W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:26 PM GMT

PDB ID	:	1OXV
Title	:	Crystal structure of GlcV, the ABC-ATPase of the glucose ABC transporter from Sulfolobus solfataricus
Authors	:	Verdon, G.; Albers, S.V.; Dijkstra, B.W.; Driessen, A.J.; Thunnissen, A.M.
Deposited on	:	2003-04-03
Resolution	:	1.95 Å(reported)

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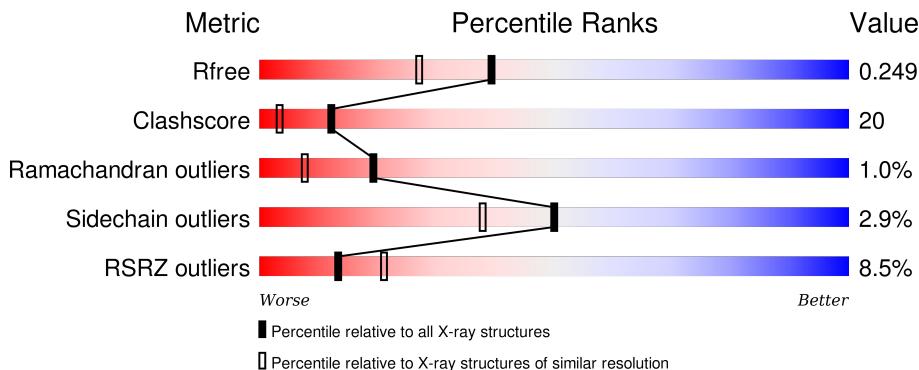
1　Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
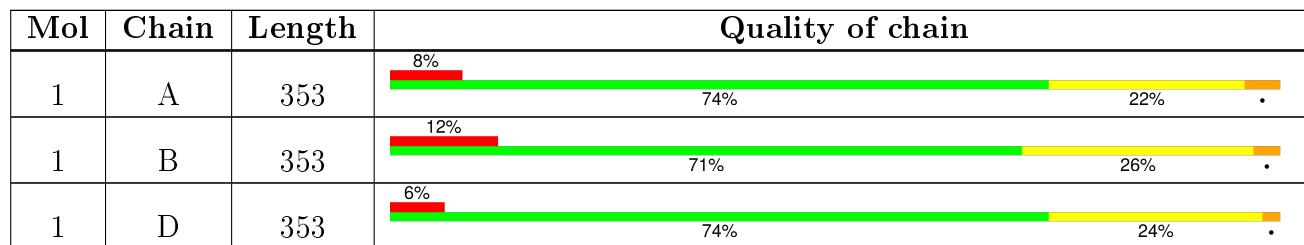
The reported resolution of this entry is 1.95 Å.

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		0.249
Clashscore		20
Ramachandran outliers		1.0%
Sidechain outliers		2.9%
RSRZ outliers		8.5%

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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	353	8% / 74% / 22% / •
1	B	353	12% / 71% / 26% / •
1	D	353	6% / 74% / 24% / •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	1202	-	-	X	-
3	IOD	A	1217	-	-	X	-
3	IOD	A	1227	-	-	X	-
3	IOD	A	1228	-	-	X	-
3	IOD	B	1221	-	-	X	-
3	IOD	B	1236	-	-	X	-
3	IOD	D	1208	-	-	X	-
3	IOD	D	1222	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9042 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 ABC transporter, ATP binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total 2702	C 1736	N 468	O 491	S 7	0	17	0
1	B	353	Total 2672	C 1717	N 464	O 485	S 6	0	11	0
1	D	353	Total 2671	C 1714	N 461	O 489	S 7	0	7	0
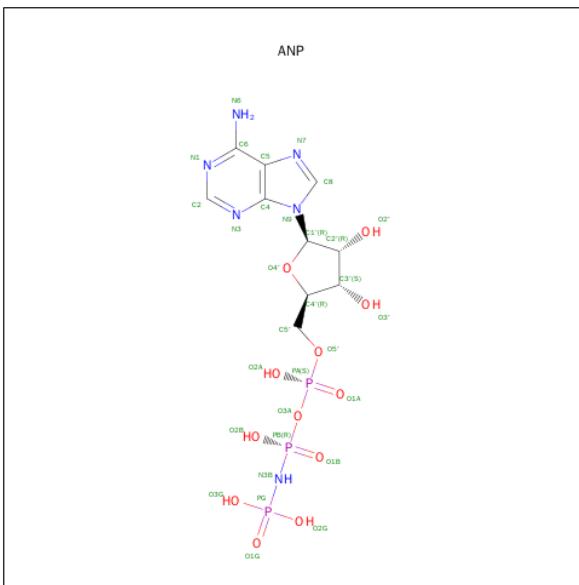
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	12	Total 12	I 12	0	0
3	A	15	Total 15	I 15	0	0
3	D	11	Total 11	I 11	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
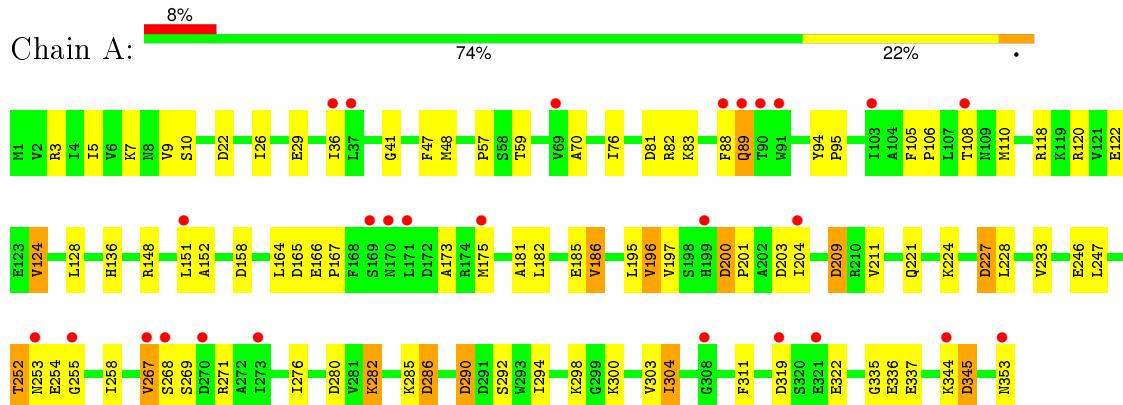
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	296	Total	O	0	3
			299	299		
5	B	239	Total	O	0	3
			242	242		
5	D	318	Total	O	0	4
			322	322		
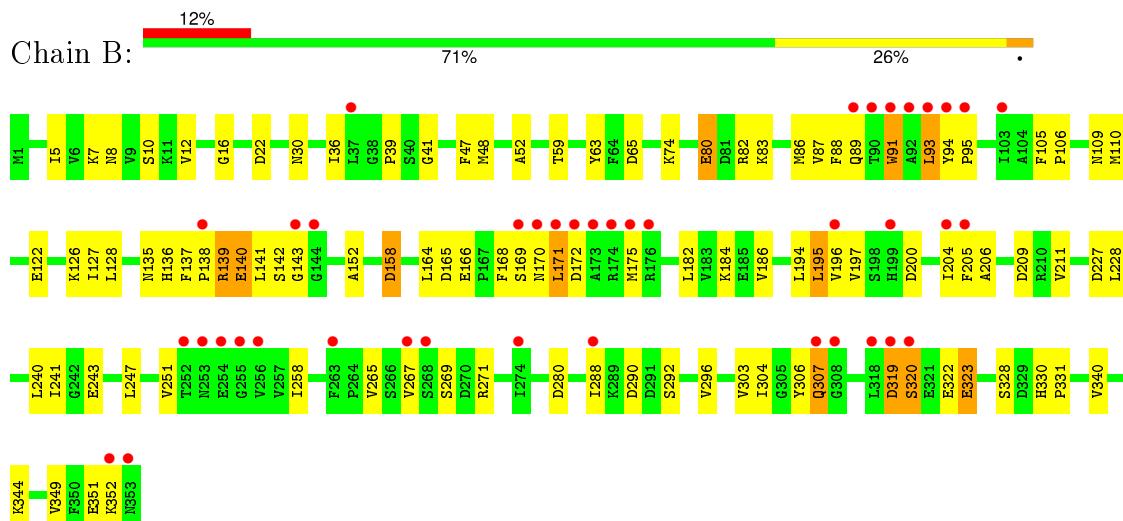
3 Residue-property plots (i)

