Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 12:38 PM EDT

PDB ID	:	1QVI
Title	:	Crystal structure of scallop myosin S1 in the pre-power stroke state to 2.6 Angstrom resolution: flexibility and function in the head
Authors	:	Gourinath, S.; Himmel, D.M.; Brown, J.H.; Reshetnikova, L.; Szent-Gyrgyi, A.G.; Cohen, C.
Deposited on	:	2003-08-27
Resolution	:	2.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

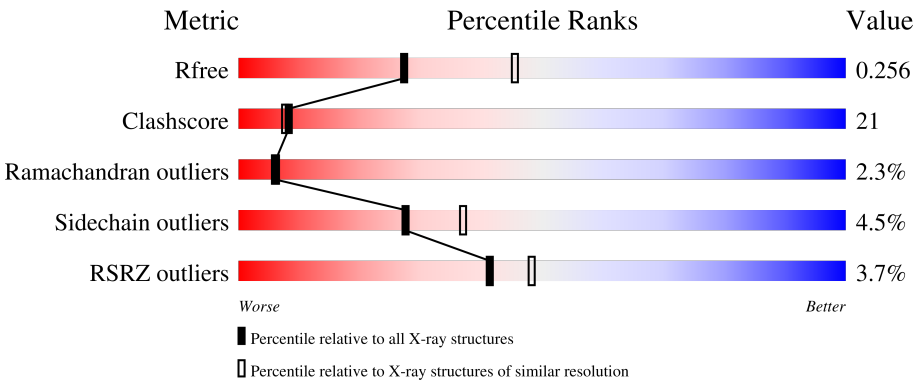
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	840	4% 59% 35%
2	Y	156	4% 49% 37% 10%
3	Z	156	% 58% 40%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8826 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 Myosin heavy chain, striated muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	806	6397	4073	1104	1182	38	0	0	0

- Molecule 2 is a protein called Myosin regulatory light chain, striated adductor muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Y	141	1117	706	179	223	9	0	0	0

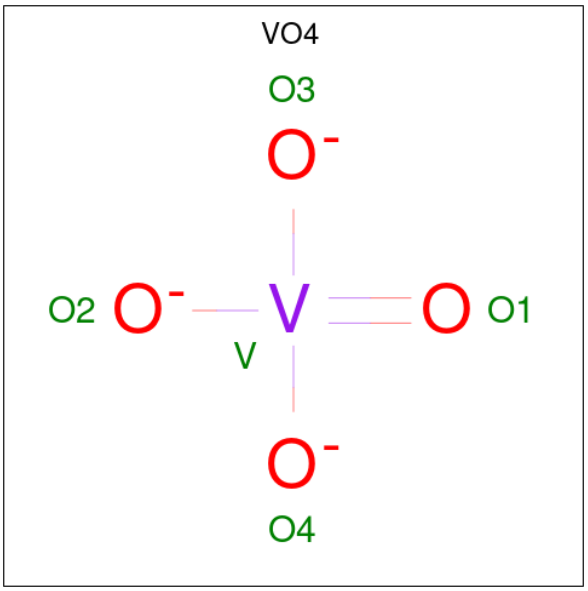
- Molecule 3 is a protein called Myosin essential light chain, striated adductor muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	Z	155	1225	776	195	247	7	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

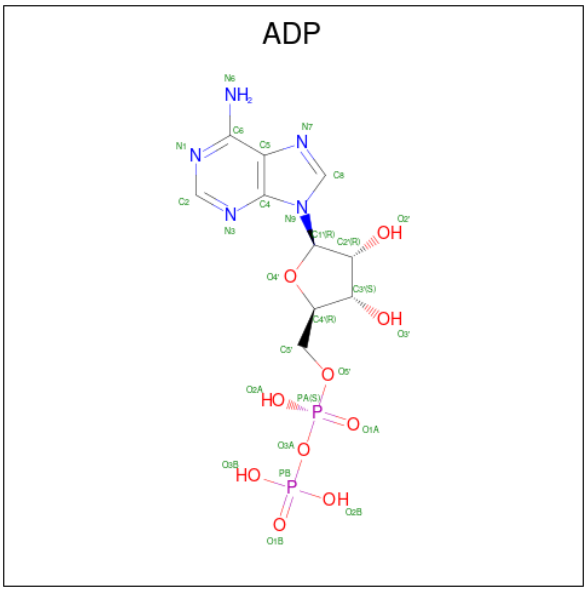
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	Y	1	1	1	0	0

- Molecule 5 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	V		
5	A	1	5	4	1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	Z	1	1	1	0	0

- Molecule 8 is water.

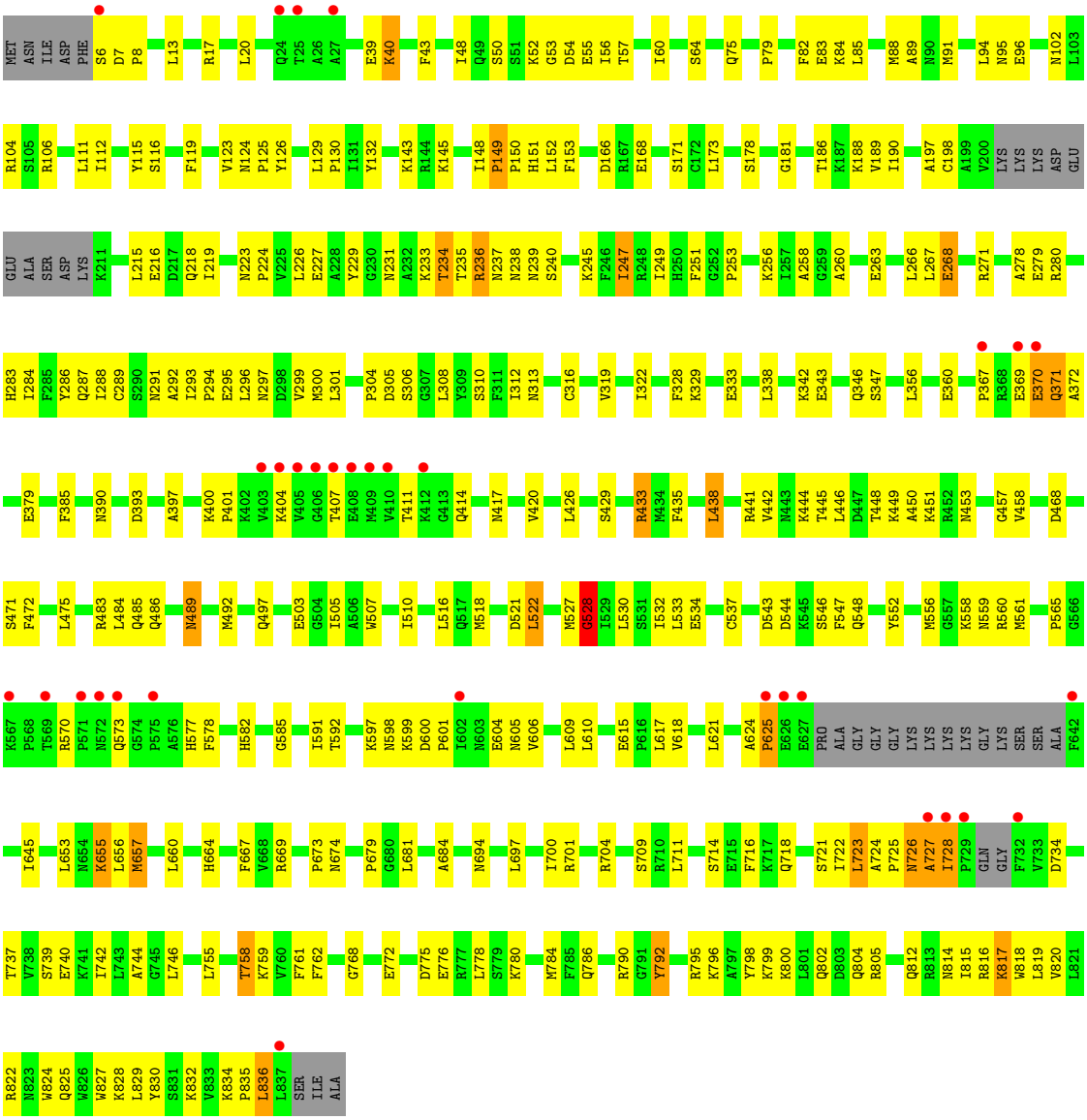
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	43	43	43	0	0
			Total	O		
8	Y	2	2	2	0	0
			Total	O		
8	Z	7	7	7	0	0

