



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:34 PM EDT

PDB ID : 1KK8 / pdb_00001kk8
Title : SCALLOP MYOSIN (S1-ADP-BeFx) IN THE ACTIN-DETACHED CONFORMATION
Authors : Himmel, M.; Gourinath, S.; Reshetnikova, L.; Shen, Y.; Szent-Gyorgyi, G.; Cohen, C.
Deposited on : 2001-12-06
Resolution : 2.30 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

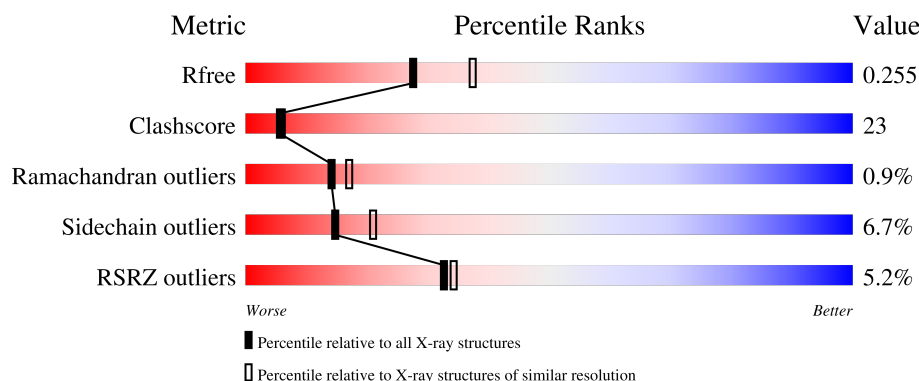
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	837	6% 56% 34% 5% 5%
2	B	139	4% 58% 34% 8%
3	C	154	2% 71% 24% 5%

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
7	GOL	A	998	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8702 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
1	A	793	Total	C	N	O	S	3	0	0
			6231	3971	1069	1154	37			

- Molecule 2 is a protein called Myosin Regulatory Light Chain, Striated adductor muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1059	673	167	210	9			

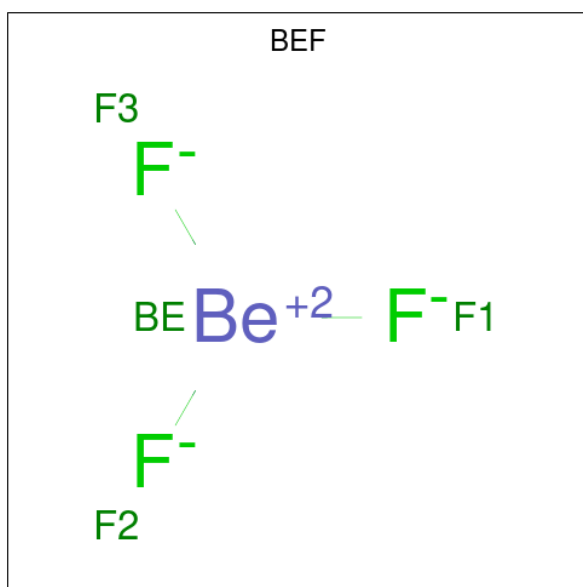
- Molecule 3 is a protein called Myosin Essential Light Chain, Striated adductor muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	154	Total	C	N	O	S	3	0	0
			1187	757	192	231	7			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

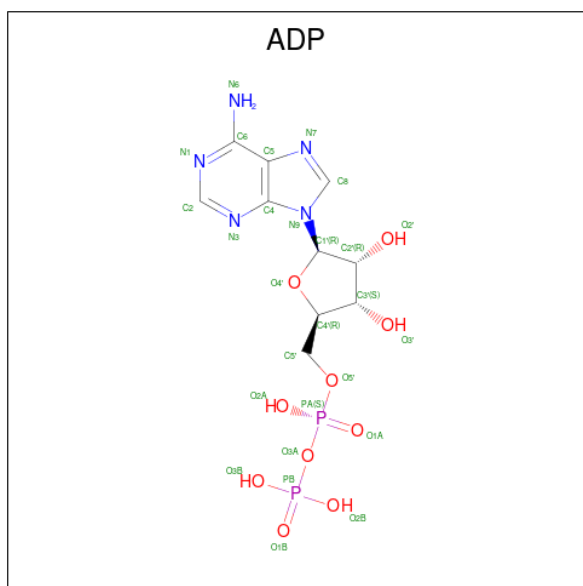
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Be	F		0	0
			4	1	3			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca	0	0
			1	1		