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.
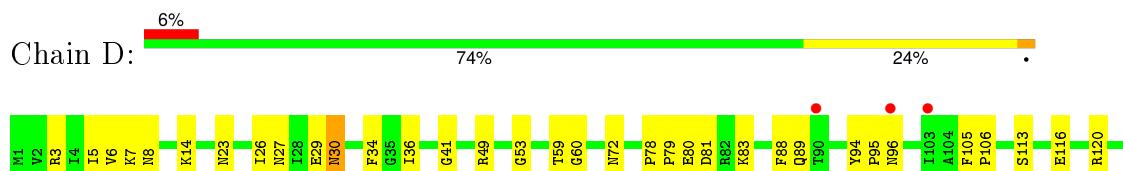
- Molecule 1: ABC transporter, ATP binding protein
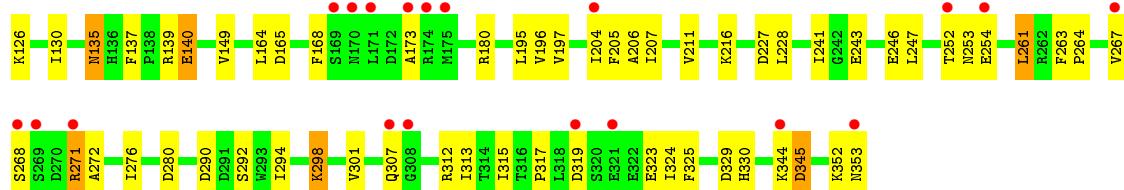
- Molecule 1: ABC transporter, ATP binding protein

- Molecule 1: ABC transporter, ATP binding protein

K126 I130 N135 H136 F137 P138 R139 E140 V149 L164 D165 F168 S169 N170 L171 D172 A173 R174 M175 R180 L195 V196 V197 I204 F205 A206 I207 V211 K216 D227 L228 I241 G242 E243 E246 L247 T252 N253 E254 L261 R262 F263 P264 V267

S268 S269 D270 R271 A272 I276 D280 D290 D291 S292 W293 I294 K298 V301 Q307 G308 R312 I313 T314 I315 T316 P317 L318 D319 S320 E321 E322 E323 I324 F325 D329 H330 K344 D345 K352 N353

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.09Å　　148.78Å　　176.71Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	20.00　　–　　1.95 19.99　　–　　1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.95) 95.9 (19.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$<I/\sigma(I)>$ [1]	3.27 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.188　　,　　0.240 0.202　　,　　0.249	Depositor DCC
R_{free} test set	4465 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\lvert L \rvert> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	3 of 87766 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9042	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.8814e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<\lvert L \rvert>$, $<L^2>$ 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: MG, IOD, ANP

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	0.51	2/2832 (0.1%)	0.75	12/3828 (0.3%)
1	B	0.43	1/2772 (0.0%)	0.74	10/3748 (0.3%)
1	D	0.42	0/2758	0.71	6/3730 (0.2%)
All	All	0.46	3/8362 (0.0%)	0.73	28/11306 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282[A]	LYS	C-N	-10.51	1.09	1.34
1	A	282[B]	LYS	C-N	-10.51	1.09	1.34
1	B	139	ARG	C-N	9.99	1.57	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	GLU	O-C-N	-10.43	106.01	122.70
1	B	65	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	140	GLU	CA-C-N	6.58	131.67	117.20
1	A	22	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	290	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	200	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	286	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	227	ASP	CB-CG-OD2	5.84	123.55	118.30
1	D	280	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	319	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	280	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	319	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	345	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	209	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	81	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	158	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	319	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	22	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	200	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	345	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	81	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	227	ASP	CB-CG-OD2	5.16	122.95	118.30
1	D	329	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	158	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	227	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	203	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	209	ASP	CB-CG-OD2	5.03	122.83	118.30

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	2702	0	2778	105	1
1	B	2672	0	2734	110	2
1	D	2671	0	2727	106	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	0	13	1
3	B	12	0	0	6	0
3	D	11	0	0	6	0
4	A	31	0	13	1	0
4	B	31	0	13	1	0
4	D	31	0	13	1	0
5	A	299	0	0	18	4
5	B	242	0	0	13	0
5	D	322	0	0	22	1
All	All	9042	0	8278	328	6

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 20.