3 Residue-property plots (i)

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

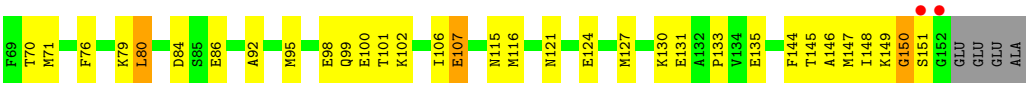
• Molecule 1: Myosin heavy chain, striated muscle

Chain A: 4% 59% 35%



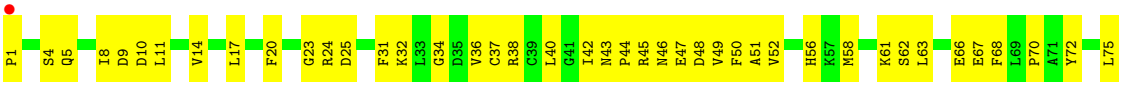
• Molecule 2: Myosin regulatory light chain, striated adductor muscle

Chain Y:



- Molecule 3: Myosin essential light chain, striated adductor muscle

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.38Å 285.62Å 59.83Å 90.00° 114.50° 90.00°	Depositor
Resolution (Å)	45.58 – 2.54 45.58 – 2.54	Depositor EDS
% Data completeness (in resolution range)	80.5 (45.58-2.54) 80.7 (45.58-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	5.59 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.266 0.203 , 0.256	Depositor DCC
R_{free} test set	2544 reflections (5.94%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8826	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, MG, VO4, 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	0.38	0/6525	0.61	2/8799 (0.0%)
2	Y	0.39	0/1134	0.64	1/1515 (0.1%)
3	Z	0.40	0/1250	0.60	0/1683
All	All	0.39	0/8909	0.61	3/11997 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	51	PRO	N-CA-C	-7.07	93.72	112.10
1	A	528	GLY	N-CA-C	6.94	130.45	113.10
1	A	625	PRO	N-CA-CB	5.50	109.90	103.30

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	6397	0	6342	266	0
2	Y	1117	0	1099	57	0
3	Z	1225	0	1154	60	0
4	A	1	0	0	0	0
4	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	1	0
6	A	27	0	12	1	0
7	Z	1	0	0	0	0
8	A	43	0	0	1	0
8	Y	2	0	0	0	0
8	Z	7	0	0	0	0
All	All	8826	0	8607	366	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 21.

