:592:MET:HG3	1.76	0.67
2:B:331:ILE:HD11	2:B:387:ALA:HA	1.75	0.66
1:A:513:LEU:H	1:A:513:LEU:HD23	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASN:O	1:A:257:VAL:HG13	1.95	0.66
1:A:530:GLU:O	1:A:533:LEU:HB2	1.96	0.66
1:A:346:ILE:HA	1:A:691:ILE:HD11	1.76	0.66
2:B:576:LEU:O	2:B:922:ILE:HD13	1.95	0.66
3:D:9:DT:H2"	3:D:10:DG:C8	2.31	0.65
1:A:242:ASN:ND2	1:A:255:SER:H	1.94	0.65
1:A:271:SER:O	1:A:275:LYS:HG2	1.97	0.65
2:B:679:ILE:HD11	2:B:801:PHE:HE1	1.61	0.65
1:A:522:TYR:CE1	1:A:550:LYS:HD3	2.32	0.65
2:B:865:GLN:HE21	2:B:868:TYR:HB2	1.62	0.65
1:A:880:GLY:HA2	1:A:883:ILE:HD12	1.77	0.65
2:B:286:ARG:HH11	2:B:335:VAL:HG13	1.61	0.65
1:A:351:MET:O	1:A:704:ILE:HD13	1.96	0.64
2:B:761:LYS:HD3	2:B:764:SER:HB3	1.80	0.64
2:B:865:GLN:HE21	2:B:868:TYR:H	1.45	0.64
1:A:801:HIS:CD2	1:A:803:THR:HG23	2.32	0.64
1:A:764:TRP:CE2	2:B:1080:LYS:HE3	2.32	0.64
2:B:747:ILE:HD11	2:B:771:PHE:HE2	1.63	0.64
2:B:537:GLU:HG2	2:B:542:GLN:HG2	1.80	0.64
2:B:530:GLY:O	2:B:534:ARG:HD3	1.98	0.64
1:A:496:LEU:HD22	1:A:513:LEU:HD22	1.80	0.64
1:A:677:THR:O	1:A:681:GLN:HB3	1.99	0.63
2:B:531:THR:HA	2:B:534:ARG:HH11	1.63	0.63
1:A:825:SER:HB3	2:B:976:ASP:OD2	1.99	0.63
1:A:387:LEU:HD11	1:A:595:LEU:HD23	1.80	0.62
2:B:836:ASP:HB2	2:B:854:ARG:HH12	1.63	0.62
2:B:702:LEU:HD23	2:B:703:ILE:HG12	1.80	0.62
2:B:497:ILE:HG22	2:B:510:LEU:HD11	1.82	0.62
1:A:337:GLN:HG2	1:A:596:ASN:OD1	2.00	0.62
1:A:202:PRO:C	1:A:204:GLY:N	2.53	0.62
4:E:26:DT:C2'	4:E:27:DC:H5'	2.30	0.62
1:A:29:LYS:HE2	1:A:49:ASP:OD2	1.99	0.62
2:B:501:LEU:HD21	2:B:509:MET:CE	2.29	0.62
2:B:541:ASN:HD21	2:B:544:ASP:HB3	1.65	0.61
1:A:364:GLU:HG2	1:A:429:GLN:HE21	1.65	0.61
1:A:13:SER:HB2	1:A:16:GLU:HB2	1.82	0.61
1:A:832:GLU:HG2	1:A:841:ILE:HD12	1.83	0.61
1:A:534:ARG:HD3	1:A:534:ARG:N	2.16	0.61
1:A:589:VAL:O	1:A:592:MET:HG2	2.01	0.61
2:B:836:ASP:HB2	2:B:854:ARG:NH1	2.15	0.61
1:A:752:ARG:NH2	1:A:783[A]:HIS:HD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:SER:HB3	2:B:493:SER:HB3	1.83	0.61
1:A:666:ILE:HB	1:A:799:ASN:ND2	2.16	0.61
1:A:411:ILE:HD13	1:A:447:PHE:CG	2.36	0.60
1:A:145:ILE:HD11	1:A:165:TYR:HB2	1.83	0.60
2:B:869:VAL:HG23	2:B:870:PRO:HD2	1.84	0.60
2:B:232:GLN:HA	2:B:235:LYS:HE3	1.81	0.60
2:B:650:VAL:HG13	2:B:654:ILE:HD12	1.82	0.60
2:B:598:VAL:HG22	2:B:649:ALA:HB1	1.82	0.60
2:B:511:SER:O	2:B:512:LYS:HB2	2.01	0.60
2:B:452:ILE:HD12	2:B:452:ILE:H	1.65	0.60
1:A:234:THR:O	1:A:237:ILE:HG22	2.01	0.60
2:B:450:ASP:HB3	2:B:452:ILE:HD13	1.83	0.60
1:A:462:GLN:HA	1:A:465:ASN:HD22	1.65	0.60
2:B:832:ALA:HB2	2:B:912:TYR:HB2	1.85	0.59
2:B:930:MET:HB3	2:B:966:ASP:HB3	1.85	0.59
1:A:165:TYR:CE2	1:A:174:GLY:HA3	2.38	0.59
2:B:314:SER:HB3	4:E:29:DT:OP2	2.03	0.59
1:A:436:PHE:HZ	1:A:602:LEU:HB2	1.67	0.59
1:A:427:LYS:HA	1:A:430:LYS:HB2	1.84	0.59
2:B:302:GLU:OE2	2:B:307:LYS:HE2	2.03	0.59
1:A:891:VAL:HG11	2:B:1101:LEU:HD21	1.85	0.58
1:A:20:VAL:HG21	1:A:68:GLY:CA	2.32	0.58
1:A:622:PRO:HD3	1:A:695:VAL:HG22	1.86	0.58
1:A:165:TYR:CZ	1:A:174:GLY:HA3	2.39	0.58
1:A:126:GLY:O	1:A:147:VAL:HG23	2.04	0.58
2:B:532:THR:HG23	2:B:928:THR:HG23	1.86	0.58
1:A:422:GLU:HA	1:A:425:GLU:HB2	1.84	0.57
2:B:246:LYS:HZ3	4:E:35:DG:H1'	1.69	0.57
1:A:361:ASN:O	1:A:364:GLU:HB3	2.04	0.57
2:B:987:TYR:CE2	2:B:992:VAL:HG23	2.39	0.57
1:A:124:SER:HB2	1:A:125:PRO:HD2	1.85	0.57
1:A:723:SER:HB2	1:A:726:MET:HB3	1.85	0.57
1:A:213:LEU:O	1:A:217:ILE:HG13	2.05	0.57