All (328) 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:B:194:LEU:HD21	1:B:196[B]:VAL:CG2	1.69	1.23
1:D:352:LYS:HG3	1:D:353:ASN:N	1.47	1.17
1:B:211:VAL:HG13	1:B:228:LEU:HD11	1.26	1.16
3:A:1228:IOD:I	5:A:1446:HOH:O	2.36	1.14
1:A:175:MET:HE2	5:A:1415:HOH:O	1.45	1.13
1:D:352:LYS:CG	1:D:353:ASN:H	1.59	1.12
1:D:96:ASN:O	1:D:96:ASN:OD1	1.71	1.09
1:B:140:GLU:OE2	5:B:1361:HOH:O	1.69	1.07
3:A:1230:IOD:I	5:A:1384:HOH:O	2.41	1.06
1:A:182:LEU:O	1:A:186[A]:VAL:HG13	1.60	1.01
1:B:290:ASP:OD1	1:B:292:SER:OG	1.79	1.00
1:D:140:GLU:HG3	5:D:1422:HOH:O	1.60	1.00
1:B:211:VAL:HG13	1:B:228:LEU:CD1	1.91	0.99
1:B:12[B]:VAL:HG11	1:B:16:GLY:HA2	1.46	0.98
1:B:164:LEU:HB2	1:B:196[B]:VAL:HG13	1.50	0.94
1:B:110:MET:HE2	1:B:110:MET:HA	1.49	0.93
1:B:194:LEU:HD21	1:B:196[B]:VAL:HG22	1.50	0.93
1:A:26:ILE:HD12	3:A:1202:IOD:I	2.39	0.93
1:D:14[B]:LYS:NZ	5:D:1531:HOH:O	2.03	0.91
1:B:211:VAL:CG1	1:B:228:LEU:CD1	2.49	0.90
1:A:7[B]:LYS:HB3	1:A:7[B]:LYS:NZ	1.83	0.90
1:B:194:LEU:CD2	1:B:196[B]:VAL:CG2	2.50	0.89
1:A:165:ASP:HA	1:A:197:VAL:CG2	2.03	0.89
1:A:282[B]:LYS:NZ	5:A:1506:HOH:O	2.02	0.88
1:D:83:LYS:NZ	5:D:1534:HOH:O	2.01	0.88
1:A:3[B]:ARG:NH1	1:A:29:GLU:OE2	2.08	0.86
1:A:70:ALA:HA	1:A:76:ILE:CD1	2.07	0.85
1:B:211:VAL:CG1	1:B:228:LEU:HD12	2.07	0.84
1:B:175:MET:HE2	5:B:1401:HOH:O	1.75	0.84
1:A:3[B]:ARG:NH2	5:A:1482:HOH:O	2.10	0.84
1:B:211:VAL:HG11	1:B:228:LEU:HD12	1.59	0.83
1:B:110:MET:HA	1:B:110:MET:CE	2.08	0.83
1:D:211:VAL:HG13	1:D:228:LEU:HD11	1.60	0.82
1:A:209:ASP:OD2	5:A:1281:HOH:O	1.97	0.81
1:A:165:ASP:HA	1:A:197:VAL:HG23	1.60	0.81
1:B:290:ASP:CG	1:B:292:SER:HG	1.83	0.81
1:B:168:PHE:C	1:B:170:ASN:H	1.83	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLU:OE2	5:A:1459:HOH:O	1.99	0.81
1:B:12[B]:VAL:CG1	1:B:16:GLY:HA2	2.12	0.80
1:A:82:ARG:O	3:A:1217:IOD:I	2.69	0.80
1:A:304:ILE:HG22	3:A:1227:IOD:I	2.51	0.80
3:B:1221:IOD:I	3:B:1236:IOD:I	3.40	0.79
1:B:307:GLN:HA	5:B:1405[A]:HOH:O	1.82	0.79
1:B:194:LEU:HD21	1:B:196[B]:VAL:HG23	1.65	0.79
1:A:70:ALA:CA	1:A:76:ILE:HD13	2.13	0.78
1:B:267:VAL:HG22	1:B:351:GLU:HG2	1.66	0.78
1:B:7:LYS:HE3	1:B:8:ASN:OD1	1.84	0.78
1:B:194:LEU:CD2	1:B:196[B]:VAL:HG23	2.14	0.77
1:A:294:ILE:HG13	1:A:344:LYS:HB2	1.64	0.77
3:A:1238:IOD:I	5:A:1386:HOH:O	2.73	0.76
1:A:252:THR:CG2	1:A:254:GLU:H	1.99	0.76
1:D:211:VAL:HG13	1:D:228:LEU:CD1	2.15	0.76
1:D:307:GLN:OE1	5:D:1336:HOH:O	2.03	0.75
1:B:168:PHE:O	1:B:170:ASN:N	2.18	0.75
1:A:110[A]:MET:HE3	5:A:1522:HOH:O	1.87	0.75
1:D:139:ARG:HG2	1:D:139:ARG:HH11	1.52	0.75
1:D:137:PHE:O	1:D:140:GLU:HG2	1.85	0.74
1:D:7[A]:LYS:NZ	5:D:1365:HOH:O	2.20	0.74
1:D:96:ASN:HB3	3:D:1208:IOD:I	2.58	0.74
1:B:82:ARG:O	3:B:1236:IOD:I	2.76	0.74
1:D:344:LYS:O	3:D:1233:IOD:I	2.75	0.74
1:A:118[A]:ARG:NH1	1:A:122:GLU:OE2	2.20	0.74
1:A:164:LEU:HB3	1:A:167:PRO:HG3	1.68	0.73
1:D:352:LYS:HG3	1:D:353:ASN:H	0.67	0.72
1:D:252:THR:O	1:D:254:GLU:N	2.22	0.72
1:B:135:ASN:OD1	5:B:1238:HOH:O	2.06	0.72
1:A:89:GLN:HG2	1:A:166:GLU:HB2	1.71	0.72
1:D:88:PHE:CD2	3:D:1222:IOD:I	3.13	0.72
1:B:184:LYS:HD3	1:B:206:ALA:O	1.90	0.72
1:D:23:ASN:ND2	5:D:1513:HOH:O	2.20	0.72
1:B:127:ILE:HG21	5:B:1290:HOH:O	1.90	0.72
1:A:7[B]:LYS:HB3	1:A:7[B]:LYS:HZ1	1.53	0.71
3:A:1217:IOD:I	5:A:1519:HOH:O	2.78	0.71
1:A:3[A]:ARG:HD3	5:A:1424:HOH:O	1.88	0.71
1:D:36:ILE:HB	1:D:197:VAL:HG12	1.73	0.71
1:D:267:VAL:CG2	1:D:272:ALA:HB2	2.21	0.71
1:D:352:LYS:O	1:D:353:ASN:CB	2.38	0.71
1:B:52:ALA:HB1	1:B:86:MET:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246[B]:GLU:OE1	5:D:1516:HOH:O	2.09	0.70
1:A:70:ALA:HA	1:A:76:ILE:HD12	1.74	0.70
1:A:70:ALA:HA	1:A:76:ILE:HD13	1.73	0.69
1:A:88:PHE:HB2	3:A:1218:IOD:I	2.63	0.68
1:B:83[B]:LYS:NZ	1:B:158:ASP:O	2.26	0.68
1:A:252:THR:HG22	1:A:255:GLY:H	1.58	0.68
1:D:164:LEU:HB2	1:D:196[B]:VAL:CG2	2.22	0.68
1:D:298:LYS:HB2	1:D:298:LYS:HZ2	1.59	0.68
1:D:135:ASN:H	1:D:135:ASN:HD22	1.42	0.68
1:B:344:LYS:O	3:B:1235:IOD:I	2.82	0.67
1:A:252:THR:HG22	1:A:254:GLU:H	1.58	0.67
1:B:109:ASN:O	1:B:110:MET:CE	2.42	0.67
1:D:60:GLY:H	1:D:72:ASN:ND2	1.92	0.67
1:B:247:LEU:HD12	1:B:322:GLU:HB3	1.77	0.67
1:A:120[B]:ARG:HH11	1:A:120[B]:ARG:HG2	1.57	0.67
1:A:105:PHE:HB3	1:A:106:PRO:HD3	1.77	0.67
1:B:290:ASP:CG	1:B:292:SER:OG	2.30	0.66
1:B:267:VAL:CG2	1:B:351:GLU:HG2	2.25	0.66
1:A:269:SER:CB	1:A:353:ASN:HD22	2.10	0.64
1:B:168:PHE:C	1:B:170:ASN:N	2.50	0.64
1:A:108:THR:HG22	5:A:1449:HOH:O	1.97	0.64
1:B:105:PHE:HB3	1:B:106:PRO:HD3	1.79	0.64
1:D:113:SER:OG	1:D:116:GLU:HG3	1.97	0.63
1:A:36[B]:ILE:HB	1:A:197:VAL:HG12	1.81	0.63
1:D:49:ARG:NH1	3:D:1222:IOD:I	3.00	0.63
1:D:135:ASN:H	1:D:135:ASN:ND2	1.95	0.63
1:A:201:PRO:HD3	5:A:1433:HOH:O	1.98	0.63
1:B:88:PHE:O	1:B:91:TRP:HD1	1.82	0.63
1:D:330:HIS:NE2	5:D:1519:HOH:O	2.30	0.63
1:A:164:LEU:HB2	1:A:196[B]:VAL:HG13	1.80	0.63
1:D:94:TYR:HB3	3:D:1208:IOD:I	2.69	0.62