All (366) 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)
2:Y:49:ARG:O	2:Y:51:PRO:HD3	1.55	1.06
1:A:486:GLN:HA	1:A:489:ASN:HD21	1.10	1.05
3:Z:31:PHE:HB3	3:Z:58:MET:HE2	1.42	1.02
1:A:48:ILE:HG23	1:A:56:ILE:HD11	1.42	0.98
1:A:497:GLN:HE21	1:A:507:TRP:HE1	1.00	0.97
1:A:836:LEU:HD23	1:A:836:LEU:H	1.30	0.96
1:A:722:ILE:HD11	3:Z:88:GLU:HB3	1.44	0.96
1:A:497:GLN:HE22	1:A:510:ILE:H	1.13	0.95
1:A:485:GLN:HE22	1:A:669:ARG:HH22	0.94	0.92
1:A:828:LYS:HA	1:A:828:LYS:HE2	1.51	0.90
1:A:94:LEU:HD11	1:A:704:ARG:HD3	1.56	0.88
1:A:486:GLN:HA	1:A:489:ASN:ND2	1.89	0.87
1:A:287:GLN:HB2	1:A:328:PHE:HB2	1.55	0.86
1:A:89:ALA:O	1:A:704:ARG:HD2	1.77	0.85
1:A:533:LEU:HD22	1:A:598:ASN:ND2	1.94	0.83
3:Z:36:VAL:HG11	3:Z:68:PHE:CZ	2.17	0.79
3:Z:32:LYS:HG2	3:Z:58:MET:HE1	1.65	0.79
2:Y:149:LYS:HE2	2:Y:149:LYS:HA	1.66	0.77
1:A:814:ASN:HD21	2:Y:84:ASP:H	1.29	0.77
1:A:39:GLU:HG3	1:A:40:LYS:H	1.49	0.77
1:A:577:HIS:ND1	1:A:591:ILE:HG13	2.00	0.77
1:A:310:SER:HA	1:A:313:ASN:OD1	1.86	0.75
1:A:817:LYS:O	1:A:820:VAL:HG12	1.87	0.75
3:Z:5:GLN:O	3:Z:8:ILE:HG22	1.86	0.75
1:A:75:GLN:OE1	1:A:95:ASN:HB2	1.87	0.74
1:A:85:LEU:H	1:A:102:ASN:HD21	1.34	0.74
1:A:486:GLN:CA	1:A:489:ASN:HD21	1.96	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:HG22	1:A:236:ARG:H	1.52	0.73
1:A:258:ALA:HB1	1:A:450:ALA:HB3	1.70	0.73
1:A:497:GLN:NE2	1:A:507:TRP:HE1	1.81	0.73
1:A:489:ASN:ND2	1:A:489:ASN:H	1.85	0.72
2:Y:15:LYS:HD2	2:Y:15:LYS:H	1.55	0.72
3:Z:42:ILE:HG22	3:Z:44:PRO:HD3	1.72	0.72
1:A:486:GLN:HA	1:A:486:GLN:HE21	1.55	0.72
1:A:796:LYS:HG2	3:Z:152:PRO:HB3	1.73	0.71
1:A:485:GLN:HE22	1:A:669:ARG:NH2	1.79	0.71
3:Z:126:ILE:HG23	3:Z:131:LEU:HB3	1.73	0.71
1:A:39:GLU:HG3	1:A:40:LYS:N	2.06	0.70
3:Z:11:LEU:HD13	3:Z:40:LEU:HD11	1.73	0.70
3:Z:111:THR:CG2	3:Z:122:VAL:HG21	2.22	0.70
1:A:291:ASN:HB2	1:A:304:PRO:HB3	1.75	0.69
2:Y:92:ALA:HA	2:Y:95:MET:HE3	1.72	0.69
3:Z:32:LYS:HG2	3:Z:58:MET:CE	2.23	0.69
2:Y:149:LYS:O	2:Y:151:SER:N	2.26	0.68
1:A:527:MET:HG3	1:A:528:GLY:N	2.07	0.68
3:Z:116:ARG:HH11	3:Z:116:ARG:HB2	1.58	0.68
1:A:301:LEU:HD11	1:A:385:PHE:HD2	1.59	0.68
1:A:369:GLU:O	1:A:369:GLU:HG3	1.93	0.68
1:A:598:ASN:O	1:A:645:ILE:HG13	1.92	0.68
3:Z:31:PHE:HB3	3:Z:58:MET:CE	2.23	0.67
1:A:219:ILE:HD11	1:A:260:ALA:HB3	1.77	0.67
1:A:50:SER:O	1:A:56:ILE:HD12	1.96	0.66
1:A:256:LYS:HE2	3:Z:95:ARG:HH22	1.61	0.66
1:A:417:ASN:HA	1:A:420:VAL:HG22	1.77	0.65
1:A:484:LEU:HD23	1:A:484:LEU:O	1.95	0.65
1:A:790:ARG:NH1	3:Z:117:LEU:HD23	2.11	0.65
1:A:369:GLU:O	1:A:371:GLN:N	2.28	0.65
1:A:426:LEU:HD11	1:A:610:LEU:HD11	1.78	0.65
1:A:830:TYR:O	1:A:834:LYS:HB2	1.96	0.65
1:A:497:GLN:HE22	1:A:510:ILE:N	1.92	0.65
1:A:50:SER:HB2	1:A:57:THR:HB	1.80	0.64
1:A:485:GLN:NE2	1:A:669:ARG:HH22	1.79	0.64
1:A:776:GLU:O	1:A:780:LYS:HG2	1.97	0.64
1:A:219:ILE:HD13	1:A:446:LEU:HD22	1.79	0.64
2:Y:36:SER:OG	2:Y:38:GLU:HG2	1.98	0.63
2:Y:99:GLN:CD	2:Y:99:GLN:H	2.00	0.63
2:Y:41:LYS:HG2	2:Y:45:GLU:OE2	1.99	0.63
3:Z:34:GLY:O	3:Z:38:ARG:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:CYS:HB3	1:A:216:GLU:HG2	1.81	0.63
1:A:271:ARG:HH12	1:A:279:GLU:CG	2.12	0.63
1:A:758:THR:HG22	1:A:759:LYS:HG2	1.81	0.62
1:A:360:GLU:HB2	1:A:379:GLU:HG2	1.80	0.62
1:A:296:LEU:HA	1:A:299:VAL:HG23	1.81	0.62
1:A:814:ASN:HD21	2:Y:84:ASP:N	1.98	0.62
3:Z:61:LYS:HE3	3:Z:63:LEU:HD21	1.82	0.61
1:A:740:GLU:OE1	1:A:755:LEU:HD11	2.00	0.61
1:A:674:ASN:ND2	1:A:681:LEU:HB3	2.15	0.61
1:A:836:LEU:H	1:A:836:LEU:CD2	2.10	0.61
1:A:617:LEU:HD23	1:A:621:LEU:HG	1.83	0.61
1:A:249:ILE:HD12	1:A:249:ILE:N	2.16	0.60
1:A:234:THR:HG22	1:A:236:ARG:N	2.17	0.60
1:A:429:SER:O	1:A:433:ARG:HB2	2.00	0.60
1:A:758:THR:HG22	1:A:759:LYS:CG	2.31	0.60
1:A:216:GLU:H	1:A:216:GLU:CD	2.05	0.60
1:A:280:ARG:HH21	1:A:283:HIS:HD1	1.50	0.60
1:A:796:LYS:O	1:A:796:LYS:HD3	2.02	0.60
2:Y:26:MET:O	2:Y:43:ILE:HD12	2.02	0.60
2:Y:86:GLU:HG3	2:Y:145:THR:HG22	1.84	0.60
1:A:190:ILE:CD1	1:A:247:ILE:HD13	2.32	0.59
1:A:556:MET:O	1:A:558:LYS:HG2	2.02	0.59
2:Y:37:LYS:HG3	2:Y:60:LEU:HD12	1.82	0.59
1:A:173:LEU:HD12	1:A:667:PHE:CE2	2.36	0.59