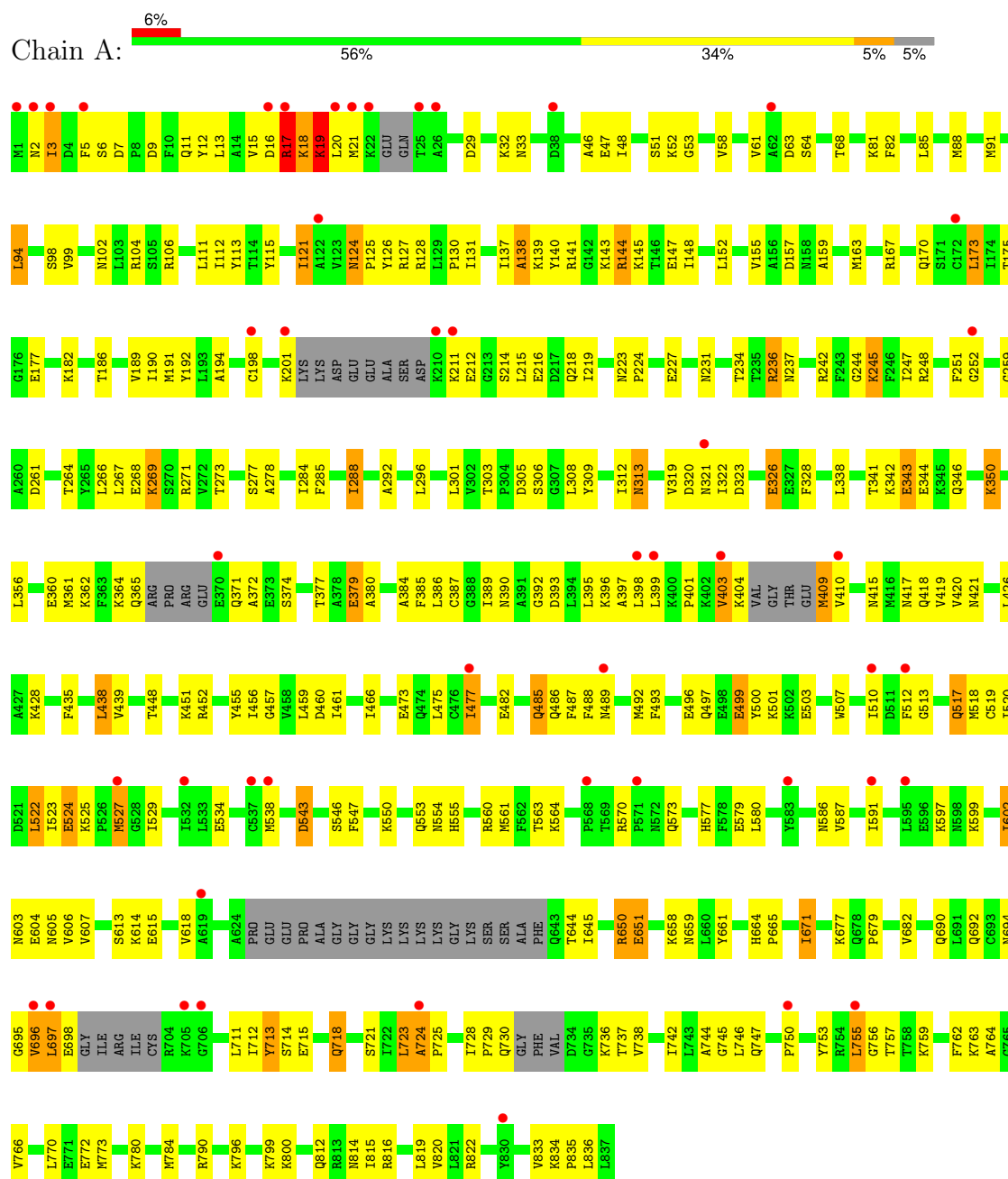
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	145	Total	O	0	0
			145	145		
9	B	20	Total	O	0	0
			20	20		
9	C	20	Total	O	0	0
			20	20		

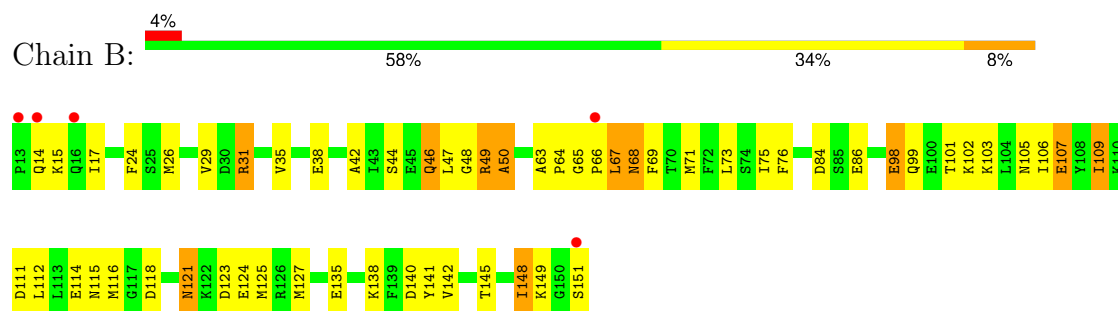
3 Residue-property plots

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.

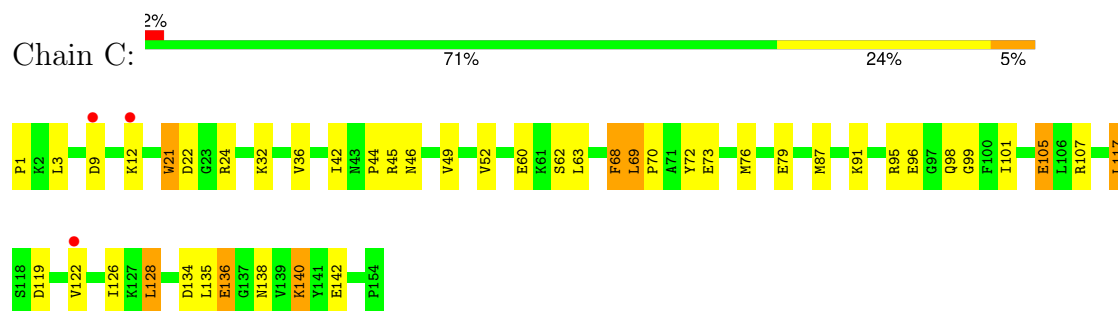
- Molecule 1: Myosin Heavy Chain, Striated muscle



- Molecule 2: Myosin Regulatory Light Chain, Striated adductor muscle



- Molecule 3: Myosin Essential Light Chain, Striated adductor muscle



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.60Å 58.53Å 133.29Å 81.08° 84.94° 67.24°	Depositor
Resolution (Å)	29.84 – 2.30 29.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.9 (29.84-2.30) 77.9 (29.84-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.29Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.230 , 0.269 0.217 , 0.255	Depositor DCC
R_{free} test set	2520 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8702	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, ADP, BEF, CA, MG