1:B:52:ALA:HB1	1:B:86:MET:HE2	1.81	0.62
1:A:3[B]:ARG:HG2	1:A:5:ILE:HD11	1.81	0.62
1:D:204:ILE:HG22	1:D:205:PHE:N	2.13	0.62
1:A:247:LEU:HB3	1:A:258:ILE:HD13	1.81	0.62
1:D:298:LYS:NZ	1:D:298:LYS:CB	2.62	0.62
1:A:95:PRO:HD2	3:A:1232:IOD:I	2.69	0.62
1:A:247:LEU:HB3	1:A:258:ILE:CD1	2.29	0.61
1:A:285:LYS:CE	1:A:336:GLU:OE1	2.49	0.61
1:A:5:ILE:HD12	1:A:5:ILE:N	2.15	0.61
1:B:109:ASN:O	1:B:110:MET:HE2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36[A]:ILE:HB	1:A:197:VAL:HG12	1.81	0.61
1:B:89[B]:GLN:HG3	1:B:165:ASP:O	2.01	0.60
1:A:36[B]:ILE:HD11	1:A:47:PHE:CE2	2.37	0.60
1:D:3:ARG:NH1	1:D:29:GLU:OE2	2.34	0.60
1:B:74:LYS:HE3	5:B:1327:HOH:O	2.01	0.60
1:A:221:GLN:HE22	1:A:233:VAL:H	1.47	0.60
1:B:319:ASP:O	1:B:320:SER:O	2.19	0.60
1:B:241:ILE:HG13	1:B:241:ILE:O	2.02	0.60
1:B:88:PHE:O	1:B:91:TRP:CD1	2.56	0.59
1:D:26:ILE:HD11	1:D:34:PHE:CZ	2.38	0.59
1:B:194:LEU:HD23	1:B:194:LEU:C	2.23	0.59
1:B:122:GLU:O	1:B:126[B]:LYS:HG3	2.02	0.59
1:D:164:LEU:HB2	1:D:196[B]:VAL:HG22	1.83	0.58
1:A:108:THR:CG2	5:A:1510:HOH:O	2.52	0.58
1:D:137:PHE:HB2	1:D:140:GLU:OE2	2.04	0.58
1:A:48[B]:MET:SD	1:A:197:VAL:HG22	2.43	0.58
1:D:294:ILE:HD12	1:D:344:LYS:CB	2.33	0.58
1:A:344:LYS:NZ	1:A:345:ASP:OD2	2.37	0.58
1:A:269:SER:HB3	1:A:353:ASN:HD22	1.69	0.58
1:D:30:ASN:HD22	1:D:30:ASN:H	1.51	0.57
1:D:139:ARG:HG2	1:D:139:ARG:NH1	2.19	0.57
1:A:120[B]:ARG:HG2	1:A:120[B]:ARG:NH1	2.18	0.57
1:D:30:ASN:ND2	1:D:30:ASN:H	2.03	0.57
1:B:136:HIS:HB2	1:B:141:LEU:HD21	1.86	0.57
1:A:290:ASP:OD2	1:A:292:SER:OG	2.20	0.57
1:D:345:ASP:HB3	5:D:1550:HOH:O	2.04	0.57
1:B:122:GLU:O	1:B:126[A]:LYS:HG3	2.04	0.57
1:B:251:VAL:HG21	1:B:267:VAL:HG12	1.87	0.56
1:B:194:LEU:HD21	1:B:196[B]:VAL:HG21	1.78	0.56
1:A:89:GLN:CG	1:A:166:GLU:HB2	2.35	0.56
1:D:3:ARG:HH11	1:D:29:GLU:CD	2.08	0.56
1:B:93:LEU:O	1:B:94:TYR:C	2.44	0.56
1:B:265:VAL:HB	1:B:349:VAL:HG21	1.87	0.56
1:B:306:TYR:O	1:B:307:GLN:HG3	2.06	0.56
1:A:105:PHE:O	1:A:108:THR:HG23	2.06	0.56
1:D:6:VAL:HB	1:D:26:ILE:HG22	1.87	0.56
1:B:306:TYR:C	1:B:307:GLN:HG3	2.26	0.56
1:B:269:SER:OG	1:B:271:ARG:O	2.22	0.55
1:D:8:ASN:HD22	1:D:23:ASN:HD21	1.54	0.55
1:B:48:MET:SD	1:B:197:VAL:HG13	2.46	0.55
1:A:48[B]:MET:SD	1:A:197:VAL:CG2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:CE	1:D:216:LYS:HA	2.37	0.55
1:D:261:LEU:HD22	1:D:317:PRO:HG3	1.88	0.55
1:B:110:MET:CA	1:B:110:MET:CE	2.84	0.55
1:B:247:LEU:HB3	1:B:258:ILE:HD13	1.89	0.55
1:B:182:LEU:O	1:B:186:VAL:HG23	2.06	0.55
1:B:205:PHE:CE1	1:B:241:ILE:HD11	2.42	0.55
1:D:72:ASN:ND2	5:D:1517:HOH:O	2.40	0.55
1:A:247:LEU:HD12	1:A:322:GLU:HB3	1.89	0.55
1:A:285:LYS:NZ	1:A:336:GLU:OE1	2.39	0.55
1:A:221:GLN:NE2	1:A:233:VAL:H	2.04	0.55
1:B:93:LEU:HD23	1:B:138:PRO:HG3	1.87	0.55
1:A:3[A]:ARG:HG2	1:A:5:ILE:HD11	1.89	0.54
1:D:164:LEU:HB2	1:D:196[B]:VAL:HG23	1.88	0.54
1:A:211:VAL:HG13	1:A:228:LEU:HD11	1.90	0.54
1:A:48[B]:MET:CE	1:A:195[B]:LEU:HG	2.37	0.54
1:D:14[B]:LYS:HE2	5:D:1364:HOH:O	2.07	0.54
1:A:76:ILE:HD12	1:A:76:ILE:N	2.23	0.54
1:D:216:LYS:HA	1:D:216:LYS:HE2	1.90	0.53
1:A:252:THR:HG22	1:A:254:GLU:N	2.22	0.53
1:D:180:ARG:HD3	1:D:206:ALA:CB	2.39	0.53
1:B:175:MET:CE	5:B:1401:HOH:O	2.46	0.53
1:D:120:ARG:HD3	5:D:1465:HOH:O	2.09	0.53
1:B:89[A]:GLN:HG2	1:B:166:GLU:HB2	1.92	0.52
1:B:89[B]:GLN:NE2	5:B:1375:HOH:O	2.35	0.52
1:D:211:VAL:CG1	1:D:228:LEU:CD1	2.86	0.52
1:A:118[A]:ARG:NH1	1:A:122:GLU:CD	2.63	0.52
1:D:211:VAL:CG1	1:D:228:LEU:HD12	2.39	0.52
1:D:139:ARG:NH1	5:D:1265:HOH:O	2.42	0.52
1:A:70:ALA:CA	1:A:76:ILE:CD1	2.75	0.52
1:B:8:ASN:HA	5:B:1457:HOH:O	2.10	0.52
1:B:211:VAL:HG11	1:B:228:LEU:CD1	2.28	0.51
1:B:165:ASP:HA	1:B:197:VAL:HG22	1.92	0.51
1:D:3:ARG:HG2	1:D:30:ASN:HD22	1.75	0.51
1:A:303:VAL:HG23	3:A:1227:IOD:I	2.81	0.51
1:B:109:ASN:O	1:B:110:MET:HE3	2.11	0.51
1:B:52:ALA:HB1	1:B:86:MET:HE1	1.91	0.51
1:D:41:GLY:H	4:D:1106:ANP:HNB1	1.57	0.51
1:B:12[B]:VAL:HG11	1:B:16:GLY:CA	2.31	0.51
1:B:36:ILE:HB	1:B:197:VAL:HG12	1.93	0.51
1:A:7[B]:LYS:HB3	1:A:7[B]:LYS:HZ2	1.73	0.51
1:D:8:ASN:ND2	1:D:23:ASN:HD21	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ILE:HG13	1:D:241:ILE:O	2.10	0.51
1:A:108:THR:HG22	5:A:1510:HOH:O	2.11	0.50
1:D:247:LEU:HD21	1:D:323:GLU:O	2.12	0.50
1:A:108:THR:HG21	5:A:1510:HOH:O	2.11	0.50
1:A:9:VAL:HG13	1:A:57:PRO:HB3	1.94	0.50
1:D:140:GLU:CG	5:D:1422:HOH:O	2.37	0.49
1:D:298:LYS:HG2	5:D:1375:HOH:O	2.11	0.49
1:B:205:PHE:HE1	1:B:241:ILE:HD11	1.78	0.49
3:B:1221:IOD:I	5:B:1341:HOH:O	2.90	0.49
1:A:224:LYS:HE2	1:A:227:ASP:OD1	2.12	0.49
1:B:48:MET:CG	1:B:197:VAL:HG11	2.42	0.49
1:D:352:LYS:CG	1:D:353:ASN:N	2.32	0.49
1:A:252:THR:HG23	1:A:254:GLU:H	1.73	0.49
1:B:170:ASN:O	1:B:171:LEU:O	2.30	0.49
1:D:105:PHE:HB3	1:D:106:PRO:HD3	1.95	0.49
1:A:48[B]:MET:HE1	1:A:195[B]:LEU:HG	1.94	0.48
1:A:252:THR:HG23	1:A:253:ASN:N	2.28	0.48