2:Y:41:LYS:O	2:Y:45:GLU:HG3	2.01	0.59
1:A:486:GLN:HA	1:A:486:GLN:NE2	2.17	0.59
1:A:404:LYS:HE2	1:A:604:GLU:OE1	2.03	0.59
1:A:301:LEU:HD11	1:A:385:PHE:CD2	2.38	0.59
1:A:489:ASN:ND2	1:A:489:ASN:N	2.49	0.58
2:Y:86:GLU:OE2	2:Y:146:ALA:HA	2.03	0.58
1:A:223:ASN:O	1:A:227:GLU:HG3	2.04	0.58
3:Z:1:PRO:HG3	3:Z:77:ASP:OD1	2.04	0.58
2:Y:15:LYS:HD2	2:Y:15:LYS:N	2.18	0.58
1:A:289:CYS:SG	1:A:356:LEU:HD21	2.43	0.57
2:Y:44:SER:OG	2:Y:51:PRO:HD2	2.03	0.57
1:A:223:ASN:HB2	1:A:224:PRO:HD3	1.86	0.57
1:A:390:ASN:HB3	1:A:393:ASP:HB2	1.87	0.57
1:A:342:LYS:O	1:A:346:GLN:HG3	2.05	0.57
2:Y:131:GLU:HG2	2:Y:131:GLU:O	2.05	0.56
1:A:229:TYR:CZ	1:A:284:ILE:HG12	2.40	0.56
1:A:799:LYS:HA	1:A:802:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:LYS:HE2	1:A:656:LEU:N	2.21	0.56
1:A:489:ASN:N	1:A:489:ASN:HD22	2.03	0.56
1:A:552:TYR:HD1	1:A:556:MET:HB2	1.71	0.56
1:A:234:THR:CG2	1:A:236:ARG:H	2.19	0.56
1:A:800:LYS:O	1:A:804:GLN:HG3	2.06	0.55
3:Z:14:VAL:HG12	3:Z:36:VAL:HG13	1.89	0.55
1:A:768:GLY:O	1:A:772:GLU:HG2	2.06	0.55
1:A:226:LEU:HD23	1:A:438:LEU:HD13	1.88	0.55
2:Y:76:PHE:O	2:Y:80:LEU:HB3	2.07	0.55
3:Z:11:LEU:CD1	3:Z:40:LEU:HD11	2.36	0.55
1:A:288:ILE:HG13	1:A:300:MET:SD	2.47	0.55
3:Z:31:PHE:HD2	3:Z:58:MET:HG2	1.70	0.55
3:Z:11:LEU:HD11	3:Z:68:PHE:CE2	2.42	0.55
1:A:88:MET:CE	1:A:116:SER:HB3	2.37	0.55
1:A:527:MET:HG3	1:A:528:GLY:H	1.70	0.55
1:A:186:THR:HG23	1:A:458:VAL:HG11	1.89	0.55
1:A:52:LYS:O	1:A:54:ASP:N	2.40	0.54
1:A:190:ILE:HD13	1:A:247:ILE:HD13	1.89	0.54
1:A:152:LEU:HD21	1:A:189:VAL:HG23	1.88	0.54
1:A:372:ALA:HB3	1:A:414:GLN:O	2.08	0.54
1:A:497:GLN:NE2	1:A:510:ILE:H	1.94	0.54
3:Z:111:THR:HG23	3:Z:122:VAL:HG21	1.89	0.54
1:A:278:ALA:HA	1:A:316:CYS:SG	2.47	0.54
1:A:556:MET:C	1:A:558:LYS:H	2.11	0.54
1:A:268:GLU:OE1	1:A:271:ARG:NE	2.33	0.54
1:A:215:LEU:HD22	1:A:448:THR:HG21	1.90	0.54
1:A:828:LYS:HA	1:A:828:LYS:CE	2.30	0.53
3:Z:40:LEU:HD12	3:Z:72:TYR:CE1	2.42	0.53
1:A:784:MET:SD	3:Z:79:GLU:HG2	2.48	0.53
1:A:106:ARG:HB3	1:A:111:LEU:HB2	1.89	0.53
1:A:237:ASN:HB3	1:A:240:SER:HB2	1.91	0.53
1:A:724:ALA:HB1	1:A:726:ASN:ND2	2.23	0.53
2:Y:92:ALA:HA	2:Y:95:MET:CE	2.36	0.53
1:A:834:LYS:HB3	1:A:835:PRO:HD3	1.91	0.53
1:A:544:ASP:OD2	1:A:592:THR:HA	2.08	0.53
1:A:617:LEU:CD2	1:A:621:LEU:HG	2.39	0.53
2:Y:38:GLU:HG3	2:Y:39:ASP:N	2.23	0.53
1:A:288:ILE:HG13	1:A:300:MET:CE	2.38	0.52
2:Y:15:LYS:H	2:Y:15:LYS:CD	2.21	0.52
3:Z:31:PHE:CD2	3:Z:58:MET:HG2	2.44	0.52
1:A:468:ASP:OD1	1:A:570:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LYS:O	1:A:645:ILE:HD12	2.09	0.52
1:A:727:ALA:O	1:A:728:ILE:HB	2.10	0.52
2:Y:13:PRO:O	2:Y:17:ILE:HG12	2.09	0.52
3:Z:36:VAL:HG11	3:Z:68:PHE:HZ	1.67	0.52
3:Z:5:GLN:NE2	3:Z:9:ASP:OD2	2.42	0.52
3:Z:36:VAL:CG1	3:Z:68:PHE:HZ	2.22	0.52
1:A:148:ILE:CG1	1:A:149:PRO:HD2	2.40	0.52
1:A:560:ARG:HG3	1:A:561:MET:HE2	1.92	0.52
1:A:836:LEU:HD23	1:A:836:LEU:N	2.12	0.52
3:Z:124:GLU:HG3	3:Z:127:LYS:HE2	1.92	0.52
1:A:734:ASP:OD1	1:A:737:THR:HG23	2.10	0.52
1:A:104:ARG:HH22	1:A:684:ALA:HB2	1.75	0.51
1:A:817:LYS:HE3	1:A:817:LYS:HA	1.92	0.51
1:A:85:LEU:N	1:A:102:ASN:HD21	2.06	0.51
1:A:503:GLU:HG3	1:A:761:PHE:CZ	2.45	0.51
1:A:742:ILE:O	1:A:746:LEU:HG	2.10	0.51
1:A:124:ASN:O	1:A:673:PRO:HG2	2.11	0.51
1:A:438:LEU:O	1:A:442:VAL:HG23	2.10	0.51
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.76	0.51
2:Y:58:ALA:HA	2:Y:61:LYS:HB2	1.93	0.51
2:Y:121:ASN:OD1	2:Y:124:GLU:HG3	2.10	0.51
1:A:197:ALA:HB1	1:A:251:PHE:HE2	1.76	0.51
1:A:400:LYS:HE2	1:A:411:THR:CG2	2.41	0.51
1:A:533:LEU:HD22	1:A:598:ASN:HD22	1.72	0.51
1:A:96:GLU:HG2	1:A:697:LEU:HD22	1.92	0.51
1:A:186:THR:HG23	1:A:458:VAL:CG1	2.41	0.51
2:Y:12:LEU:HD11	2:Y:16:GLN:HG2	1.93	0.51
1:A:815:ILE:O	1:A:819:LEU:HG	2.11	0.50
1:A:573:GLN:O	1:A:573:GLN:HG3	2.10	0.50
2:Y:49:ARG:O	2:Y:51:PRO:CD	2.44	0.50
3:Z:62:SER:O	3:Z:63:LEU:HD23	2.10	0.50
1:A:319:VAL:HB	1:A:322:ILE:HB	1.92	0.50
1:A:548:GLN:HG2	1:A:552:TYR:CD2	2.46	0.50
1:A:795:ARG:HD3	3:Z:38:ARG:O	2.12	0.50
3:Z:154:PRO:O	3:Z:155:ASP:HB2	2.11	0.50