1:A:838:LYS:O	1:A:842:GLU:HG2	2.05	0.57
1:A:574:GLN:O	1:A:578:VAL:HG23	2.04	0.57
2:B:629:PHE:CE2	2:B:633:VAL:HG21	2.39	0.57
2:B:1063:VAL:HG23	2:B:1066:LEU:HD12	1.86	0.57
2:B:1060:GLY:O	2:B:1063:VAL:HG12	2.05	0.57
4:E:37:DA:H2''	4:E:38:DG:O5'	2.05	0.57
1:A:534:ARG:HE	2:B:752:VAL:HB	1.70	0.57
1:A:193:GLN:HE22	1:A:299:TYR:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:MET:HE1	2:B:1063:VAL:HG13	1.87	0.56
4:E:39:DC:H2'	4:E:40:DT:C6	2.40	0.56
4:E:39:DC:H2"	4:E:40:DT:H5'	1.87	0.56
1:A:148:VAL:HG23	1:A:165:TYR:HB3	1.88	0.56
2:B:702:LEU:H	2:B:702:LEU:HD22	1.69	0.56
2:B:1057:ARG:NH1	2:B:1082:LYS:HA	2.20	0.56
1:A:236:ASP:HB3	1:A:240:ASP:OD1	2.04	0.56
2:B:501:LEU:HD21	2:B:509:MET:HE3	1.87	0.56
2:B:942:THR:HG23	2:B:945:GLU:H	1.71	0.56
1:A:607:SER:O	1:A:611:VAL:HG23	2.04	0.56
1:A:785[B]:HIS:HE1	1:A:822:CYS:HB3	1.70	0.56
1:A:147:VAL:HG12	1:A:148:VAL:N	2.20	0.56
1:A:425:GLU:CA	1:A:430:LYS:HG2	2.31	0.56
3:D:7:DT:H2"	3:D:8:DC:H5'	1.87	0.56
1:A:125:PRO:HG2	1:A:223:LEU:HD21	1.88	0.56
1:A:836:PHE:HB3	1:A:841:ILE:HG23	1.87	0.56
1:A:472:PRO:O	1:A:479:SER:HB2	2.06	0.56
1:A:658:GLU:HG2	1:A:661:LYS:HG3	1.87	0.55
1:A:400:ASN:OD1	1:A:402:GLN:HB3	2.06	0.55
1:A:534:ARG:CB	1:A:534:ARG:HH21	2.14	0.55
2:B:987:TYR:HE2	2:B:992:VAL:HG23	1.71	0.55
1:A:681:GLN:O	1:A:685:ILE:HG12	2.06	0.55
2:B:978:ILE:HD13	2:B:1004:PRO:HG2	1.87	0.55
1:A:29:LYS:HB3	1:A:35:ARG:CZ	2.36	0.55
2:B:1006:CYS:HB3	2:B:1018:ASN:HD21	1.69	0.55
1:A:430:LYS:HA	1:A:433:LEU:HB2	1.89	0.55
2:B:439:VAL:CG1	2:B:440:GLN:H	2.20	0.55
1:A:439:PRO:O	1:A:443:LEU:HD23	2.07	0.55
3:D:11:DA:H2'	3:D:12:DA:C8	2.41	0.54
2:B:890[A]:MET:HE3	2:B:892:GLY:HA3	1.89	0.54
1:A:788:THR:HG22	1:A:799:ASN:ND2	2.22	0.54
2:B:512:LYS:HD2	2:B:514:GLU:OE1	2.07	0.54
1:A:709:LEU:HD12	1:A:739:ALA:HB2	1.89	0.54
2:B:571:VAL:HA	2:B:909:ILE:HD11	1.90	0.54
2:B:833:LYS:O	2:B:833:LYS:HG2	2.06	0.54
2:B:513:PRO:HA	2:B:516:PHE:CE1	2.43	0.54
2:B:521:SER:OG	2:B:524:GLU:HG3	2.08	0.54
1:A:359:ARG:O	1:A:363:VAL:HG23	2.07	0.54
1:A:514:ASP:O	1:A:521:TYR:HA	2.08	0.54
1:A:617:VAL:HG22	1:A:638:ARG:NH2	2.23	0.54
4:E:28:DA:H2'	4:E:29:DT:H71	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:TYR:O	2:B:278:THR:HG23	2.08	0.53
1:A:678:TYR:CD1	1:A:817:VAL:HG21	2.43	0.53
1:A:789:ALA:HB2	1:A:855:GLN:OE1	2.08	0.53
2:B:413:GLN:N	2:B:414:PRO:HD3	2.23	0.53
2:B:985:LEU:O	2:B:989:ILE:HG13	2.08	0.53
1:A:807:THR:HB	1:A:810:THR:HB	1.89	0.53
2:B:854:ARG:HE	2:B:859:ASP:CG	2.11	0.53
2:B:364:GLU:HB3	2:B:379:ILE:HG12	1.89	0.53
3:D:11:DA:H4'	3:D:12:DA:OP1	2.08	0.53
1:A:425:GLU:HA	1:A:430:LYS:CG	2.34	0.53
1:A:916:ILE:HD11	2:B:1102:TRP:HZ2	1.73	0.53
1:A:436:PHE:CZ	1:A:602:LEU:HD13	2.44	0.53
1:A:819:LYS:HG2	1:A:820:GLY:H	1.72	0.53
2:B:575:LEU:HD11	2:B:584:ARG:CZ	2.38	0.53
1:A:424:HIS:HE1	1:A:428:HIS:CE1	2.27	0.53
1:A:639:HIS:HD2	1:A:641:CYS:H	1.56	0.53
2:B:896:TYR:O	2:B:900:VAL:HG23	2.08	0.53
2:B:904:THR:CG2	2:B:926:ILE:HD11	2.38	0.53
2:B:286:ARG:NH1	2:B:335:VAL:HG13	2.24	0.53
2:B:282:PHE:CE1	2:B:337:PRO:HG3	2.43	0.53
1:A:782:THR:HG21	1:A:787:LEU:HD23	1.91	0.52
1:A:679:ILE:HD12	1:A:746:ILE:HG23	1.91	0.52
3:D:16:DG:H2'	3:D:17:DA:C8	2.43	0.52
2:B:778:GLU:HG3	2:B:779:ASN:N	2.24	0.52
1:A:726:MET:HE2	1:A:726:MET:HA	1.90	0.52
2:B:949:ASP:O	2:B:953:ILE:HG13	2.08	0.52
1:A:145:ILE:HD11	1:A:147:VAL:O	2.09	0.52