1:D:130:ILE:HD12	1:D:149:VAL:HG22	1.95	0.48
1:B:288:ILE:HG22	1:B:290:ASP:H	1.78	0.48
1:D:267:VAL:HG21	1:D:272:ALA:HB2	1.93	0.48
1:B:109:ASN:C	1:B:110:MET:HE3	2.34	0.48
1:D:243:GLU:OE2	5:D:1300:HOH:O	2.20	0.48
1:B:80:GLU:HG3	1:B:80:GLU:H	1.35	0.48
1:D:78:PRO:HB2	1:D:80:GLU:OE1	2.13	0.48
1:B:5[A]:ILE:HB	1:B:63:TYR:HB2	1.96	0.48
1:A:41:GLY:H	4:A:1104:ANP:HNB1	1.61	0.48
1:B:5[B]:ILE:HB	1:B:63:TYR:HB2	1.96	0.48
1:B:127:ILE:HD13	5:B:1442:HOH:O	2.15	0.47
1:A:252:THR:HB	1:A:255:GLY:O	2.15	0.47
1:D:79:PRO:HD2	1:D:80:GLU:OE1	2.14	0.47
3:B:1223:IOD:I	5:B:1295:HOH:O	2.91	0.47
1:B:41:GLY:H	4:B:1105:ANP:HNB1	1.61	0.47
1:A:300:LYS:HE3	1:A:335:GLY:HA2	1.95	0.47
1:D:5:ILE:HG23	1:D:27:ASN:OD1	2.14	0.47
1:D:307:GLN:NE2	1:D:312:ARG:HD2	2.30	0.46
1:B:128:LEU:HD12	1:B:152:ALA:HB2	1.97	0.46
1:A:124[A]:VAL:CG1	1:A:152:ALA:HB1	2.45	0.46
1:B:194:LEU:CD2	1:B:196[B]:VAL:HG22	2.30	0.46
1:D:263:PHE:HA	1:D:264:PRO:HD3	1.73	0.46
1:A:3[B]:ARG:NE	5:A:1424:HOH:O	2.26	0.46
1:D:8:ASN:HB3	5:D:1513:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12[B]:VAL:CG1	1:B:16:GLY:CA	2.91	0.45
1:B:303:VAL:HG22	1:B:304:ILE:N	2.31	0.45
1:A:285:LYS:HE2	1:A:336:GLU:OE1	2.17	0.45
1:D:8:ASN:ND2	5:D:1354:HOH:O	2.49	0.45
1:D:3:ARG:CG	1:D:30:ASN:HD22	2.30	0.45
1:B:290:ASP:OD1	1:B:292:SER:N	2.40	0.45
1:D:352:LYS:HE2	1:D:353:ASN:O	2.17	0.45
1:A:304:ILE:HD11	1:A:311:PHE:CD2	2.53	0.44
1:D:307:GLN:HE22	1:D:312:ARG:HD2	1.83	0.44
1:A:303:VAL:HG22	1:A:304:ILE:N	2.33	0.44
1:A:269:SER:HB2	1:A:353:ASN:HD22	1.82	0.44
1:B:48:MET:SD	1:B:197:VAL:CG1	3.05	0.44
1:A:151[B]:LEU:HD13	3:A:1206:IOD:I	2.87	0.44
1:D:211:VAL:HG11	1:D:228:LEU:HD12	2.00	0.44
1:D:252:THR:O	1:D:252:THR:OG1	2.29	0.43
1:D:3:ARG:CD	1:D:30:ASN:HD22	2.31	0.43
1:D:5:ILE:HG22	1:D:7[B]:LYS:HG3	1.99	0.43
1:D:298:LYS:HB3	1:D:298:LYS:NZ	2.32	0.43
1:D:53:GLY:O	1:D:79:PRO:HG3	2.19	0.43
1:D:26:ILE:HG13	1:D:27:ASN:N	2.34	0.43
1:D:216:LYS:CA	1:D:216:LYS:HE2	2.48	0.43
1:A:83:LYS:HB2	3:A:1217:IOD:I	2.89	0.43
1:A:246:GLU:O	1:A:247:LEU:HD13	2.19	0.43
1:A:211:VAL:HG13	1:A:228:LEU:CD1	2.48	0.43
1:A:70:ALA:C	1:A:76:ILE:HD13	2.39	0.43
1:D:345:ASP:OD2	1:D:345:ASP:N	2.51	0.43
1:B:137:PHE:O	1:B:140:GLU:N	2.52	0.43
1:A:276:ILE:O	1:A:276:ILE:HG23	2.19	0.42
1:A:204:ILE:N	1:A:204:ILE:HD12	2.34	0.42
1:B:47:PHE:HE2	1:B:195:LEU:HD11	1.84	0.42
1:D:14[A]:LYS:HD3	5:D:1328:HOH:O	2.18	0.42
1:D:276:ILE:O	1:D:276:ILE:HG23	2.19	0.42
1:D:290:ASP:OD1	1:D:292:SER:OG	2.36	0.42
1:D:271:ARG:HB3	1:D:352:LYS:HB3	2.02	0.42
1:D:95:PRO:HD2	3:D:1208:IOD:I	2.90	0.42
1:B:127:ILE:CG2	5:B:1290:HOH:O	2.57	0.42
1:A:298:LYS:NZ	5:A:1459:HOH:O	2.51	0.42
1:A:269:SER:OG	1:A:271:ARG:O	2.27	0.42
1:B:138:PRO:HA	1:B:141:LEU:HD12	2.02	0.42
1:B:10:SER:HB2	1:B:59:THR:OG1	2.20	0.42
1:B:87:VAL:HB	1:B:164:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:VAL:HG22	1:B:340:VAL:O	2.20	0.42
1:D:301:VAL:HA	1:D:315:ILE:HG22	2.00	0.42
1:A:10:SER:HB2	1:A:59:THR:OG1	2.20	0.42
1:B:330:HIS:HA	1:B:331:PRO:HD3	1.92	0.42
1:A:252:THR:CG2	1:A:253:ASN:N	2.81	0.42
1:D:89:GLN:HB2	5:D:1426:HOH:O	2.20	0.42
1:A:36[B]:ILE:CD1	1:A:47:PHE:CE2	3.02	0.41
1:A:70:ALA:N	1:A:76:ILE:HD13	2.34	0.41
1:D:8:ASN:HD22	1:D:23:ASN:ND2	2.18	0.41
1:D:165:ASP:HA	1:D:197:VAL:HG22	2.01	0.41
1:D:126:LYS:HD2	5:D:1401:HOH:O	2.20	0.41
1:A:3[B]:ARG:HH11	1:A:29:GLU:CD	2.22	0.41
1:D:164:LEU:HB2	1:D:196[A]:VAL:HG23	2.01	0.41
1:A:94:TYR:HA	1:A:95:PRO:HD3	1.88	0.41
1:A:181:ALA:O	1:A:185[A]:GLU:HG3	2.21	0.41
1:D:313:ILE:O	1:D:325:PHE:HA	2.21	0.41
1:A:221:GLN:HE22	1:A:233:VAL:N	2.17	0.41
1:B:139:ARG:CG	1:B:140:GLU:N	2.84	0.41
1:D:267:VAL:HG22	1:D:272:ALA:HB2	2.00	0.41
1:D:168:PHE:HE1	1:D:207:ILE:CD1	2.34	0.41
1:D:298:LYS:CB	1:D:298:LYS:HZ2	2.20	0.41
1:D:59:THR:HA	1:D:72:ASN:HD22	1.85	0.41
1:B:142:SER:O	1:B:143:GLY:C	2.59	0.41
1:B:89[A]:GLN:CG	1:B:166:GLU:HB2	2.51	0.40
1:B:93:LEU:HD23	1:B:138:PRO:HB3	2.03	0.40
1:D:247:LEU:HD11	1:D:324:ILE:HD11	2.03	0.40
1:A:128:LEU:O	1:A:148:ARG:HD3	2.21	0.40
1:B:328:SER:HB2	3:B:1211:IOD:I	2.91	0.40
1:D:83:LYS:CE	5:D:1534:HOH:O	2.62	0.40
1:B:94:TYR:HA	1:B:95:PRO:HD3	1.75	0.40
1:B:39:PRO:HG3	1:B:240:LEU:HD21	2.02	0.40
1:A:48[B]:MET:HE1	1:A:197:VAL:HG13	2.03	0.40
1:B:247:LEU:HD11	1:B:323:GLU:O	2.22	0.40
1:A:200:ASP:HA	1:A:201:PRO:HD2	1.94	0.40
1:B:271:ARG:HB2	1:B:352:LYS:HB3	2.03	0.40
1:A:26:ILE:CD1	3:A:1202:IOD:I	3.27	0.40
1:A:5:ILE:CD1	1:A:5:ILE:N	2.83	0.40
1:A:166:GLU:N	1:A:167:PRO:HD3	2.36	0.40
1:D:96:ASN:C	1:D:96:ASN:OD1	2.53	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1228:IOD:I	5:A:1497:HOH:O[1_455]	1.01	1.19
1:B:7:LYS:NZ	1:D:96:ASN:OD1[1_565]	1.86	0.34
1:B:8:ASN:ND2	1:D:96:ASN:ND2[1_565]	1.93	0.27
5:A:1446:HOH:O	5:A:1497:HOH:O[1_455]	2.02	0.18
1:A:282[B]:LYS:NZ	5:A:1492:HOH:O[1_455]	2.09	0.11
5:A:1383:HOH:O	5:D:1310:HOH:O[4_456]	2.17	0.03