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	0.62	0/6354	1.03	33/8575 (0.4%)
2	B	0.52	0/1076	0.97	2/1444 (0.1%)
3	C	0.55	0/1211	0.96	4/1633 (0.2%)
All	All	0.60	0/8641	1.01	39/11652 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	LYS	N-CA-C	-9.59	90.38	110.80
1	A	692	GLN	N-CA-C	8.49	121.48	111.71
1	A	21	MET	N-CA-C	-8.14	93.47	110.80
1	A	696	VAL	N-CA-C	-7.92	98.23	108.93
3	C	21	TRP	N-CA-C	7.66	120.52	111.71
1	A	448	THR	N-CA-C	-7.55	99.86	110.50
1	A	266	LEU	N-CA-C	7.51	121.76	111.17
1	A	664	HIS	N-CA-C	-7.20	98.10	109.04
2	B	50	ALA	N-CA-C	7.09	119.86	110.08
1	A	527	MET	N-CA-C	-6.88	102.32	113.19
1	A	124	ASN	CA-C-N	6.86	126.11	118.97
1	A	124	ASN	C-N-CA	6.86	126.11	118.97
1	A	61	VAL	N-CA-C	6.59	118.14	110.62
1	A	421	ASN	N-CA-C	-6.58	105.41	113.50
1	A	524	GLU	N-CA-C	6.44	121.31	113.38
3	C	1	PRO	N-CA-CB	6.31	109.94	103.00
1	A	143	LYS	N-CA-C	6.25	119.74	110.48
1	A	99	VAL	N-CA-C	-6.19	104.25	111.00
1	A	252	GLY	CA-C-N	6.10	125.58	119.24
1	A	252	GLY	C-N-CA	6.10	125.58	119.24
1	A	815	ILE	N-CA-C	-5.96	105.26	111.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	LYS	N-CA-C	5.92	117.73	111.28
3	C	22	ASP	N-CA-C	-5.83	106.08	112.72
1	A	744	ALA	N-CA-C	-5.71	105.06	111.28
1	A	499	GLU	N-CA-C	-5.65	105.12	112.23
1	A	144	ARG	N-CA-C	-5.54	103.08	110.55
2	B	67	LEU	N-CA-C	5.47	118.27	107.98
1	A	155	VAL	N-CA-C	-5.40	105.23	110.42
1	A	138	ALA	N-CA-C	-5.37	105.08	111.69
3	C	117	LEU	N-CA-C	-5.29	101.94	110.14
1	A	46	ALA	N-CA-C	5.17	116.85	109.14
1	A	512	PHE	N-CA-C	5.17	120.45	114.04
1	A	2	ASN	N-CA-C	5.13	116.79	109.14
1	A	477	ILE	CB-CA-C	-5.12	105.42	111.97
1	A	303	THR	N-CA-C	-5.09	101.31	109.04
1	A	724	ALA	CA-C-N	5.02	124.80	119.28
1	A	724	ALA	C-N-CA	5.02	124.80	119.28
1	A	175	THR	N-CA-C	5.01	117.91	110.14
1	A	131	ILE	N-CA-C	5.00	119.75	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6231	0	6104	299	0
2	B	1059	0	1009	68	0
3	C	1187	0	1109	39	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
6	A	27	0	12	0	0
7	A	6	0	8	9	0
8	C	1	0	0	0	0
9	A	145	0	0	47	0
9	B	20	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	20	0	0	3	0
All	All	8702	0	8242	391	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 23.