1:A:530:LEU:O	1:A:534:GLU:HG3	2.12	0.49
1:A:724:ALA:HB1	1:A:726:ASN:HD22	1.78	0.49
1:A:400:LYS:O	1:A:400:LYS:HG3	2.12	0.49
1:A:231:ASN:HD22	1:A:239:ASN:ND2	2.10	0.49
1:A:772:GLU:HA	1:A:772:GLU:OE2	2.13	0.49
1:A:822:ARG:HH22	2:Y:150:GLY:HA3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG12	1:A:673:PRO:HG3	1.95	0.49
2:Y:99:GLN:HG2	2:Y:101:THR:HG23	1.93	0.49
1:A:126:TYR:O	1:A:679:PRO:HG3	2.13	0.49
1:A:537:CYS:HB3	1:A:599:LYS:HD3	1.95	0.49
2:Y:12:LEU:CG	2:Y:16:GLN:HG2	2.42	0.49
3:Z:45:ARG:NH2	3:Z:47:GLU:OE2	2.46	0.49
3:Z:112:ALA:HA	3:Z:116:ARG:HD3	1.93	0.49
3:Z:122:VAL:O	3:Z:126:ILE:HG13	2.12	0.49
1:A:50:SER:HB2	1:A:57:THR:CB	2.44	0.48
3:Z:36:VAL:CG1	3:Z:68:PHE:CZ	2.93	0.48
1:A:60:ILE:HD12	1:A:60:ILE:N	2.28	0.48
1:A:238:ASN:HB3	1:A:319:VAL:HG11	1.95	0.48
1:A:292:ALA:HB3	1:A:328:PHE:HD2	1.78	0.48
1:A:709:SER:HB2	1:A:762:PHE:HB2	1.96	0.48
3:Z:154:PRO:O	3:Z:155:ASP:CB	2.61	0.48
3:Z:42:ILE:HD11	3:Z:76:MET:CE	2.44	0.48
1:A:286:TYR:CD1	1:A:286:TYR:N	2.81	0.48
1:A:486:GLN:CA	1:A:489:ASN:ND2	2.68	0.48
1:A:293:ILE:HD12	1:A:328:PHE:CE2	2.48	0.48
1:A:548:GLN:O	1:A:552:TYR:HD2	1.97	0.48
1:A:115:TYR:CE1	1:A:145:LYS:HD3	2.49	0.47
1:A:123:VAL:CG1	1:A:673:PRO:HG3	2.44	0.47
1:A:825:GLN:CA	1:A:825:GLN:HE21	2.27	0.47
2:Y:101:THR:O	2:Y:102:LYS:HB2	2.14	0.47
1:A:148:ILE:HG12	1:A:149:PRO:HD2	1.95	0.47
1:A:219:ILE:CD1	1:A:446:LEU:HD22	2.44	0.47
1:A:505:ILE:HD11	1:A:761:PHE:CD1	2.49	0.47
1:A:297:ASN:N	1:A:297:ASN:HD22	2.12	0.47
1:A:112:ILE:HG21	1:A:125:PRO:HB3	1.97	0.47
1:A:306:SER:C	1:A:308:LEU:H	2.17	0.47
1:A:582:HIS:HB2	1:A:585:GLY:O	2.14	0.47
1:A:697:LEU:HD21	1:A:701:ARG:HH22	1.80	0.47
2:Y:106:ILE:HG23	2:Y:107:GLU:OE1	2.15	0.47
3:Z:37:CYS:SG	3:Z:75:LEU:HD12	2.54	0.47
3:Z:124:GLU:O	3:Z:128:LEU:HG	2.15	0.47
1:A:91:MET:O	1:A:704:ARG:NH1	2.47	0.47
1:A:786:GLN:HE22	3:Z:115:GLU:N	2.13	0.47
1:A:115:TYR:CZ	1:A:150:PRO:HA	2.50	0.47
1:A:198:CYS:HB3	1:A:216:GLU:CG	2.45	0.47
3:Z:11:LEU:HD13	3:Z:40:LEU:CD1	2.43	0.47
3:Z:116:ARG:HH11	3:Z:116:ARG:CB	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:HA	1:A:527:MET:CE	2.45	0.46
1:A:825:GLN:NE2	1:A:825:GLN:HA	2.30	0.46
2:Y:148:ILE:C	2:Y:150:GLY:H	2.18	0.46
1:A:369:GLU:O	1:A:370:GLU:C	2.53	0.46
1:A:832:LYS:HB3	2:Y:47:LEU:HD13	1.97	0.46
1:A:124:ASN:HB3	1:A:673:PRO:HD3	1.96	0.46
1:A:722:ILE:O	1:A:722:ILE:CG2	2.64	0.46
1:A:615:GLU:HG3	1:A:618:VAL:H	1.81	0.46
1:A:79:PRO:HD2	1:A:82:PHE:CE1	2.51	0.46
1:A:116:SER:OG	1:A:119:PHE:CE1	2.67	0.46
2:Y:12:LEU:HD12	2:Y:13:PRO:HD2	1.97	0.46
1:A:556:MET:C	1:A:558:LYS:N	2.69	0.46
1:A:800:LYS:HE2	1:A:804:GLN:NE2	2.30	0.46
2:Y:34:PHE:CE1	2:Y:68:ASN:HB3	2.51	0.46
2:Y:127:MET:O	2:Y:130:LYS:HG2	2.16	0.46
1:A:503:GLU:HG3	1:A:761:PHE:CE1	2.51	0.45
1:A:716:PHE:HD1	1:A:739:SER:HG	1.64	0.45
1:A:329:LYS:O	1:A:333:GLU:HG2	2.16	0.45
1:A:697:LEU:HG	1:A:701:ARG:NH1	2.32	0.45
1:A:166:ASP:HB2	1:A:168:GLU:HG2	1.99	0.45
3:Z:11:LEU:HD11	3:Z:68:PHE:HE2	1.81	0.45
1:A:518:MET:HE2	1:A:560:ARG:NH1	2.32	0.45
2:Y:12:LEU:HG	2:Y:16:GLN:HG2	1.98	0.45
1:A:565:PRO:HD3	1:A:578:PHE:HA	1.98	0.45
1:A:824:TRP:CE2	2:Y:79:LYS:HD2	2.51	0.45
3:Z:50:PHE:CE1	3:Z:56:HIS:NE2	2.85	0.45
1:A:94:LEU:HD22	1:A:700:ILE:HG21	1.99	0.45
1:A:468:ASP:HA	1:A:570:ARG:HH11	1.81	0.45
1:A:245:LYS:HA	1:A:263:GLU:O	2.17	0.45
2:Y:144:PHE:CZ	2:Y:148:ILE:HD11	2.51	0.45
2:Y:144:PHE:O	2:Y:148:ILE:HG12	2.16	0.45
1:A:296:LEU:HA	1:A:299:VAL:CG2	2.46	0.45
2:Y:52:ASP:OD1	2:Y:54:LYS:HG3	2.17	0.45
1:A:190:ILE:HD11	1:A:247:ILE:HD13	1.96	0.45
1:A:532:ILE:HG22	1:A:547:PHE:CE1	2.52	0.45
1:A:657:MET:CE	1:A:660:LEU:HD12	2.46	0.45
1:A:798:TYR:CE1	3:Z:17:LEU:HD23	2.52	0.44
2:Y:37:LYS:CG	2:Y:60:LEU:HD12	2.46	0.44
1:A:234:THR:HG22	1:A:237:ASN:H	1.81	0.44
1:A:312:ILE:HD13	1:A:356:LEU:HD11	1.99	0.44
1:A:591:ILE:C	1:A:591:ILE:HD12	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:ARG:HG3	3:Z:20:PHE:CE1	2.53	0.44
1:A:441:ARG:O	1:A:444:LYS:HB2	2.18	0.44
1:A:485:GLN:O	1:A:489:ASN:ND2	2.51	0.44
1:A:527:MET:CG	1:A:528:GLY:N	2.78	0.44