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	368/353 (104%)	358 (97%)	8 (2%)	2 (0%)	34	21
1	B	362/353 (102%)	346 (96%)	10 (3%)	6 (2%)	11	3
1	D	359/353 (102%)	350 (98%)	6 (2%)	3 (1%)	24	11
All	All	1089/1059 (103%)	1054 (97%)	24 (2%)	11 (1%)	19	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	LEU
1	B	320	SER
1	D	253	ASN
1	A	173	ALA
1	B	169	SER
1	D	173	ALA
1	A	267	VAL
1	B	91	TRP
1	B	172	ASP
1	B	93	LEU
1	D	268	SER

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	296/307 (96%)	283 (96%)	13 (4%)	35	19
1	B	288/307 (94%)	281 (98%)	7 (2%)	57	47
1	D	290/307 (94%)	283 (98%)	7 (2%)	57	47
All	All	874/921 (95%)	847 (97%)	27 (3%)	50	34

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	124[A]	VAL
1	A	124[B]	VAL
1	A	136	HIS
1	A	186[A]	VAL
1	A	186[B]	VAL
1	A	196[A]	VAL
1	A	196[B]	VAL
1	A	252	THR
1	A	267	VAL
1	A	268	SER
1	A	286	ASP
1	A	304	ILE
1	B	30	ASN
1	B	80	GLU
1	B	195	LEU
1	B	204	ILE
1	B	243	GLU
1	B	307	GLN
1	B	323	GLU
1	D	30	ASN
1	D	135	ASN
1	D	140	GLU
1	D	195	LEU
1	D	261	LEU
1	D	271	ARG