2:B:282:PHE:CD1	2:B:337:PRO:HG3	2.45	0.52
1:A:519:PHE:HE1	1:A:542:VAL:HG12	1.74	0.52
2:B:747:ILE:HD12	2:B:747:ILE:O	2.09	0.52
1:A:589:VAL:HA	1:A:592:MET:SD	2.50	0.52
1:A:171:ARG:NH2	1:A:392:LYS:HE3	2.25	0.52
1:A:658:GLU:HG2	1:A:661:LYS:CG	2.40	0.52
2:B:1019:TYR:CD2	2:B:1052:ARG:HA	2.45	0.52
4:E:40:DT:H2"	4:E:41:DT:H5"	1.90	0.52
1:A:196:PRO:HG2	1:A:222:ILE:HD13	1.92	0.51
1:A:907:LYS:HB2	1:A:907:LYS:HZ3	1.75	0.51
2:B:265:CYS:HA	2:B:273:THR:O	2.11	0.51
1:A:413:GLN:HA	1:A:413:GLN:OE1	2.11	0.51
1:A:284:SER:O	1:A:288:GLN:HG3	2.10	0.51
1:A:454:ILE:HG23	1:A:458:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:CG	1:A:711:ARG:NH2	2.61	0.51
1:A:668:THR:O	1:A:801:HIS:HB2	2.09	0.51
1:A:419:GLN:HG2	1:A:423:LYS:HE3	1.91	0.51
1:A:887:PHE:O	1:A:891:VAL:HG23	2.10	0.51
1:A:484:ILE:HG21	1:A:566:ASN:ND2	2.26	0.51
2:B:865:GLN:NE2	2:B:868:TYR:HB2	2.24	0.51
2:B:632:ILE:O	2:B:636:LEU:HG	2.11	0.51
1:A:601:GLN:O	1:A:605:VAL:HG13	2.10	0.51
1:A:535:ASN:CG	1:A:536:ASN:N	2.63	0.51
1:A:638:ARG:HA	1:A:650:PHE:HE2	1.76	0.51
2:B:604:ASN:HA	2:B:607:ARG:HG3	1.92	0.51
1:A:532:VAL:HG12	1:A:535:ASN:ND2	2.25	0.51
1:A:438:THR:HB	1:A:439:PRO:HD3	1.92	0.51
2:B:232:GLN:O	2:B:235:LYS:HD2	2.12	0.50
1:A:220:GLY:HA2	1:A:304:ILE:HD12	1.92	0.50
3:D:4:DC:H2"	3:D:5:DT:OP2	2.11	0.50
1:A:651:ILE:HG13	1:A:651:ILE:O	2.11	0.50
1:A:831:ALA:O	1:A:836:PHE:HB2	2.11	0.50
1:A:210:MET:O	1:A:214:ARG:HG3	2.11	0.50
1:A:525:VAL:HG23	1:A:551:PHE:HE2	1.76	0.50
1:A:481:LEU:HD23	1:A:570:TYR:HA	1.93	0.50
4:E:40:DT:H2"	4:E:41:DT:C5'	2.42	0.50
2:B:1089:ASN:O	2:B:1093:LYS:HD2	2.10	0.50
2:B:1104:MET:HB3	2:B:1109:ASP:HB3	1.92	0.50
1:A:534:ARG:HE	2:B:752:VAL:CG1	2.25	0.50
1:A:849:LEU:O	1:A:852:GLU:HG2	2.11	0.50
4:E:28:DA:C2'	4:E:29:DT:H5'	2.37	0.50
1:A:533:LEU:HA	1:A:536:ASN:OD1	2.11	0.50
1:A:728:GLU:OE2	1:A:750:LEU:HD12	2.12	0.50
2:B:539:LEU:HD11	2:B:572:THR:HG22	1.93	0.50
1:A:132:GLU:HG2	1:A:389:ARG:HH21	1.75	0.50
1:A:513:LEU:CD2	1:A:513:LEU:H	2.24	0.50
2:B:865:GLN:NE2	2:B:868:TYR:H	2.10	0.50
1:A:58:PHE:O	1:A:60:THR:HG22	2.12	0.50
2:B:765:THR:HG22	2:B:767:ALA:H	1.77	0.50
1:A:804:ALA:HB2	1:A:813:MET:SD	2.52	0.49
1:A:21:ARG:HA	1:A:21:ARG:HE	1.75	0.49
2:B:660:ARG:O	2:B:664:LEU:HG	2.12	0.49
3:D:13:DG:H2'	3:D:14:DC:O4'	2.12	0.49
1:A:780:PHE:CE1	1:A:782:THR:HB	2.47	0.49
1:A:24:GLN:HA	1:A:24:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:CG1	1:A:148:VAL:N	2.74	0.49
1:A:811:LEU:HD12	1:A:829:HIS:HD2	1.77	0.49
2:B:671:SER:OG	2:B:672:PRO:HD3	2.13	0.49
1:A:899:MET:CE	1:A:903:ASN:HB3	2.42	0.49
2:B:439:VAL:CG1	2:B:440:GLN:N	2.75	0.49
1:A:685:ILE:HD12	1:A:696:PRO:HD2	1.93	0.49
4:E:30:DC:H2"	4:E:31:DG:OP2	2.13	0.49
1:A:823:ASP:OD2	1:A:824:GLN:HG2	2.12	0.49
1:A:421:LEU:CD2	1:A:437:VAL:HG23	2.42	0.49
1:A:421:LEU:HD22	1:A:437:VAL:HG23	1.94	0.49
1:A:769:TYR:CE2	1:A:773:LYS:HG2	2.48	0.49
1:A:684:VAL:O	1:A:688:MET:HG3	2.13	0.49
1:A:638:ARG:HD3	1:A:638:ARG:N	2.27	0.49
1:A:144:SER:HB2	1:A:167:ASP:OD1	2.12	0.49
2:B:598:VAL:O	2:B:602:ILE:HG13	2.13	0.49
1:A:625:LEU:HD22	1:A:631:ARG:HB2	1.95	0.49
1:A:650:PHE:HA	5:A:935:ADP:C2	2.47	0.48
1:A:193:GLN:NE2	1:A:299:TYR:HB2	2.28	0.48
1:A:153:SER:O	1:A:160:GLN:HB3	2.14	0.48
2:B:431:ILE:HD12	2:B:432:HIS:N	2.28	0.48
1:A:712:VAL:HA	1:A:748:ASP:HB3	1.94	0.48
4:E:47:DA:H2"	4:E:48:DG:C8	2.48	0.48
1:A:301:LYS:O	1:A:302:LEU:HD23	2.13	0.48