All (391) 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:523:ILE:HD11	1:A:580:LEU:HD21	1.33	1.08
1:A:98:SER:HB2	9:A:1127:HOH:O	1.57	1.02
1:A:16:ASP:OD2	1:A:19:LYS:HB3	1.60	1.01
1:A:591:ILE:HD13	9:A:1138:HOH:O	1.63	0.97
1:A:833:VAL:C	1:A:835:PRO:HD2	1.90	0.97
1:A:350:LYS:HG2	1:A:386:LEU:HD22	1.45	0.95
1:A:29:ASP:H	1:A:33:ASN:HD22	1.17	0.91
2:B:111:ASP:HA	9:B:1012:HOH:O	1.69	0.91
1:A:390:ASN:ND2	1:A:393:ASP:H	1.69	0.90
1:A:390:ASN:HD22	1:A:393:ASP:H	1.04	0.90
1:A:836:LEU:HD11	2:B:47:LEU:HD21	1.52	0.90
1:A:234:THR:HG21	7:A:998:GOL:O2	1.74	0.88
1:A:603:ASN:HB3	9:A:1117:HOH:O	1.73	0.87
1:A:546:SER:O	9:A:1118:HOH:O	1.93	0.87
1:A:497:GLN:O	1:A:501:LYS:HD3	1.75	0.86
3:C:96:GLU:HG3	3:C:98:GLN:HG2	1.56	0.86
1:A:599:LYS:HD2	1:A:644:THR:HG22	1.57	0.85
1:A:605:ASN:HB3	9:A:1117:HOH:O	1.75	0.85
1:A:755:LEU:H	1:A:755:LEU:HD23	1.42	0.85
1:A:403:VAL:HG22	1:A:404:LYS:H	1.42	0.84
1:A:755:LEU:H	1:A:755:LEU:CD2	1.90	0.84
1:A:527:MET:HE2	1:A:555:HIS:NE2	1.93	0.83
2:B:121:ASN:HD22	2:B:123:ASP:H	1.23	0.83
1:A:518:MET:HE1	1:A:560:ARG:NH1	1.92	0.83
1:A:137:ILE:O	9:A:1104:HOH:O	1.96	0.81
1:A:577:HIS:ND1	1:A:591:ILE:HG13	1.96	0.81
3:C:42:ILE:HG22	3:C:44:PRO:HD3	1.63	0.81
1:A:29:ASP:H	1:A:33:ASN:ND2	1.78	0.80
1:A:547:PHE:HD2	9:A:1138:HOH:O	1.62	0.80
3:C:9:ASP:O	3:C:12:LYS:HG3	1.82	0.80
1:A:323:ASP:OD2	1:A:326:GLU:HB2	1.84	0.78
1:A:518:MET:HE2	1:A:561:MET:HG2	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HA	2:B:116:MET:HE3	1.67	0.77
3:C:101:ILE:HD11	3:C:105:GLU:HG2	1.66	0.77
1:A:248:ARG:HB2	9:A:1100:HOH:O	1.85	0.76
1:A:485:GLN:NE2	1:A:489:ASN:ND2	2.33	0.76
1:A:550:LYS:HB2	9:A:1118:HOH:O	1.85	0.76
1:A:836:LEU:HD11	2:B:47:LEU:CD2	2.17	0.75
1:A:343:GLU:HG3	1:A:344:GLU:H	1.51	0.74
1:A:755:LEU:HD23	1:A:755:LEU:N	2.00	0.74
1:A:16:ASP:O	1:A:18:LYS:N	2.22	0.73
3:C:36:VAL:HG11	3:C:68:PHE:HE2	1.53	0.73
2:B:121:ASN:ND2	2:B:123:ASP:H	1.87	0.73
1:A:466:ILE:HG12	1:A:587:VAL:HG22	1.71	0.73
1:A:814:ASN:HD21	2:B:84:ASP:H	1.35	0.72
1:A:140:TYR:N	9:A:1104:HOH:O	2.22	0.72
1:A:215:LEU:HD21	1:A:259:GLY:HA2	1.70	0.72
3:C:3:LEU:HD21	3:C:76:MET:SD	2.29	0.72
1:A:11:GLN:NE2	9:A:1141:HOH:O	2.22	0.71
1:A:538:MET:HG2	1:A:599:LYS:NZ	2.05	0.71
1:A:390:ASN:HD22	1:A:393:ASP:N	1.85	0.71
1:A:603:ASN:O	1:A:607:VAL:HG23	1.90	0.71
1:A:460:ASP:OD2	9:A:1012:HOH:O	2.09	0.71
1:A:342:LYS:O	1:A:346:GLN:HG3	1.90	0.70
1:A:770:LEU:HD23	1:A:773:MET:HE3	1.72	0.70
1:A:790:ARG:NH1	3:C:117:LEU:HD23	2.05	0.70
1:A:696:VAL:C	1:A:698:GLU:H	1.98	0.70
1:A:501:LYS:HD2	1:A:501:LYS:N	2.07	0.69
1:A:485:GLN:HE22	1:A:489:ASN:HD21	1.37	0.69
1:A:756:GLY:HA3	1:A:759:LYS:O	1.92	0.69
1:A:714:SER:O	1:A:718:GLN:HG2	1.92	0.69
2:B:44:SER:OG	2:B:50:ALA:HA	1.92	0.69
1:A:145:LYS:HD2	9:A:1123:HOH:O	1.92	0.69
3:C:36:VAL:HG11	3:C:68:PHE:CE2	2.28	0.69
1:A:721:SER:HA	1:A:742:ILE:CD1	2.23	0.69
1:A:485:GLN:NE2	1:A:489:ASN:HD21	1.92	0.68
1:A:538:MET:HG2	1:A:599:LYS:HZ1	1.58	0.68
1:A:834:LYS:N	1:A:835:PRO:HD2	2.10	0.67
1:A:350:LYS:HG2	1:A:386:LEU:CD2	2.22	0.67
1:A:360:GLU:O	1:A:362:LYS:HD2	1.95	0.67
2:B:138:LYS:HE3	9:B:1003:HOH:O	1.94	0.67
1:A:834:LYS:N	1:A:835:PRO:CD	2.58	0.67
1:A:836:LEU:CD1	2:B:47:LEU:HD21	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:GLU:OE2	9:B:1000:HOH:O	2.13	0.66
1:A:112:ILE:HD13	1:A:125:PRO:HG3	1.76	0.66
1:A:401:PRO:HA	1:A:605:ASN:HD22	1.60	0.66
1:A:248:ARG:CB	9:A:1100:HOH:O	2.41	0.66
2:B:140:ASP:OD1	2:B:142:VAL:HG22	1.95	0.66
1:A:88:MET:HB3	1:A:91:MET:HE2	1.76	0.66
1:A:112:ILE:HG21	1:A:125:PRO:HG3	1.77	0.66
1:A:796:LYS:HE2	3:C:128:LEU:HD11	1.78	0.66
1:A:403:VAL:HG13	1:A:404:LYS:N	2.11	0.66
1:A:658:LYS:CB	9:A:1106:HOH:O	2.44	0.65
1:A:234:THR:HG23	1:A:237:ASN:H	1.62	0.65
1:A:485:GLN:HE22	1:A:489:ASN:ND2	1.93	0.65
1:A:522:LEU:HD13	1:A:580:LEU:HD11	1.78	0.65
3:C:9:ASP:HA	3:C:12:LYS:HG2	1.79	0.65
1:A:403:VAL:HG12	1:A:410:VAL:HB	1.79	0.65
1:A:52:LYS:O	9:A:1053:HOH:O	2.15	0.64
2:B:86:GLU:HG3	2:B:145:THR:HG22	1.79	0.64
1:A:417:ASN:HA	1:A:420:VAL:HG22	1.80	0.64
2:B:35:VAL:HB	2:B:67:LEU:HD23	1.79	0.64
3:C:136:GLU:HB2	3:C:138:ASN:OD1	1.98	0.64
2:B:63:ALA:HB1	2:B:71:MET:HG2	1.81	0.63
1:A:390:ASN:ND2	1:A:393:ASP:N	2.45	0.63
1:A:341:THR:HB	1:A:343:GLU:HG3	1.80	0.63
1:A:696:VAL:O	1:A:698:GLU:N	2.32	0.63
1:A:242:ARG:HH22	7:A:998:GOL:H12	1.62	0.63