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Mol	Chain	Res	Type
1	D	298	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	199	HIS
1	A	221	GLN
1	A	353	ASN
1	B	136	HIS
1	B	307	GLN
1	B	353	ASN
1	D	8	ASN
1	D	23	ASN
1	D	30	ASN
1	D	72	ASN
1	D	96	ASN
1	D	135	ASN
1	D	146	GLN
1	D	199	HIS
1	D	307	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)

Of 44 ligands modelled in this entry, 41 are monoatomic - leaving 3 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	$\#|Z| > 2$
4	ANP	A	1104	2	27,33,33	1.64	6 (22%)	30,52,52	2.11	7 (23%)
4	ANP	B	1105	2	27,33,33	1.74	6 (22%)	30,52,52	2.00	4 (13%)
4	ANP	D	1106	2	27,33,33	1.65	7 (25%)	30,52,52	2.08	6 (20%)

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
4	ANP	A	1104	2	-	0/12/38/38	0/3/3/3
4	ANP	B	1105	2	-	0/12/38/38	0/3/3/3
4	ANP	D	1106	2	-	1/12/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1105	ANP	PB-O3A	-4.86	1.53	1.59
4	D	1106	ANP	PB-O3A	-3.79	1.54	1.59
4	A	1104	ANP	PG-O3G	-3.09	1.48	1.56
4	A	1104	ANP	PB-O2B	-2.77	1.49	1.56
4	D	1106	ANP	PG-O3G	-2.57	1.49	1.56
4	B	1105	ANP	PG-O3G	-2.39	1.50	1.56
4	A	1104	ANP	PB-O3A	-2.20	1.56	1.59
4	D	1106	ANP	PB-O2B	-2.18	1.50	1.56
4	A	1104	ANP	PG-O2G	-2.16	1.50	1.56
4	D	1106	ANP	PG-O2G	-2.10	1.50	1.56
4	B	1105	ANP	PG-O2G	-2.05	1.51	1.56
4	D	1106	ANP	PB-O1B	2.04	1.48	1.46
4	B	1105	ANP	PB-O1B	2.15	1.48	1.46
4	B	1105	ANP	C5-C4	2.74	1.46	1.40
4	A	1104	ANP	C5-C4	2.74	1.46	1.40
4	D	1106	ANP	C5-C4	2.79	1.46	1.40
4	B	1105	ANP	PG-O1G	3.34	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1106	ANP	PG-O1G	3.35	1.49	1.46
4	A	1104	ANP	PG-O1G	3.41	1.50	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1104	ANP	N3-C2-N1	-8.62	122.29	128.89
4	D	1106	ANP	N3-C2-N1	-8.03	122.74	128.89
4	B	1105	ANP	N3-C2-N1	-7.53	123.12	128.89
4	B	1105	ANP	C4-C5-N7	-3.08	106.65	109.48
4	A	1104	ANP	C1'-N9-C4	-2.45	123.24	126.94
4	D	1106	ANP	C4-C5-N7	-2.35	107.32	109.48
4	D	1106	ANP	C1'-N9-C4	-2.20	123.61	126.94
4	A	1104	ANP	C4-C5-N7	-2.17	107.48	109.48
4	D	1106	ANP	O2A-PA-O3A	2.12	114.71	105.09
4	A	1104	ANP	O3A-PA-O5'	2.13	108.60	102.94
4	D	1106	ANP	C2-N1-C6	2.14	122.60	118.77
4	A	1104	ANP	C2-N1-C6	2.35	122.96	118.77
4	A	1104	ANP	O2A-PA-O3A	2.44	116.16	105.09
4	B	1105	ANP	O3A-PA-O5'	2.56	109.73	102.94
4	A	1104	ANP	C4'-O4'-C1'	3.20	113.23	109.72
4	B	1105	ANP	C4'-O4'-C1'	3.72	113.80	109.72
4	D	1106	ANP	C4'-O4'-C1'	4.20	114.33	109.72