1:A:335:THR:HB	1:A:337:GLN:OE1	2.13	0.48
1:A:132:GLU:HG2	1:A:389:ARG:NH2	2.28	0.48
2:B:738:VAL:HB	2:B:744:MET:HE1	1.94	0.48
1:A:424:HIS:CE1	1:A:428:HIS:CE1	3.02	0.48
1:A:904:ILE:HG21	2:B:1107:ALA:HA	1.95	0.48
2:B:219:ILE:HD13	2:B:219:ILE:H	1.77	0.48
2:B:312:ASN:H	2:B:312:ASN:HD22	1.60	0.48
1:A:531:LYS:O	1:A:534:ARG:NH2	2.47	0.48
2:B:246:LYS:HZ2	4:E:35:DG:H1'	1.76	0.48
1:A:838:LYS:HA	1:A:841:ILE:HD11	1.95	0.48
1:A:66:TYR:OH	2:B:340:LYS:HB2	2.14	0.48
1:A:274:ILE:HG23	1:A:279:LEU:HD12	1.95	0.48
2:B:580:GLU:O	2:B:583:ALA:HB3	2.12	0.48
3:D:9:DT:H2"	3:D:10:DG:N7	2.28	0.48
2:B:987:TYR:C	2:B:987:TYR:CD2	2.86	0.48
2:B:1096:LYS:O	2:B:1100:LYS:HG3	2.14	0.48
2:B:822:VAL:O	2:B:826:PHE:HD1	1.97	0.48
2:B:408:ARG:O	2:B:412:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:LYS:HE2	1:A:742:ASP:CG	2.34	0.47
2:B:883:MET:HG3	2:B:1019:TYR:CD1	2.49	0.47
1:A:630:GLY:HA2	1:A:777:PHE:HZ	1.79	0.47
1:A:436:PHE:C	1:A:439:PRO:HD2	2.35	0.47
1:A:899:MET:HE2	1:A:903:ASN:HB3	1.96	0.47
1:A:723:SER:HB2	1:A:726:MET:CB	2.43	0.47
1:A:424:HIS:CE1	1:A:428:HIS:NE2	2.82	0.47
1:A:371:GLU:OE2	1:A:423:LYS:HG2	2.15	0.47
2:B:501:LEU:HD21	2:B:509:MET:HE2	1.95	0.47
1:A:807:THR:HG22	1:A:808:GLU:N	2.30	0.47
1:A:900:SER:O	1:A:904:ILE:HD12	2.14	0.47
1:A:337:GLN:CD	1:A:337:GLN:H	2.18	0.47
2:B:346:ASN:CG	2:B:347:VAL:H	2.18	0.47
2:B:958:THR:O	2:B:994:SER:HB3	2.14	0.47
1:A:46:HIS:HD1	1:A:77:SER:HB3	1.79	0.47
1:A:564:THR:O	1:A:568:THR:HG22	2.15	0.47
1:A:568:THR:O	1:A:572:GLU:HG2	2.14	0.47
2:B:752:VAL:O	2:B:755:ILE:HG13	2.15	0.47
2:B:541:ASN:ND2	2:B:544:ASP:HB3	2.29	0.47
1:A:907:LYS:HB2	1:A:907:LYS:NZ	2.29	0.47
1:A:425:GLU:C	1:A:427:LYS:H	2.17	0.47
1:A:346:ILE:HA	1:A:691:ILE:CD1	2.45	0.47
1:A:178:PHE:HE2	1:A:190:LEU:HD22	1.79	0.47
2:B:904:THR:HG21	2:B:926:ILE:HD11	1.97	0.47
1:A:477:ASN:O	1:A:481:LEU:HD13	2.15	0.47
1:A:434:ALA:C	1:A:436:PHE:H	2.19	0.46
1:A:891:VAL:HG21	2:B:1101:LEU:HD21	1.96	0.46
1:A:419:GLN:HG2	1:A:423:LYS:CE	2.45	0.46
1:A:215:GLN:O	1:A:219:ARG:HG3	2.15	0.46
1:A:926:ILE:O	1:A:930:ILE:HG13	2.15	0.46
2:B:882:VAL:HG11	2:B:985:LEU:HD11	1.97	0.46
1:A:658:GLU:HG3	1:A:659:LYS:H	1.79	0.46
1:A:814:LEU:HB2	6:A:940:HOH:O	2.14	0.46
1:A:224:ILE:HG22	1:A:225:THR:N	2.30	0.46
1:A:534:ARG:HE	2:B:752:VAL:CB	2.28	0.46
2:B:855:HIS:HB3	2:B:858:ILE:HB	1.97	0.46
1:A:124:SER:HB2	1:A:125:PRO:CD	2.45	0.46
1:A:679:ILE:HG13	1:A:680:ARG:N	2.31	0.46
1:A:743:SER:O	1:A:776:ALA:HB1	2.15	0.46
3:D:13:DG:H4'	3:D:14:DC:OP1	2.15	0.46
2:B:382:VAL:HG23	2:B:493:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ILE:HG22	1:A:411:ILE:O	2.14	0.46
2:B:512:LYS:N	2:B:513:PRO:HD3	2.29	0.46
1:A:635:LYS:HB2	1:A:699:SER:HB3	1.97	0.46
2:B:487:GLU:HB3	2:B:489:PRO:HD2	1.97	0.46
2:B:633:VAL:HG12	2:B:677:LEU:HB2	1.97	0.46
1:A:162:GLY:HA3	1:A:265:VAL:HG12	1.97	0.46
1:A:826:PHE:O	1:A:830:VAL:HG23	2.15	0.46
1:A:78:VAL:HG12	1:A:79:VAL:N	2.30	0.46
2:B:245:TYR:HB3	3:D:14:DC:H2"	1.97	0.46
2:B:650:VAL:HG21	2:B:663:ILE:HG21	1.98	0.46
2:B:528:ILE:HG21	2:B:533:LEU:HD13	1.98	0.46
1:A:61:GLN:HB2	2:B:348:ASP:OD1	2.15	0.46
1:A:64:ILE:HG23	1:A:76:GLN:HB3	1.98	0.46
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.81	0.46
1:A:532:VAL:HG12	1:A:532:VAL:O	2.16	0.46
1:A:340:ARG:NH2	1:A:386:ASP:OD2	2.48	0.46
1:A:671:ASN:O	1:A:672:MET:HB2	2.15	0.46
2:B:246:LYS:HE3	2:B:248:ARG:HD3	1.98	0.46