1:A:137:ILE:O	1:A:141:ARG:HG3	1.99	0.62
1:A:501:LYS:HD2	1:A:501:LYS:H	1.64	0.62
1:A:780:LYS:HE3	3:C:45:ARG:NH1	2.14	0.62
1:A:182:LYS:HB3	1:A:460:ASP:OD1	2.00	0.62
1:A:17:ARG:CZ	9:A:1001:HOH:O	2.48	0.62
1:A:799:LYS:HG2	1:A:800:LYS:N	2.13	0.62
2:B:102:LYS:O	2:B:103:LYS:HD2	2.00	0.61
2:B:98:GLU:H	2:B:98:GLU:CD	2.06	0.61
1:A:51:SER:CB	3:C:95:ARG:HH21	2.14	0.61
1:A:152:LEU:HD21	1:A:189:VAL:HG23	1.83	0.61
1:A:244:GLY:HA3	1:A:461:ILE:HG22	1.81	0.61
2:B:84:ASP:O	2:B:149:LYS:NZ	2.32	0.61
1:A:137:ILE:C	9:A:1104:HOH:O	2.42	0.61
1:A:563:THR:HG22	1:A:564:LYS:N	2.15	0.61
1:A:487:PHE:HA	9:A:1074:HOH:O	2.00	0.61
1:A:361:MET:HE3	1:A:380:ALA:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:GLU:OE1	1:A:586:ASN:HB3	2.01	0.61
1:A:17:ARG:NE	9:A:1001:HOH:O	2.33	0.60
1:A:563:THR:CG2	1:A:564:LYS:N	2.65	0.60
1:A:550:LYS:CB	9:A:1118:HOH:O	2.47	0.60
2:B:63:ALA:HB1	2:B:71:MET:CG	2.32	0.60
1:A:721:SER:HA	1:A:742:ILE:HD11	1.82	0.60
1:A:390:ASN:ND2	1:A:393:ASP:OD1	2.35	0.59
2:B:84:ASP:O	2:B:149:LYS:CE	2.50	0.59
3:C:32:LYS:NZ	9:C:1019:HOH:O	2.35	0.59
1:A:53:GLY:HA3	9:A:1053:HOH:O	2.02	0.59
3:C:99:GLY:O	3:C:140:LYS:HD3	2.03	0.59
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.68	0.58
1:A:245:LYS:NZ	9:A:1113:HOH:O	2.36	0.58
1:A:360:GLU:HB2	1:A:379:GLU:HG3	1.86	0.58
1:A:486:GLN:C	9:A:1074:HOH:O	2.45	0.58
1:A:772:GLU:OE1	1:A:772:GLU:HA	2.04	0.57
2:B:63:ALA:C	2:B:71:MET:HE3	2.30	0.57
1:A:313:ASN:C	1:A:313:ASN:HD22	2.11	0.57
2:B:141:TYR:N	9:B:1011:HOH:O	2.38	0.57
1:A:712:ILE:HG13	1:A:712:ILE:O	2.05	0.57
1:A:3:ILE:HD12	1:A:3:ILE:N	2.19	0.57
1:A:523:ILE:HD13	1:A:529:ILE:HD12	1.87	0.57
1:A:63:ASP:O	1:A:64:SER:HB2	2.05	0.56
1:A:284:ILE:HG13	1:A:288:ILE:HD13	1.87	0.56
1:A:343:GLU:HG3	1:A:344:GLU:N	2.20	0.56
1:A:296:LEU:HD11	9:A:1075:HOH:O	2.03	0.56
2:B:15:LYS:HD2	2:B:15:LYS:O	2.05	0.56
1:A:718:GLN:HB2	9:A:1119:HOH:O	2.05	0.56
1:A:341:THR:HG22	1:A:342:LYS:H	1.69	0.56
1:A:513:GLY:HA2	9:A:1109:HOH:O	2.06	0.56
3:C:46:ASN:O	3:C:49:VAL:HG22	2.05	0.56
1:A:501:LYS:H	1:A:501:LYS:CD	2.19	0.56
1:A:248:ARG:CG	9:A:1100:HOH:O	2.54	0.56
1:A:121:ILE:N	1:A:121:ILE:HD12	2.21	0.55
1:A:15:VAL:HG23	9:A:1031:HOH:O	2.06	0.55
1:A:51:SER:HB3	3:C:95:ARG:HH21	1.71	0.55
1:A:341:THR:HG22	1:A:342:LYS:N	2.21	0.55
1:A:603:ASN:ND2	9:A:1130:HOH:O	2.38	0.55
2:B:145:THR:O	2:B:148:ILE:HG22	2.07	0.55
1:A:12:TYR:CD1	1:A:130:PRO:HD2	2.42	0.55
3:C:87:MET:HE1	3:C:142:GLU:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HG3	1:A:82:PHE:N	2.21	0.55
1:A:212:GLU:HG3	1:A:218:GLN:NE2	2.21	0.55
1:A:248:ARG:HG3	9:A:1100:HOH:O	2.05	0.55
3:C:62:SER:O	3:C:63:LEU:HD23	2.07	0.55
1:A:234:THR:CG2	1:A:237:ASN:H	2.20	0.54
2:B:107:GLU:CD	2:B:107:GLU:H	2.11	0.54
1:A:137:ILE:O	1:A:137:ILE:HG22	2.07	0.54
1:A:309:TYR:CG	1:A:356:LEU:HG	2.42	0.54
1:A:51:SER:HB2	3:C:95:ARG:HE	1.71	0.54
1:A:321:ASN:OD1	1:A:322:ILE:HG13	2.08	0.54
1:A:397:ALA:HA	1:A:605:ASN:ND2	2.22	0.54
2:B:38:GLU:CD	2:B:38:GLU:N	2.64	0.54
1:A:81:LYS:HD2	1:A:82:PHE:CZ	2.42	0.54
1:A:177:GLU:OE2	1:A:690:GLN:HG2	2.08	0.54
1:A:615:GLU:HG3	1:A:618:VAL:H	1.72	0.54
1:A:715:GLU:HA	1:A:718:GLN:CG	2.38	0.54
1:A:127:ARG:HE	1:A:679:PRO:HB2	1.73	0.54
1:A:301:LEU:HD11	1:A:385:PHE:HD2	1.73	0.54
1:A:374:SER:OG	1:A:395:LEU:HD22	2.08	0.53
1:A:518:MET:CE	1:A:561:MET:HG2	2.34	0.53
1:A:242:ARG:NH2	7:A:998:GOL:H12	2.24	0.53
1:A:401:PRO:HG3	1:A:603:ASN:HD21	1.73	0.53
1:A:242:ARG:HH22	7:A:998:GOL:C1	2.22	0.53
1:A:597:LYS:O	1:A:645:ILE:HD12	2.08	0.53
1:A:201:LYS:HD3	1:A:201:LYS:N	2.24	0.52
1:A:534:GLU:CD	1:A:650:ARG:HH21	2.17	0.52
1:A:488:PHE:O	1:A:492:MET:HG2	2.09	0.52
1:A:320:ASP:O	1:A:321:ASN:OD1	2.27	0.52
1:A:173:LEU:HD13	1:A:459:LEU:HD23	1.90	0.52
1:A:473:GLU:O	1:A:477:ILE:HG12	2.09	0.52
2:B:121:ASN:HD22	2:B:123:ASP:N	1.99	0.51
2:B:105:ASN:HB3	2:B:107:GLU:OE1	2.10	0.51
2:B:69:PHE:CE2	2:B:73:LEU:HD11	2.46	0.51
2:B:105:ASN:ND2	9:B:999:HOH:O	2.43	0.51
1:A:5:PHE:CG	1:A:6:SER:N	2.72	0.51
1:A:399:LEU:HD23	1:A:419:VAL:HG21	1.93	0.51
1:A:721:SER:HB2	1:A:728:ILE:CD1	2.41	0.51
1:A:306:SER:C	1:A:308:LEU:H	2.19	0.51
1:A:292:ALA:HB3	1:A:328:PHE:HD2	1.76	0.51
1:A:563:THR:HG22	1:A:564:LYS:O	2.10	0.51
1:A:7:ASP:OD1	1:A:9:ASP:HB2	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD22	1:A:435:PHE:CG	2.46	0.50
1:A:361:MET:HE3	1:A:380:ALA:CB	2.42	0.50