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1106	ANP	O1B-PB-N3B-PG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1104	ANP	1	0
4	B	1105	ANP	1	0
4	D	1106	ANP	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(Å^2)	Q<0.9
1	A	353/353 (100%)	0.38	27 (7%)	17	26	10, 20, 36, 71	0
1	B	353/353 (100%)	0.56	41 (11%)	6	10	8, 19, 38, 56	0
1	D	353/353 (100%)	0.35	22 (6%)	24	34	7, 20, 37, 76	0
All	All	1059/1059 (100%)	0.43	90 (8%)	13	21	7, 20, 37, 76	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170	ASN	6.6
1	B	173	ALA	6.5
1	A	170	ASN	5.8
1	D	353	ASN	5.7
1	B	253	ASN	5.6
1	D	267	VAL	5.2
1	B	92	ALA	5.1
1	B	254	GLU	4.6
1	A	353	ASN	4.3
1	D	171	LEU	4.2
1	B	171	LEU	4.0
1	B	320	SER	4.0
1	B	95	PRO	3.9
1	B	176	ARG	3.8
1	A	267	VAL	3.8
1	B	353	ASN	3.7
1	A	171	LEU	3.7
1	A	169	SER	3.7
1	D	175[A]	MET	3.7
1	B	93	LEU	3.6
1	A	90	THR	3.5
1	D	268	SER	3.5
1	D	173	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	143	GLY	3.4
1	B	169	SER	3.4
1	A	175	MET	3.4
1	B	252	THR	3.4
1	D	103	ILE	3.4
1	A	199	HIS	3.4
1	D	308	GLY	3.3
1	D	90	THR	3.3
1	B	94	TYR	3.3
1	B	268	SER	3.2
1	B	90	THR	3.2
1	A	108	THR	3.2
1	A	321	GLU	3.2
1	D	319	ASP	3.1
1	A	253	ASN	3.0
1	A	37	LEU	3.0
1	A	103	ILE	3.0
1	B	319	ASP	3.0
1	A	270	ASP	3.0
1	B	267	VAL	3.0
1	A	319	ASP	2.9
1	D	252	THR	2.7
1	A	89	GLN	2.7
1	B	307	GLN	2.7
1	D	254	GLU	2.7
1	B	196[A]	VAL	2.7
1	D	271	ARG	2.7
1	D	321	GLU	2.6
1	B	204	ILE	2.6
1	B	91	TRP	2.6
1	B	255	GLY	2.6
1	D	174	ARG	2.6
1	B	89[A]	GLN	2.6
1	B	256	VAL	2.6
1	B	144	GLY	2.6
1	B	170	ASN	2.5
1	D	344	LYS	2.5
1	B	352	LYS	2.5
1	D	96	ASN	2.4
1	B	174	ARG	2.4
1	B	172	ASP	2.4
1	A	91	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	308	GLY	2.3
1	A	273	ILE	2.3
1	B	103	ILE	2.3
1	B	199	HIS	2.3
1	A	88	PHE	2.3
1	B	288	ILE	2.2
1	A	255	GLY	2.2
1	A	151[A]	LEU	2.2
1	A	204	ILE	2.2
1	B	263	PHE	2.2
1	B	318	LEU	2.1
1	D	269	SER	2.1
1	B	175	MET	2.1
1	B	274	ILE	2.1
1	D	169	SER	2.1
1	D	204	ILE	2.1
1	D	307	GLN	2.1
1	A	69	VAL	2.1
1	A	268	SER	2.1
1	B	138	PRO	2.1
1	B	205	PHE	2.0
1	B	37	LEU	2.0
1	A	308	GLY	2.0
1	A	344	LYS	2.0
1	A	36[A]	ILE	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
3	IOD	D	1233	1/1	0.97	0.17	-0.13	60,60,60,60	1
4	ANP	B	1105	31/31	0.98	0.10	-0.20	24,34,45,48	0
3	IOD	B	1236	1/1	0.99	0.14	-0.48	58,58,58,58	1
4	ANP	A	1104	31/31	0.99	0.08	-0.67	18,26,38,38	0
3	IOD	B	1235	1/1	0.97	0.10	-0.85	60,60,60,60	1
4	ANP	D	1106	31/31	0.98	0.07	-1.25	18,26,35,38	0
2	MG	B	1103	1/1	0.98	0.03	-1.52	33,33,33,33	0
3	IOD	B	1220	1/1	0.91	0.08	-1.54	42,42,42,42	1
3	IOD	A	1237	1/1	0.92	0.08	-1.62	50,50,50,50	1
3	IOD	B	1223	1/1	0.93	0.06	-1.67	45,45,45,45	1
3	IOD	B	1211	1/1	0.99	0.08	-1.97	28,28,28,28	1
3	IOD	A	1206	1/1	0.98	0.05	-2.33	41,41,41,41	1
3	IOD	D	1203	1/1	0.99	0.04	-2.55	34,34,34,34	1
3	IOD	A	1217	1/1	0.97	0.04	-2.66	37,37,37,37	1
3	IOD	A	1201	1/1	0.99	0.03	-2.95	31,31,31,31	1
3	IOD	B	1224	1/1	0.97	0.05	-3.03	43,43,43,43	1
3	IOD	A	1216	1/1	0.99	0.03	-3.06	35,35,35,35	1
3	IOD	B	1221	1/1	0.98	0.06	-3.39	50,50,50,50	1
3	IOD	D	1234	1/1	0.86	0.07	-3.86	57,57,57,57	1
3	IOD	D	1204	1/1	0.99	0.06	-4.18	36,36,36,36	1
3	IOD	D	1215	1/1	0.99	0.03	-5.18	29,29,29,29	1
3	IOD	B	1210	1/1	0.98	0.03	-5.86	48,48,48,48	1
3	IOD	D	1209	1/1	0.93	0.06	-	46,46,46,46	1
3	IOD	D	1205	1/1	0.99	0.05	-	42,42,42,42	1
3	IOD	A	1231	1/1	1.00	0.02	-	42,42,42,42	1
3	IOD	B	1226	1/1	0.89	0.17	-	67,67,67,67	1
3	IOD	D	1222	1/1	0.96	0.07	-	54,54,54,54	1
3	IOD	A	1227	1/1	0.98	0.10	-	48,48,48,48	1
3	IOD	D	1208	1/1	0.98	0.04	-	48,48,48,48	1
3	IOD	A	1219	1/1	0.96	0.10	-	34,34,34,34	1
2	MG	D	1101	1/1	0.98	0.07	-	25,25,25,25	0
3	IOD	A	1218	1/1	0.98	0.07	-	44,44,44,44	1
3	IOD	B	1207	1/1	0.98	0.04	-	33,33,33,33	1
3	IOD	A	1228	1/1	0.94	0.13	-	47,47,47,47	1
3	IOD	A	1232	1/1	0.93	0.13	-	46,46,46,46	1
2	MG	A	1102	1/1	0.98	0.04	-	25,25,25,25	0
3	IOD	D	1213	1/1	0.96	0.09	-	41,41,41,41	1
3	IOD	A	1238	1/1	0.93	0.10	-	57,57,57,57	1
3	IOD	A	1202	1/1	0.99	0.05	-	40,40,40,40	1
3	IOD	B	1212	1/1	0.98	0.13	-	36,36,36,36	1
3	IOD	D	1214	1/1	0.98	0.06	-	40,40,40,40	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	IOD	B	1225	1/1	0.95	0.10	-	61,61,61,61	1
3	IOD	A	1229	1/1	0.93	0.09	-	46,46,46,46	1
3	IOD	A	1230	1/1	0.97	0.06	-	42,42,42,42	1

6.5　Other polymers ⓘ

There are no such residues in this entry.