2:Y:133:PRO:HD2	2:Y:144:PHE:HB2	1.99	0.44
1:A:280:ARG:NH2	1:A:283:HIS:HD1	2.13	0.44
1:A:489:ASN:H	1:A:489:ASN:HD22	1.55	0.44
1:A:577:HIS:O	1:A:578:PHE:HB3	2.18	0.44
1:A:825:GLN:HE21	1:A:825:GLN:HA	1.81	0.44
1:A:267:LEU:HD22	1:A:435:PHE:CG	2.53	0.44
1:A:721:SER:HA	1:A:742:ILE:HD11	1.99	0.44
1:A:725:PRO:O	1:A:726:ASN:C	2.56	0.44
1:A:740:GLU:OE2	1:A:744:ALA:HB2	2.18	0.44
2:Y:45:GLU:HG2	2:Y:50:ALA:HB2	2.00	0.44
1:A:401:PRO:HG2	1:A:414:GLN:NE2	2.33	0.44
1:A:792:TYR:CD1	1:A:792:TYR:C	2.91	0.43
3:Z:42:ILE:HD11	3:Z:76:MET:HG2	2.00	0.43
1:A:17:ARG:HA	1:A:20:LEU:CB	2.48	0.43
1:A:560:ARG:HG2	1:A:560:ARG:NH1	2.34	0.43
1:A:171:SER:HA	1:A:457:GLY:O	2.18	0.43
1:A:173:LEU:N	1:A:173:LEU:HD23	2.33	0.43
2:Y:63:ALA:HB1	2:Y:71:MET:HG2	2.01	0.43
3:Z:111:THR:HG22	3:Z:117:LEU:O	2.19	0.43
1:A:6:SER:C	1:A:8:PRO:HD2	2.39	0.43
1:A:449:LYS:HD2	1:A:449:LYS:N	2.33	0.43
1:A:721:SER:HA	1:A:742:ILE:CD1	2.48	0.43
1:A:827:TRP:C	1:A:829:LEU:H	2.21	0.43
1:A:145:LYS:HG3	8:A:2035:HOH:O	2.19	0.43
1:A:52:LYS:HB2	1:A:55:GLU:O	2.19	0.43
1:A:178:SER:HA	5:A:1998:VO4:O3	2.19	0.43
1:A:814:ASN:ND2	2:Y:84:ASP:H	2.05	0.43
1:A:7:ASP:N	1:A:8:PRO:CD	2.82	0.42
1:A:218:GLN:NE2	1:A:445:THR:CG2	2.81	0.42
1:A:543:ASP:H	1:A:546:SER:HB3	1.84	0.42
1:A:669:ARG:HH21	1:A:694:ASN:CG	2.23	0.42
1:A:727:ALA:O	1:A:728:ILE:CB	2.67	0.42
2:Y:52:ASP:OD1	2:Y:53:ASP:N	2.52	0.42
2:Y:115:ASN:C	2:Y:116:MET:HG3	2.40	0.42
2:Y:131:GLU:O	2:Y:147:MET:HE1	2.19	0.42
1:A:151:HIS:CE1	1:A:153:PHE:CD2	3.07	0.42
1:A:305:ASP:HB3	1:A:308:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:46:ASN:O	3:Z:49:VAL:HG22	2.20	0.42
1:A:518:MET:HE3	1:A:559:ASN:OD1	2.18	0.42
1:A:115:TYR:CE2	1:A:150:PRO:HA	2.54	0.42
1:A:253:PRO:N	1:A:453:ASN:ND2	2.68	0.42
1:A:758:THR:HG22	1:A:759:LYS:HG3	1.99	0.42
3:Z:67:GLU:O	3:Z:70:PRO:HD2	2.19	0.42
1:A:43:PHE:CZ	1:A:75:GLN:NE2	2.87	0.42
1:A:822:ARG:HG2	1:A:822:ARG:HH11	1.84	0.42
1:A:219:ILE:CD1	1:A:260:ALA:HB3	2.46	0.42
1:A:294:PRO:C	1:A:296:LEU:H	2.22	0.42
1:A:397:ALA:CB	1:A:609:LEU:HD11	2.49	0.42
3:Z:67:GLU:C	3:Z:70:PRO:HD2	2.40	0.42
1:A:181:GLY:HA2	6:A:1999:ADP:PA	2.60	0.42
1:A:219:ILE:HD11	1:A:260:ALA:CB	2.46	0.42
1:A:249:ILE:N	1:A:249:ILE:CD1	2.81	0.42
2:Y:106:ILE:HG23	2:Y:107:GLU:N	2.34	0.42
3:Z:101:ILE:HG22	3:Z:141:TYR:HD1	1.83	0.42
1:A:471:SER:OG	1:A:472:PHE:N	2.52	0.42
2:Y:12:LEU:CD1	2:Y:16:GLN:HG2	2.50	0.42
1:A:812:GLN:O	1:A:816:ARG:HG3	2.20	0.42
2:Y:23:ALA:O	2:Y:27:ILE:HG13	2.20	0.42
1:A:600:ASP:HA	1:A:601:PRO:HD3	1.89	0.41
1:A:360:GLU:HB2	1:A:379:GLU:CG	2.49	0.41
1:A:129:LEU:HA	1:A:130:PRO:HD3	1.75	0.41
1:A:132:TYR:CE2	1:A:188:LYS:HG3	2.54	0.41
1:A:253:PRO:HG3	1:A:453:ASN:HD21	1.84	0.41
1:A:426:LEU:HD13	1:A:606:VAL:HG11	2.02	0.41
1:A:728:ILE:O	1:A:728:ILE:HG22	2.19	0.41
1:A:256:LYS:HE2	3:Z:95:ARG:NH2	2.33	0.41
1:A:723:LEU:HD12	1:A:723:LEU:HA	1.88	0.41
1:A:360:GLU:CB	1:A:379:GLU:HG2	2.49	0.41
1:A:83:GLU:O	1:A:84:LYS:C	2.59	0.41
1:A:657:MET:HE3	1:A:660:LEU:HD12	2.01	0.41
3:Z:23:GLY:O	3:Z:24:ARG:C	2.58	0.41
1:A:94:LEU:HD13	1:A:700:ILE:HG22	2.03	0.41
1:A:818:TRP:HB2	2:Y:148:ILE:HG23	2.02	0.41
2:Y:18:GLN:HA	2:Y:18:GLN:OE1	2.21	0.41
3:Z:42:ILE:HD11	3:Z:76:MET:HE3	2.02	0.41
3:Z:43:ASN:HD22	3:Z:80:GLN:HE21	1.67	0.41
3:Z:48:ASP:O	3:Z:51:ALA:HB3	2.20	0.41
3:Z:66:GLU:O	3:Z:70:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HH12	1:A:279:GLU:CD	2.24	0.41
2:Y:121:ASN:CG	2:Y:124:GLU:HG3	2.40	0.41
1:A:483:ARG:CZ	1:A:657:MET:HG2	2.50	0.41
1:A:532:ILE:HG22	1:A:547:PHE:HE1	1.86	0.40
1:A:548:GLN:HG2	1:A:552:TYR:HD2	1.86	0.40
1:A:343:GLU:O	1:A:347:SER:N	2.48	0.40
1:A:451:LYS:HD2	1:A:451:LYS:HA	1.75	0.40
1:A:401:PRO:HA	1:A:605:ASN:ND2	2.36	0.40
1:A:233:LYS:HG2	1:A:234:THR:N	2.37	0.40
2:Y:68:ASN:HD21	2:Y:70:THR:HB	1.86	0.40
1:A:347:SER:CB	1:A:617:LEU:HD12	2.51	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	798/840 (95%)	707 (89%)	76 (10%)	15 (2%)	8 9
2	Y	139/156 (89%)	116 (84%)	18 (13%)	5 (4%)	3 2
3	Z	153/156 (98%)	142 (93%)	6 (4%)	5 (3%)	4 2
All	All	1090/1152 (95%)	965 (88%)	100 (9%)	25 (2%)	6 6