1:A:755:LEU:HG	1:A:755:LEU:O	2.11	0.50
2:B:135:GLU:OE2	2:B:138:LYS:HD2	2.11	0.50
1:A:547:PHE:CD2	9:A:1138:HOH:O	2.48	0.50
1:A:599:LYS:HD2	1:A:644:THR:CG2	2.37	0.50
1:A:762:PHE:HB3	1:A:766:VAL:HB	1.92	0.50
2:B:116:MET:HG2	3:C:21:TRP:O	2.11	0.50
2:B:118:ASP:OD1	3:C:24:ARG:HD2	2.11	0.50
2:B:106:ILE:HG23	2:B:107:GLU:N	2.26	0.50
1:A:115:TYR:CE1	9:A:1143:HOH:O	2.55	0.50
1:A:223:ASN:HB2	1:A:224:PRO:HD3	1.94	0.50
1:A:770:LEU:HD23	1:A:773:MET:CE	2.42	0.50
1:A:784:MET:SD	3:C:79:GLU:HG2	2.52	0.50
1:A:603:ASN:CB	9:A:1117:HOH:O	2.47	0.50
1:A:729:PRO:O	1:A:730:GLN:CB	2.59	0.50
1:A:816:ARG:O	1:A:820:VAL:HG12	2.12	0.50
3:C:96:GLU:HG3	3:C:98:GLN:CG	2.36	0.49
1:A:750:PRO:HA	1:A:753:TYR:CE1	2.47	0.49
3:C:72:TYR:CE2	3:C:76:MET:SD	3.06	0.49
1:A:403:VAL:HG22	1:A:404:LYS:N	2.19	0.49
1:A:543:ASP:H	1:A:546:SER:HB3	1.78	0.49
1:A:277:SER:O	1:A:278:ALA:HB3	2.13	0.49
1:A:186:THR:O	1:A:190:ILE:HG12	2.12	0.49
1:A:384:ALA:HB1	1:A:389:ILE:O	2.12	0.48
1:A:518:MET:HE1	1:A:560:ARG:HG2	1.94	0.48
1:A:520:ILE:O	1:A:524:GLU:HG2	2.13	0.48
3:C:107:ARG:NH1	3:C:119:ASP:OD1	2.44	0.48
1:A:603:ASN:ND2	9:A:1117:HOH:O	2.47	0.48
1:A:486:GLN:HE22	1:A:517:GLN:HG2	1.77	0.48
1:A:799:LYS:HG2	9:A:1110:HOH:O	2.13	0.48
1:A:461:ILE:C	1:A:461:ILE:HD12	2.39	0.48
3:C:69:LEU:O	3:C:73:GLU:HG3	2.14	0.48
1:A:7:ASP:OD2	1:A:139:LYS:NZ	2.47	0.48
1:A:305:ASP:O	1:A:308:LEU:HB2	2.14	0.47
1:A:729:PRO:O	1:A:730:GLN:HB2	2.14	0.47
2:B:65:GLY:O	2:B:66:PRO:C	2.57	0.47
1:A:104:ARG:HG3	1:A:682:VAL:HG21	1.96	0.47
3:C:49:VAL:HA	3:C:52:VAL:HG22	1.96	0.47
1:A:602:ILE:HD12	1:A:602:ILE:O	2.14	0.47
1:A:651:GLU:OE2	1:A:651:GLU:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ASN:ND2	2:B:71:MET:H	2.12	0.47
1:A:496:GLU:HG3	1:A:500:TYR:CZ	2.49	0.47
1:A:321:ASN:OD1	1:A:321:ASN:C	2.57	0.47
1:A:451:LYS:HE2	1:A:452:ARG:O	2.14	0.47
2:B:109:ILE:O	2:B:109:ILE:HD12	2.14	0.47
1:A:236:ARG:HB2	7:A:998:GOL:C3	2.44	0.47
1:A:415:ASN:HD21	1:A:418:GLN:HG3	1.80	0.47
1:A:438:LEU:HD23	1:A:438:LEU:C	2.40	0.47
1:A:812:GLN:O	1:A:816:ARG:HG3	2.15	0.47
1:A:236:ARG:HB2	7:A:998:GOL:H31	1.96	0.47
2:B:38:GLU:CD	2:B:38:GLU:H	2.21	0.47
1:A:570:ARG:O	1:A:573:GLN:HB2	2.15	0.47
1:A:658:LYS:CA	9:A:1106:HOH:O	2.63	0.47
1:A:814:ASN:ND2	2:B:84:ASP:H	2.07	0.47
3:C:122:VAL:O	3:C:126:ILE:HG13	2.14	0.47
1:A:397:ALA:CB	1:A:605:ASN:ND2	2.78	0.47
1:A:501:LYS:N	1:A:501:LYS:CD	2.76	0.47
1:A:268:GLU:OE1	1:A:271:ARG:NE	2.39	0.46
1:A:833:VAL:HG13	2:B:26:MET:SD	2.55	0.46
1:A:85:LEU:N	1:A:102:ASN:HD21	2.14	0.46
1:A:214:SER:O	1:A:218:GLN:HG3	2.15	0.46
1:A:312:ILE:HD13	1:A:356:LEU:HD11	1.96	0.46
1:A:426:LEU:HD13	1:A:606:VAL:HG11	1.97	0.46
1:A:713:TYR:CE2	1:A:736:LYS:HG2	2.50	0.46
1:A:94:LEU:HD13	1:A:697:LEU:CB	2.45	0.46
1:A:141:ARG:N	9:A:1104:HOH:O	2.18	0.46
1:A:658:LYS:HA	9:A:1106:HOH:O	2.14	0.46
3:C:24:ARG:O	3:C:24:ARG:HG2	2.15	0.46
1:A:138:ALA:C	9:A:1104:HOH:O	2.58	0.46
1:A:493:PHE:O	1:A:496:GLU:HB3	2.14	0.46
1:A:527:MET:HE2	1:A:555:HIS:CD2	2.50	0.46
1:A:518:MET:HE1	1:A:560:ARG:CZ	2.46	0.46
2:B:121:ASN:HD22	2:B:121:ASN:C	2.24	0.46
3:C:101:ILE:CD1	3:C:105:GLU:HG2	2.42	0.46
1:A:215:LEU:O	1:A:219:ILE:HG13	2.16	0.46
1:A:756:GLY:CA	1:A:759:LYS:O	2.61	0.46
1:A:833:VAL:C	1:A:835:PRO:CD	2.75	0.46
1:A:721:SER:HA	1:A:742:ILE:HD13	1.94	0.46
1:A:455:TYR:CD1	1:A:455:TYR:C	2.93	0.46
1:A:126:TYR:CZ	1:A:677:LYS:HA	2.51	0.45
1:A:527:MET:HE3	1:A:554:ASN:OD1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:CB	9:B:1014:HOH:O	2.64	0.45
2:B:69:PHE:CZ	2:B:73:LEU:HD21	2.51	0.45
3:C:69:LEU:CB	3:C:70:PRO:HD3	2.46	0.45
1:A:212:GLU:CD	1:A:218:GLN:HE22	2.25	0.45
1:A:371:GLN:HG3	1:A:372:ALA:N	2.30	0.45
1:A:518:MET:HE2	1:A:561:MET:CG	2.40	0.45
1:A:814:ASN:O	2:B:148:ILE:HD11	2.16	0.45
2:B:35:VAL:HB	2:B:67:LEU:CD2	2.46	0.45
3:C:69:LEU:HB3	3:C:70:PRO:HD3	1.98	0.45
1:A:513:GLY:C	9:A:1109:HOH:O	2.59	0.45
1:A:157:ASP:OD2	1:A:192:TYR:OH	2.25	0.45
1:A:671:ILE:HD12	1:A:671:ILE:C	2.42	0.45
1:A:106:ARG:HB3	1:A:111:LEU:HB2	1.99	0.45
7:A:998:GOL:H11	9:A:1019:HOH:O	2.18	0.45
2:B:14:GLN:C	2:B:14:GLN:CD	2.84	0.45
1:A:251:PHE:CE1	1:A:456:ILE:HG13	2.52	0.44
1:A:404:LYS:C	1:A:404:LYS:HD2	2.42	0.44
1:A:560:ARG:NH1	1:A:560:ARG:HG2	2.31	0.44
1:A:319:VAL:HB	1:A:322:ILE:HB	1.99	0.44
2:B:99:GLN:CB	2:B:101:THR:HG23	2.47	0.44
3:C:135:LEU:HD12	3:C:135:LEU:H	1.83	0.44