1:A:785[B]:HIS:CE1	1:A:822:CYS:HB3	2.49	0.46
2:B:671:SER:N	2:B:672:PRO:CD	2.79	0.46
1:A:724:THR:HG23	2:B:889:ASN:HB3	1.98	0.46
1:A:269:SER:O	1:A:273:VAL:HG23	2.15	0.46
2:B:755:ILE:HD12	2:B:756:PRO:O	2.16	0.46
2:B:528:ILE:CG2	2:B:533:LEU:HD13	2.46	0.46
1:A:577:ILE:O	1:A:581:ILE:HG12	2.16	0.46
2:B:568:LYS:O	2:B:572:THR:HG23	2.15	0.45
1:A:554:SER:O	1:A:557:THR:HG22	2.16	0.45
1:A:821:VAL:HG12	1:A:822:CYS:N	2.31	0.45
1:A:664:PHE:HB3	1:A:797:VAL:HA	1.97	0.45
4:E:41:DT:H6	4:E:41:DT:H5'	1.80	0.45
4:E:42:DC:H2"	4:E:43:DA:C8	2.51	0.45
1:A:627:LYS:HE2	1:A:742:ASP:CB	2.46	0.45
2:B:571:VAL:HA	2:B:909:ILE:CD1	2.46	0.45
2:B:772:HIS:HB3	2:B:777:VAL:HG23	1.97	0.45
1:A:588:TYR:C	1:A:591:PRO:HD2	2.36	0.45
1:A:535:ASN:O	1:A:536:ASN:C	2.54	0.45
1:A:764:TRP:CD1	2:B:1080:LYS:HG3	2.51	0.45
1:A:29:LYS:HB3	1:A:35:ARG:NH1	2.31	0.45
1:A:173:LEU:O	1:A:291:LEU:HD12	2.17	0.45
1:A:639:HIS:HB2	1:A:681:GLN:HB2	1.99	0.45
2:B:598:VAL:CG2	2:B:649:ALA:HB1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:O	1:A:367:VAL:HG22	2.16	0.45
1:A:426:GLY:HA3	1:A:428:HIS:CE1	2.52	0.45
2:B:412:LEU:HD12	2:B:412:LEU:HA	1.72	0.45
2:B:404:GLU:OE1	2:B:404:GLU:HA	2.17	0.45
2:B:755:ILE:HG12	2:B:771:PHE:CE2	2.52	0.45
2:B:317:PHE:CE1	3:D:16:DG:H5"	2.52	0.45
2:B:452:ILE:HD12	2:B:452:ILE:N	2.31	0.45
1:A:237:ILE:HG23	1:A:238:TYR:N	2.32	0.45
2:B:795:SER:O	2:B:798:TRP:HB3	2.17	0.45
2:B:656:SER:HB3	2:B:659:LEU:HB2	1.98	0.45
2:B:218:SER:C	2:B:220:TYR:H	2.20	0.45
1:A:522:TYR:CZ	1:A:550:LYS:HD3	2.52	0.45
2:B:340:LYS:HA	2:B:344:ALA:O	2.16	0.45
1:A:224:ILE:HG22	1:A:225:THR:H	1.82	0.45
2:B:1062:ASN:O	2:B:1065:LYS:HE2	2.17	0.45
2:B:765:THR:C	2:B:767:ALA:H	2.19	0.45
4:E:47:DA:H2"	4:E:48:DG:H8	1.81	0.45
2:B:360:LEU:HB3	2:B:417:LEU:HD23	1.97	0.45
2:B:276:ILE:HG13	2:B:276:ILE:O	2.16	0.44
1:A:515:SER:HA	1:A:520:GLY:O	2.17	0.44
1:A:338:GLY:HA3	1:A:603:ASP:OD2	2.17	0.44
2:B:987:TYR:O	2:B:991:ASP:HB2	2.17	0.44
2:B:296:GLY:HA2	2:B:324:LEU:HD23	1.99	0.44
1:A:145:ILE:O	1:A:145:ILE:HG13	2.16	0.44
4:E:39:DC:H2"	4:E:40:DT:C5'	2.46	0.44
1:A:658:GLU:HG3	1:A:659:LYS:N	2.32	0.44
2:B:612:ILE:HG21	2:B:636:LEU:HD21	2.00	0.44
2:B:747:ILE:HD11	2:B:771:PHE:CE2	2.47	0.44
3:D:14:DC:H3'	3:D:15:DC:C6	2.52	0.44
1:A:375:THR:O	1:A:379:ASP:HB2	2.16	0.44
2:B:865:GLN:HE21	2:B:868:TYR:CB	2.29	0.44
1:A:366:PHE:CZ	1:A:602:LEU:HD11	2.53	0.44
1:A:642:VAL:HG12	1:A:642:VAL:O	2.17	0.44
4:E:39:DC:H3'	4:E:40:DT:H72	2.00	0.44
2:B:622:LYS:HD3	2:B:802:LEU:HB2	1.98	0.44
2:B:588:VAL:HG13	2:B:829:ALA:HA	1.98	0.44
1:A:193:GLN:HB2	1:A:348:GLN:HG2	2.00	0.44
2:B:422:ALA:H	2:B:451:ASN:HD21	1.64	0.44
1:A:311:ASN:HD22	1:A:311:ASN:HA	1.61	0.44
1:A:590:GLU:HB3	1:A:591:PRO:CD	2.45	0.44
2:B:512:LYS:HB3	2:B:512:LYS:HE3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:741:GLN:HE22	2:B:762:VAL:HB	1.83	0.44
2:B:893:LYS:O	2:B:897:ILE:HG12	2.17	0.44
2:B:675:HIS:O	2:B:679:ILE:HG23	2.18	0.44
1:A:202:PRO:C	1:A:204:GLY:H	2.20	0.44
2:B:930:MET:CB	2:B:966:ASP:HB3	2.47	0.44
2:B:987:TYR:HE2	2:B:992:VAL:CG2	2.30	0.44
2:B:746:GLU:HG2	2:B:768:VAL:HG21	2.00	0.44
2:B:843:GLN:HE22	2:B:847:LYS:NZ	2.16	0.44
1:A:711:ARG:HG3	1:A:711:ARG:O	2.18	0.43
2:B:398:ASP:CG	2:B:404:GLU:HB2	2.37	0.43
1:A:563:TYR:O	1:A:567:LYS:HB2	2.18	0.43
1:A:387:LEU:CD1	1:A:595:LEU:HD23	2.46	0.43
4:E:40:DT:C2'	4:E:41:DT:H5"	2.48	0.43
1:A:807:THR:O	1:A:829:HIS:CE1	2.71	0.43