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	GLU
1	A	624	ALA
1	A	625	PRO
2	Y	100	GLU
2	Y	150	GLY
3	Z	154	PRO

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Mol	Chain	Res	Type
1	A	53	GLY
1	A	266	LEU
1	A	407	THR
1	A	528	GLY
2	Y	80	LEU
1	A	268	GLU
1	A	367	PRO
1	A	726	ASN
2	Y	13	PRO
3	Z	116	ARG
3	Z	25	ASP
1	A	40	LYS
1	A	727	ALA
3	Z	4	SER
3	Z	52	VAL
1	A	295	GLU
1	A	728	ILE
2	Y	30	ASP
1	A	149	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	684/732 (93%)	653 (96%)	31 (4%)	27	37
2	Y	122/133 (92%)	115 (94%)	7 (6%)	20	27
3	Z	130/132 (98%)	126 (97%)	4 (3%)	40	54
All	All	936/997 (94%)	894 (96%)	42 (4%)	27	37

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	64	SER
1	A	143	LYS

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Mol	Chain	Res	Type
1	A	234	THR
1	A	235	THR
1	A	236	ARG
1	A	247	ILE
1	A	338	LEU
1	A	371	GLN
1	A	433	ARG
1	A	438	LEU
1	A	475	LEU
1	A	489	ASN
1	A	492	MET
1	A	516	LEU
1	A	521	ASP
1	A	522	LEU
1	A	653	LEU
1	A	655	LYS
1	A	657	MET
1	A	664	HIS
1	A	711	LEU
1	A	714	SER
1	A	718	GLN
1	A	723	LEU
1	A	758	THR
1	A	775	ASP
1	A	778	LEU
1	A	792	TYR
1	A	817	LYS
1	A	836	LEU
2	Y	20	MET
2	Y	49	ARG
2	Y	51	PRO
2	Y	53	ASP
2	Y	98	GLU
2	Y	107	GLU
2	Y	135	GLU
3	Z	10	ASP
3	Z	76	MET
3	Z	91	LYS
3	Z	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	102	ASN
1	A	162	ASN
1	A	238	ASN
1	A	239	ASN
1	A	297	ASN
1	A	371	GLN
1	A	417	ASN
1	A	436	ASN
1	A	453	ASN
1	A	485	GLN
1	A	486	GLN
1	A	489	ASN
1	A	497	GLN
1	A	581	HIS
1	A	654	ASN
1	A	718	GLN
1	A	726	ASN
1	A	786	GLN
1	A	802	GLN
1	A	812	GLN
1	A	814	ASN
1	A	825	GLN
2	Y	91	ASN
2	Y	115	ASN
3	Z	80	GLN
3	Z	138	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	1999	5,4	24,29,29	1.75	6 (25%)	29,45,45	2.47	9 (31%)
5	VO4	A	1998	4,6	1,4,4	2.23	1 (100%)	-		

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	1999	5,4	-	6/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1999	ADP	O4'-C1'	3.88	1.46	1.41
6	A	1999	ADP	C3'-C4'	3.75	1.62	1.53
6	A	1999	ADP	C2-N3	2.69	1.36	1.32
6	A	1999	ADP	C5-N7	-2.46	1.30	1.39
6	A	1999	ADP	PB-O3B	-2.45	1.45	1.54
6	A	1999	ADP	C5'-C4'	2.34	1.58	1.51
5	A	1998	VO4	O1-V	2.23	1.76	1.63

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1999	ADP	N3-C2-N1	-6.76	118.12	128.68
6	A	1999	ADP	O3B-PB-O3A	-5.69	85.56	104.64
6	A	1999	ADP	O3B-PB-O1B	3.73	125.28	110.68
6	A	1999	ADP	O2B-PB-O3A	-3.48	92.97	104.64
6	A	1999	ADP	O2A-PA-O5'	-3.46	91.67	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1999	ADP	O3A-PB-O1B	-3.36	92.53	111.19
6	A	1999	ADP	O3B-PB-O2B	3.31	120.30	107.64
6	A	1999	ADP	O5'-C5'-C4'	-3.08	98.40	108.99
6	A	1999	ADP	O5'-PA-O1A	2.78	119.91	109.07

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1999	ADP	PA-O3A-PB-O3B
6	A	1999	ADP	C5'-O5'-PA-O2A
6	A	1999	ADP	C5'-O5'-PA-O3A
6	A	1999	ADP	O4'-C4'-C5'-O5'
6	A	1999	ADP	C3'-C4'-C5'-O5'
6	A	1999	ADP	C5'-O5'-PA-O1A