1:A:12:TYR:HD1	1:A:130:PRO:HD2	1.82	0.44
1:A:661:TYR:OH	9:A:1074:HOH:O	1.95	0.44
1:A:387:CYS:O	1:A:613:SER:OG	2.34	0.44
1:A:461:ILE:HD12	1:A:461:ILE:O	2.16	0.44
2:B:107:GLU:OE1	2:B:107:GLU:N	2.41	0.44
2:B:121:ASN:ND2	2:B:123:ASP:N	2.62	0.44
1:A:507:TRP:CZ3	1:A:763:LYS:HG3	2.53	0.44
2:B:142:VAL:HG22	9:B:1011:HOH:O	2.17	0.44
1:A:712:ILE:O	1:A:713:TYR:C	2.59	0.44
2:B:44:SER:O	2:B:48:GLY:N	2.49	0.44
1:A:242:ARG:HD2	1:A:271:ARG:NE	2.33	0.44
1:A:738:VAL:O	1:A:742:ILE:HG13	2.18	0.44
1:A:247:ILE:O	1:A:457:GLY:HA2	2.19	0.43
1:A:409:MET:HA	9:A:1116:HOH:O	2.17	0.43
1:A:390:ASN:ND2	1:A:392:GLY:N	2.66	0.43
1:A:713:TYR:HE2	1:A:756:GLY:O	2.02	0.43
1:A:799:LYS:CG	1:A:800:LYS:N	2.81	0.43
1:A:211:LYS:HB3	1:A:211:LYS:HE2	1.62	0.43
1:A:159:ALA:O	1:A:170:GLN:HG3	2.18	0.43
1:A:527:MET:CE	1:A:554:ASN:HB3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:GLU:HA	1:A:607:VAL:CG2	2.48	0.43
2:B:17:ILE:CD1	2:B:73:LEU:HD22	2.48	0.43
2:B:42:ALA:O	2:B:46:GLN:HB2	2.19	0.43
2:B:114:GLU:HB2	2:B:125:MET:SD	2.59	0.43
2:B:29:VAL:C	2:B:31:ARG:H	2.27	0.43
2:B:68:ASN:ND2	2:B:68:ASN:H	2.16	0.43
2:B:121:ASN:ND2	2:B:121:ASN:C	2.77	0.43
1:A:284:ILE:HG23	1:A:285:PHE:N	2.34	0.43
2:B:24:PHE:CD1	2:B:24:PHE:C	2.96	0.43
1:A:106:ARG:NH2	1:A:113:TYR:O	2.47	0.42
1:A:659:ASN:HD22	1:A:659:ASN:HA	1.57	0.42
2:B:145:THR:HA	2:B:148:ILE:HG22	2.00	0.42
1:A:29:ASP:N	1:A:33:ASN:HD22	2.00	0.42
1:A:497:GLN:O	1:A:501:LYS:CD	2.58	0.42
1:A:724:ALA:N	1:A:725:PRO:HD3	2.34	0.42
1:A:799:LYS:HG2	1:A:800:LYS:H	1.84	0.42
1:A:711:LEU:O	1:A:759:LYS:HB2	2.19	0.42
1:A:822:ARG:HE	1:A:822:ARG:HB3	1.46	0.42
2:B:84:ASP:O	2:B:149:LYS:HE3	2.18	0.42
1:A:234:THR:CG2	7:A:998:GOL:O2	2.58	0.42
1:A:721:SER:HB2	1:A:728:ILE:HD13	2.01	0.42
2:B:101:THR:O	2:B:102:LYS:HB2	2.20	0.42
1:A:148:ILE:HG23	9:A:1088:HOH:O	2.20	0.42
1:A:503:GLU:O	1:A:757:THR:HG23	2.19	0.42
1:A:763:LYS:O	1:A:766:VAL:HG23	2.19	0.42
3:C:134:ASP:OD1	3:C:136:GLU:HG2	2.19	0.42
1:A:194:ALA:O	1:A:198:CYS:HB3	2.19	0.42
2:B:99:GLN:HB2	2:B:101:THR:HG23	2.01	0.42
1:A:377:THR:HG22	1:A:395:LEU:HD11	2.01	0.42
1:A:264:THR:HG21	1:A:439:VAL:HG21	2.02	0.42
1:A:170:GLN:O	1:A:456:ILE:HA	2.20	0.42
1:A:261:ASP:OD1	9:A:1100:HOH:O	2.22	0.42
1:A:415:ASN:ND2	1:A:418:GLN:HG3	2.35	0.42
1:A:745:GLY:C	1:A:747:GLN:N	2.77	0.42
3:C:36:VAL:HG21	3:C:68:PHE:CZ	2.55	0.42
1:A:126:TYR:CE2	1:A:677:LYS:HA	2.55	0.41
1:A:522:LEU:CD1	1:A:580:LEU:HD11	2.48	0.41
1:A:309:TYR:O	1:A:313:ASN:CG	2.63	0.41
1:A:763:LYS:O	1:A:764:ALA:C	2.63	0.41
2:B:75:ILE:HG13	2:B:76:PHE:N	2.34	0.41
1:A:236:ARG:HB2	7:A:998:GOL:O3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:LEU:HD23	1:A:819:LEU:HA	1.93	0.41
2:B:68:ASN:C	2:B:68:ASN:HD22	2.27	0.41
1:A:48:ILE:HA	1:A:58:VAL:HG12	2.03	0.41
1:A:124:ASN:C	1:A:124:ASN:OD1	2.63	0.41
1:A:553:GLN:HB3	9:A:1047:HOH:O	2.20	0.41
1:A:723:LEU:HB3	1:A:746:LEU:HD21	2.02	0.41
1:A:32:LYS:O	1:A:47:GLU:HA	2.20	0.41
1:A:137:ILE:O	1:A:137:ILE:CG2	2.69	0.41
1:A:216:GLU:HA	1:A:219:ILE:HD12	2.03	0.41
1:A:227:GLU:O	1:A:231:ASN:HB2	2.20	0.41
1:A:438:LEU:HD23	1:A:438:LEU:O	2.20	0.41
1:A:163:MET:HE2	1:A:163:MET:HB3	1.82	0.41
1:A:242:ARG:HD2	1:A:271:ARG:HE	1.85	0.41
2:B:140:ASP:OD1	2:B:142:VAL:CG2	2.66	0.41
1:A:234:THR:HG22	1:A:237:ASN:O	2.21	0.41
1:A:273:THR:OG1	1:A:428:LYS:HE2	2.21	0.41
1:A:364:LYS:O	1:A:365:GLN:C	2.63	0.41
1:A:695:GLY:O	1:A:696:VAL:C	2.62	0.41
3:C:91:LYS:HB3	3:C:91:LYS:HE2	1.76	0.41
1:A:141:ARG:HE	1:A:141:ARG:HB3	1.69	0.41
1:A:396:LYS:C	1:A:398:LEU:H	2.29	0.40
1:A:473:GLU:H	1:A:473:GLU:CD	2.29	0.40
2:B:115:ASN:C	2:B:116:MET:HG3	2.45	0.40
1:A:650:ARG:NH1	1:A:650:ARG:HG2	2.36	0.40
2:B:123:ASP:O	2:B:127:MET:HG2	2.21	0.40
1:A:438:LEU:C	1:A:438:LEU:CD2	2.95	0.40
1:A:650:ARG:HG2	1:A:650:ARG:HH11	1.85	0.40
1:A:713:TYR:CE2	1:A:756:GLY:O	2.75	0.40
2:B:121:ASN:ND2	2:B:124:GLU:HG3	2.36	0.40
3:C:60:GLU:HB2	9:C:1011:HOH:O	2.22	0.40
3:C:98:GLN:HB2	9:C:1015:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	777/837 (93%)	723 (93%)	47 (6%)	7 (1%)	14	17
2	B	137/139 (99%)	124 (90%)	10 (7%)	3 (2%)	5	4
3	C	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
All	All	1066/1130 (94%)	992 (93%)	64 (6%)	10 (1%)	14	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	697	LEU
1	A	18	LYS
1	A	20	LEU
1	A	713	TYR
2	B	31	ARG
2	B	49	ARG
1	A	19	LYS
1	A	403	VAL
2	B	64	PRO