2:B:581:ILE:HD13	2:B:908:GLN:HA	2.00	0.43
2:B:762:VAL:HG11	2:B:772:HIS:CD2	2.53	0.43
2:B:1020:HIS:CE1	2:B:1051:THR:HB	2.53	0.43
2:B:990:ARG:HG3	2:B:991:ASP:OD1	2.18	0.43
4:E:30:DC:H1'	4:E:31:DG:H5"	1.99	0.43
1:A:769:TYR:O	1:A:773:LYS:HB3	2.16	0.43
1:A:30:PRO:HD2	1:A:33:THR:HB	2.01	0.43
2:B:513:PRO:HA	2:B:516:PHE:CD1	2.53	0.43
2:B:665:GLU:HB3	2:B:818:HIS:HD2	1.84	0.43
1:A:377:GLN:HB3	1:A:377:GLN:HE21	1.57	0.43
2:B:402:ARG:NH2	2:B:426:GLN:HB2	2.34	0.43
1:A:638:ARG:HA	1:A:650:PHE:CE2	2.53	0.43
1:A:557:THR:O	1:A:561:GLU:HG3	2.19	0.43
1:A:425:GLU:O	1:A:425:GLU:HG2	2.18	0.43
2:B:392:VAL:HG11	2:B:519:LEU:HD13	1.99	0.43
1:A:435:VAL:HG12	1:A:435:VAL:O	2.19	0.43
1:A:608:PHE:CD1	1:A:693:CYS:HB2	2.53	0.43
2:B:575:LEU:HB2	2:B:581:ILE:HG12	2.00	0.43
1:A:545:GLN:NE2	1:A:545:GLN:HA	2.32	0.43
2:B:593:HIS:O	2:B:594:SER:C	2.57	0.43
2:B:883:MET:HG3	2:B:1019:TYR:CE1	2.54	0.43
2:B:720:HIS:CD2	2:B:724:ILE:HG13	2.54	0.43
1:A:83:MET:HB3	2:B:262:ASN:HB3	2.01	0.43
2:B:223:LEU:HA	2:B:316:LEU:HD21	1.99	0.43
1:A:627:LYS:HE2	1:A:742:ASP:OD2	2.18	0.43
2:B:514:GLU:CD	2:B:514:GLU:H	2.22	0.43
1:A:401:LEU:HG	1:A:458:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:HIS:HD2	1:A:803:THR:HG23	1.80	0.43
1:A:752:ARG:HH22	1:A:783[A]:HIS:HD2	1.63	0.43
1:A:188:GLU:OE2	1:A:304:ILE:HG12	2.18	0.43
1:A:481:LEU:HD21	1:A:569:GLU:OE1	2.19	0.43
1:A:251:GLU:HG3	1:A:252:GLN:H	1.83	0.43
2:B:755:ILE:HA	2:B:756:PRO:HD3	1.94	0.42
1:A:332:LYS:HD2	1:A:332:LYS:N	2.33	0.42
2:B:702:LEU:CD2	2:B:702:LEU:N	2.82	0.42
1:A:462:GLN:HA	1:A:465:ASN:ND2	2.33	0.42
1:A:682:THR:O	1:A:686:VAL:HG23	2.20	0.42
1:A:492:MET:HE1	1:A:560:ASN:HD22	1.85	0.42
2:B:577:LYS:HA	2:B:577:LYS:NZ	2.34	0.42
1:A:171:ARG:HH21	1:A:392:LYS:HG3	1.83	0.42
1:A:877:ARG:HG3	1:A:922:PHE:CD1	2.54	0.42
1:A:381:LEU:C	1:A:383:ARG:H	2.23	0.42
2:B:880:GLU:OE1	2:B:1017:GLY:HA3	2.20	0.42
2:B:534:ARG:HA	2:B:542:GLN:NE2	2.34	0.42
2:B:354:THR:HG21	2:B:413:GLN:HB2	2.02	0.42
2:B:575:LEU:O	2:B:581:ILE:HD11	2.19	0.42
1:A:534:ARG:NE	2:B:752:VAL:HB	2.32	0.42
1:A:534:ARG:HD2	2:B:752:VAL:HB	2.01	0.42
3:D:11:DA:C2'	3:D:12:DA:C8	3.03	0.42
2:B:701:PRO:C	2:B:703:ILE:H	2.21	0.42
1:A:204:GLY:O	1:A:205:GLU:O	2.37	0.42
1:A:619:TYR:HB3	1:A:694:PHE:HB3	2.01	0.42
2:B:513:PRO:HD2	2:B:514:GLU:OE2	2.19	0.42
4:E:41:DT:H2"	4:E:42:DC:C6	2.55	0.42
3:D:14:DC:H5"	3:D:15:DC:H5	1.79	0.42
1:A:783[B]:HIS:H	1:A:783[B]:HIS:CD2	2.38	0.42
2:B:532:THR:HG23	2:B:928:THR:CG2	2.49	0.42
1:A:166:VAL:HG22	1:A:173:LEU:HD22	2.02	0.42
2:B:441:ASP:OD2	2:B:442:ASP:N	2.41	0.42
1:A:390:LEU:HD21	1:A:407:LEU:HB2	2.01	0.42
1:A:801:HIS:CD2	1:A:822:CYS:HA	2.54	0.41
1:A:423:LYS:HE3	1:A:423:LYS:HB2	1.82	0.41
1:A:651:ILE:HD11	1:A:815:TYR:O	2.20	0.41
1:A:313:PHE:CZ	1:A:347:LYS:HG2	2.54	0.41
2:B:721:LEU:O	2:B:725:ARG:HG3	2.20	0.41
1:A:687:LEU:C	1:A:687:LEU:HD23	2.40	0.41
1:A:630:GLY:HA2	1:A:777:PHE:CZ	2.56	0.41
1:A:526:THR:O	1:A:527:CYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:CYS:HB3	2:B:248:ARG:HG3	2.03	0.41
1:A:175:LEU:HD12	1:A:291:LEU:HD11	2.03	0.41
2:B:867:GLN:HG2	2:B:1045:THR:O	2.20	0.41
4:E:44:DG:H2"	4:E:45:DA:OP2	2.19	0.41
1:A:807:THR:CB	1:A:810:THR:HB	2.50	0.41
1:A:384:PHE:CZ	1:A:413:GLN:HB2	2.56	0.41
2:B:842:VAL:HG12	2:B:843:GLN:N	2.36	0.41
1:A:245:LEU:O	1:A:287:GLY:HA2	2.21	0.41
3:D:13:DG:H2'	3:D:14:DC:C6	2.56	0.41