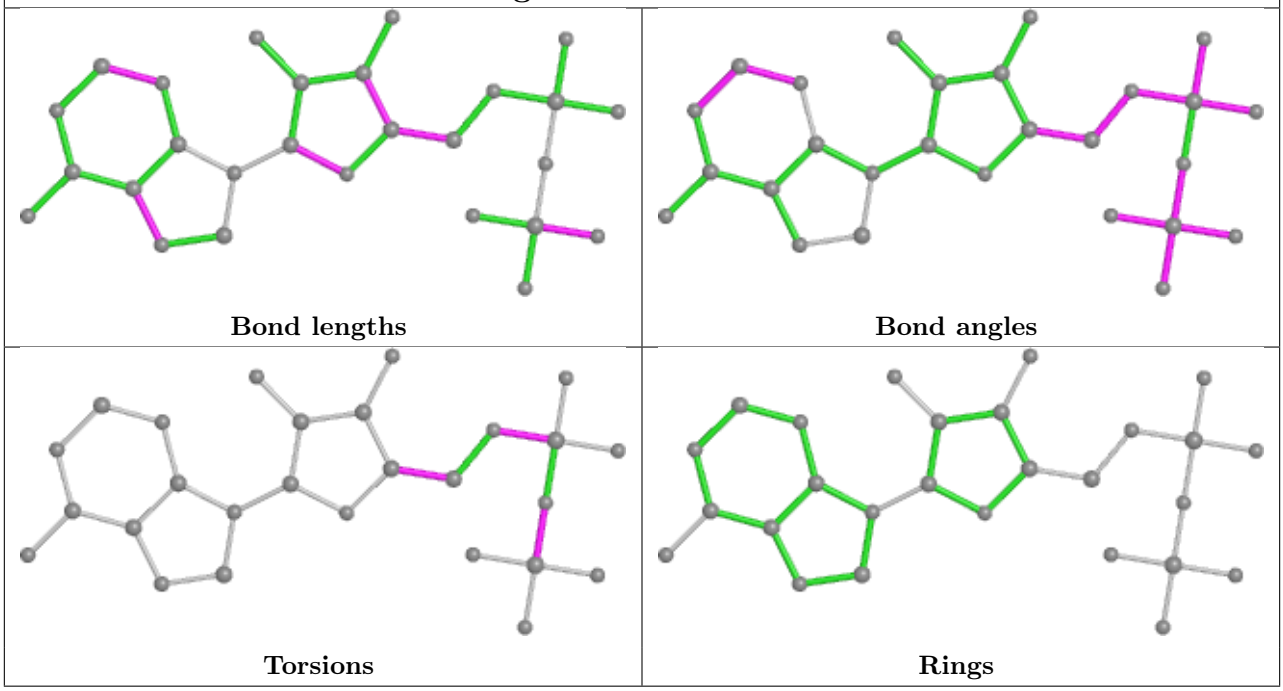
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1999	ADP	1	0
5	A	1998	VO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 1999



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	806/840 (95%)	0.08	32 (3%)	38	45	11, 41, 94, 154	0
2	Y	141/156 (90%)	0.28	7 (4%)	28	34	21, 59, 102, 127	0
3	Z	155/156 (99%)	-0.07	2 (1%)	77	82	16, 47, 72, 90	0
All	All	1102/1152 (95%)	0.08	41 (3%)	41	48	11, 45, 94, 154	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	GLY	7.4
1	A	407	THR	7.3
1	A	728	ILE	6.3
1	A	6	SER	6.0
1	A	405	VAL	5.8
1	A	625	PRO	4.9
1	A	642	PHE	4.9
1	A	409	MET	4.8
1	A	408	GLU	4.6
1	A	627	GLU	4.4
1	A	567	LYS	4.4
2	Y	152	GLY	4.2
1	A	410	VAL	4.1
1	A	403	VAL	4.0
1	A	727	ALA	3.9
1	A	837	LEU	3.8
3	Z	1	PRO	3.7
1	A	25	THR	3.5
2	Y	65	GLY	3.5
1	A	369	GLU	3.3
1	A	404	LYS	3.3
1	A	370	GLU	3.1
1	A	571	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	602	ILE	3.0
2	Y	151	SER	3.0
1	A	24	GLN	2.8
2	Y	15	LYS	2.7
2	Y	53	ASP	2.7
1	A	732	PHE	2.6
1	A	575	PRO	2.5
1	A	626	GLU	2.5
1	A	367	PRO	2.4
1	A	572	ASN	2.4
1	A	569	THR	2.3
1	A	27	ALA	2.2
1	A	573	GLN	2.1
1	A	412	LYS	2.1
2	Y	54	LYS	2.1
3	Z	154	PRO	2.1
2	Y	52	ASP	2.1
1	A	729	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

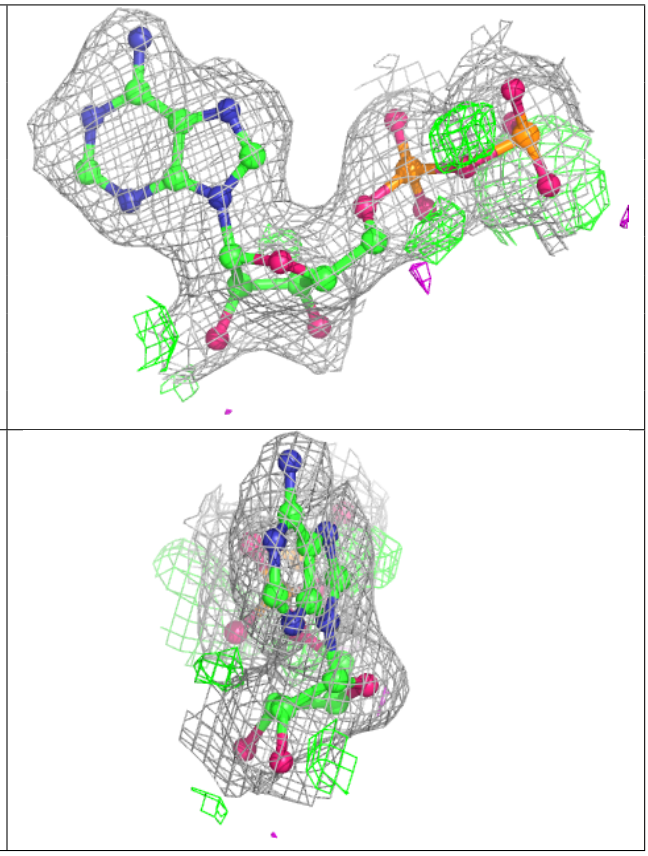
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

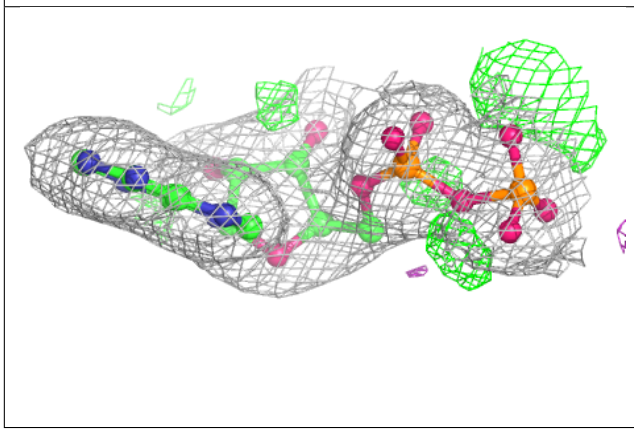
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1997	1/1	0.81	0.38	28,28,28,28	0
7	CA	Z	503	1/1	0.91	0.14	41,41,41,41	0
4	MG	Y	502	1/1	0.93	0.10	52,52,52,52	0
6	ADP	A	1999	27/27	0.97	0.17	2,22,29,32	0
5	VO4	A	1998	5/5	0.98	0.17	20,24,31,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1999:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.