1:A:391:ALA:HB1	1:A:589:VAL:HG13	2.01	0.41
2:B:679:ILE:HD11	2:B:801:PHE:CE1	2.48	0.41
2:B:346:ASN:CG	2:B:347:VAL:N	2.74	0.41
1:A:76:GLN:H	1:A:76:GLN:CD	2.24	0.41
2:B:1006:CYS:HB3	2:B:1018:ASN:ND2	2.35	0.41
1:A:378:GLU:HG2	1:A:379:ASP:OD2	2.20	0.41
2:B:456:TYR:HA	2:B:492:CYS:SG	2.61	0.41
1:A:324:GLN:HG2	1:A:325:SER:H	1.86	0.41
1:A:534:ARG:HG2	2:B:753:SER:HB3	2.03	0.41
2:B:700:PHE:CB	2:B:703:ILE:HB	2.51	0.41
1:A:899:MET:HB2	1:A:904:ILE:HD11	2.03	0.41
1:A:144:SER:HA	1:A:169:ILE:HG13	2.02	0.41
1:A:615:ALA:O	1:A:616:PRO:C	2.59	0.41
1:A:673:GLY:O	1:A:802:VAL:HG21	2.21	0.41
2:B:483:ILE:HG22	2:B:483:ILE:O	2.21	0.41
1:A:901:GLU:HA	1:A:901:GLU:OE2	2.21	0.41
2:B:602:ILE:HG12	2:B:646:ILE:HD13	2.04	0.41
2:B:880:GLU:HG2	2:B:880:GLU:H	1.61	0.41
1:A:352:ASP:OD2	1:A:354:ASN:HB2	2.21	0.41
1:A:886:GLU:OE2	1:A:890:LYS:HE3	2.21	0.41
2:B:317:PHE:CD1	3:D:16:DG:H5"	2.56	0.40
1:A:420:ALA:O	1:A:423:LYS:HB3	2.21	0.40
3:D:8:DC:H1'	3:D:9:DT:H5'	2.02	0.40
1:A:807:THR:HG22	1:A:808:GLU:H	1.86	0.40
1:A:46:HIS:ND1	1:A:77:SER:HB3	2.35	0.40
1:A:524:ARG:C	1:A:525:VAL:HG22	2.41	0.40
1:A:424:HIS:CE1	1:A:426:GLY:HA3	2.56	0.40
1:A:450:PHE:HD2	1:A:451:GLN:HE21	1.69	0.40
1:A:80:LEU:HD23	1:A:84:ASN:HB3	2.03	0.40
1:A:619:TYR:N	1:A:619:TYR:CD2	2.89	0.40
1:A:309:ALA:O	1:A:680:ARG:HD2	2.22	0.40
1:A:687:LEU:HD23	1:A:688:MET:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:826:PHE:O	2:B:830:LYS:HG2	2.21	0.40
1:A:615:ALA:HB1	1:A:616:PRO:HD2	2.03	0.40
2:B:299:LYS:HB2	2:B:322:THR:HG21	2.03	0.40
2:B:658:LEU:O	2:B:662:VAL:HG23	2.22	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	875/934 (94%)	778 (89%)	86 (10%)	11 (1%)	15	46
2	B	850/918 (93%)	754 (89%)	90 (11%)	6 (1%)	26	63
All	All	1725/1852 (93%)	1532 (89%)	176 (10%)	17 (1%)	19	54

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLU
1	A	645	GLN
1	A	235	LYS
1	A	525	VAL
1	A	536	ASN
1	A	544	ILE
1	A	854	PHE
1	A	155	VAL
1	A	509	LYS
2	B	311	ASP
1	A	612	SER
1	A	749	GLU
2	B	870	PRO
2	B	437	VAL

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Mol	Chain	Res	Type
2	B	1044	VAL
2	B	922	ILE
2	B	756	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	742/808 (92%)	691 (93%)	51 (7%)	19	48
2	B	752/818 (92%)	714 (95%)	38 (5%)	29	65
All	All	1494/1626 (92%)	1405 (94%)	89 (6%)	24	57

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	24	GLN
1	A	32	THR
1	A	61	GLN
1	A	96	ARG
1	A	106	ARG
1	A	119	LEU
1	A	138	ASN
1	A	145	ILE
1	A	148	VAL
1	A	223	LEU
1	A	239	GLN
1	A	257	VAL
1	A	283	ASP
1	A	314	GLN
1	A	337	GLN
1	A	359	ARG
1	A	377	GLN
1	A	382	ARG
1	A	388	ASN

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	437	VAL
1	A	452	GLU
1	A	458	LEU
1	A	459	ASP
1	A	464	GLU
1	A	486	ASN
1	A	516	SER
1	A	525	VAL
1	A	534	ARG
1	A	535	ASN
1	A	538	ASN
1	A	549	VAL
1	A	560	ASN
1	A	567	LYS
1	A	569	GLU
1	A	579	LYS
1	A	617	VAL
1	A	638	ARG
1	A	644	VAL
1	A	651	ILE
1	A	661	LYS
1	A	711	ARG
1	A	724	THR
1	A	780	PHE
1	A	836	PHE
1	A	852	GLU
1	A	853	GLU
1	A	898	GLU
1	A	907	LYS
1	A	925	GLU
2	B	219	ILE
2	B	248	ARG
2	B	309	ILE
2	B	311	ASP
2	B	312	ASN
2	B	347	VAL
2	B	404	GLU
2	B	442	ASP
2	B	507	GLU
2	B	533	LEU
2	B	534	ARG

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Mol	Chain	Res	Type
2	B	577	LYS
2	B	604	ASN
2	B	614	ARG
2	B	627	GLN
2	B	632	ILE
2	B	646	ILE
2	B	702	LEU
2	B	718	ARG
2	B	719	MET
2	B	778	GLU
2	B	781	ARG
2	B	787	ARG
2	B	845	GLU
2	B	846	ARG
2	B	851	LYS
2	B	866	ASP
2	B	869	VAL
2	B	894	SER
2	B	899	GLN
2	B	904	THR
2	B	929	ARG
2	B	930	MET
2	B	970	ARG
2	B	1059	TYR
2	B	1075	LYS
2	B	1090	THR
2	B	1110	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	170	GLN
1	A	186	ASN
1	A	193	GLN
1	A	239	GLN
1	A	242	ASN
1	A	285	ASN
1	A	288	GLN
1	A	311	ASN
1	A	314	GLN
1	A	409	GLN

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Mol	Chain	Res	Type
1	A	419	GLN
1	A	429	GLN
1	A	451	GLN
1	A	465	ASN
1	A	535	ASN
1	A	560	ASN
1	A	639	HIS
1	A	645	GLN
1	A	799	ASN
1	A	801	HIS
1	A	829	HIS
2	B	312	ASN
2	B	461	GLN
2	B	515	ASN
2	B	582	ASN
2	B	627	GLN
2	B	655	GLN
2	B	720	HIS
2	B	734	GLN
2	B	741	GLN
2	B	772	HIS
2	B	784	ASN
2	B	785	GLN
2	B	810	HIS
2	B	843	GLN
2	B	865	GLN
2	B	867	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	ADP	A	935	-	22,29,29	0.98	1 (4%)	27,45,45	1.86	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
5	ADP	A	935	-	-	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)
5	A	935	ADP	C5-C4	3.18	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	935	ADP	N3-C2-N1	-6.38	124.01	128.89
5	A	935	ADP	PA-O3A-PB	-3.25	121.77	132.67
5	A	935	ADP	C2'-C1'-N9	-3.20	109.40	114.29
5	A	935	ADP	C4-C5-N7	-2.98	106.74	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	935	ADP	1	0

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	A	883/934 (94%)	0.13	56 (6%)	23 17	32, 83, 179, 343	1 (0%)
2	B	857/918 (93%)	-0.16	19 (2%)	65 60	30, 69, 133, 222	1 (0%)
3	D	21/24 (87%)	0.34	3 (14%)	4 2	67, 124, 266, 297	0
4	E	24/24 (100%)	0.13	2 (8%)	14 9	58, 118, 196, 244	0
All	All	1785/1900 (93%)	-0.01	80 (4%)	37 31	30, 75, 162, 343	2 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	ARG	10.0
1	A	529	GLU	6.0
1	A	552	THR	5.9
1	A	112	SER	5.7
1	A	533	LEU	5.7
1	A	535	ASN	5.5
1	A	553	ASN	5.5
2	B	1043	PHE	5.4
1	A	536	ASN	5.3
1	A	569	GLU	5.0
1	A	873	CYS	4.9
1	A	547	ASN	4.8
2	B	766	LYS	4.3
1	A	538	ASN	4.2
1	A	466	HIS	4.2
1	A	540	SER	4.2
2	B	750	SER	4.2
1	A	510	GLN	4.0
1	A	204	GLY	3.9
2	B	1026	SER	3.9
2	B	217	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	3	DT	3.7
1	A	541	THR	3.6
1	A	144	SER	3.6
1	A	428	HIS	3.5
1	A	519	PHE	3.4
1	A	549	VAL	3.4
1	A	68	GLY	3.4
1	A	507	PRO	3.4
1	A	542	VAL	3.2
2	B	866	ASP	3.2
1	A	71	GLY	3.1
1	A	531	LYS	3.1
1	A	556	LEU	3.1
2	B	864	GLU	3.1
1	A	551	PHE	3.0
1	A	423	LYS	3.0
1	A	208	GLY	3.0
1	A	499	ALA	3.0
1	A	525	VAL	3.0
1	A	874	TYR	2.9
1	A	537	LYS	2.9
1	A	528	LYS	2.9
2	B	752	VAL	2.9
1	A	205	GLU	2.8
1	A	496	LEU	2.8
3	D	6	DA	2.8
2	B	437	VAL	2.8
4	E	49	DG	2.8
4	E	26	DT	2.8
1	A	522	TYR	2.8
1	A	515	SER	2.7
1	A	461	ASP	2.7
1	A	521	TYR	2.6
1	A	530	GLU	2.6
1	A	856	TYR	2.6
1	A	543	ASP	2.5
2	B	1044	VAL	2.5
1	A	508	GLY	2.5
1	A	559	LEU	2.4
2	B	865	GLN	2.4
1	A	502	ASP	2.4
2	B	699	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	867	GLN	2.3
3	D	5	DT	2.3
2	B	1046	PHE	2.3
2	B	425	GLU	2.2
1	A	152	MET	2.2
1	A	478	LEU	2.2
2	B	749	ASN	2.2
1	A	539	PHE	2.1
1	A	206	THR	2.1
1	A	523	PHE	2.1
1	A	500	ALA	2.1
1	A	156	ASP	2.1
1	A	506	ASP	2.0
2	B	1023	PHE	2.0
2	B	747	ILE	2.0
1	A	425	GLU	2.0
2	B	932	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, 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($\mathring{A}^2$)	Q<0.9
5	ADP	A	935	27/27	0.92	0.18	0.34	74,94,97,98	0

6.5 Other polymers (i)

There are no such residues in this entry.