5.3.2 Protein sidechains ⓘ

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	657/730 (90%)	612 (93%)	45 (7%)	14	20
2	B	110/122 (90%)	102 (93%)	8 (7%)	13	18
3	C	120/130 (92%)	114 (95%)	6 (5%)	22	33
All	All	887/982 (90%)	828 (93%)	59 (7%)	15	21

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	13	LEU
1	A	17	ARG
1	A	68	THR
1	A	94	LEU
1	A	121	ILE
1	A	128	ARG
1	A	144	ARG
1	A	147	GLU
1	A	167	ARG
1	A	173	LEU
1	A	191	MET
1	A	236	ARG
1	A	245	LYS
1	A	269	LYS
1	A	288	ILE
1	A	313	ASN
1	A	326	GLU
1	A	338	LEU
1	A	343	GLU
1	A	350	LYS
1	A	379	GLU
1	A	409	MET
1	A	438	LEU
1	A	475	LEU
1	A	482	GLU
1	A	485	GLN
1	A	499	GLU
1	A	510	ILE
1	A	517	GLN
1	A	519	CYS
1	A	522	LEU
1	A	525	LYS
1	A	543	ASP
1	A	602	ILE
1	A	614	LYS
1	A	650	ARG
1	A	651	GLU
1	A	665	PRO
1	A	671	ILE
1	A	694	ASN
1	A	718	GLN
1	A	723	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	737	THR
1	A	755	LEU
2	B	46	GLN
2	B	68	ASN
2	B	98	GLU
2	B	107	GLU
2	B	109	ILE
2	B	121	ASN
2	B	148	ILE
2	B	151	SER
3	C	68	PHE
3	C	69	LEU
3	C	105	GLU
3	C	128	LEU
3	C	136	GLU
3	C	140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	33	ASN
1	A	49	GLN
1	A	102	ASN
1	A	162	ASN
1	A	170	GLN
1	A	218	GLN
1	A	221	GLN
1	A	238	ASN
1	A	313	ASN
1	A	371	GLN
1	A	390	ASN
1	A	415	ASN
1	A	417	ASN
1	A	421	ASN
1	A	485	GLN
1	A	486	GLN
1	A	489	ASN
1	A	491	HIS
1	A	497	GLN
1	A	603	ASN
1	A	605	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	643	GLN
1	A	659	ASN
1	A	694	ASN
1	A	747	GLN
1	A	769	ASN
1	A	814	ASN
2	B	68	ASN
2	B	91	ASN
2	B	121	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 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	$\# Z > 2$
6	ADP	A	996	4,5	28,29,29	1.56	6 (21%)	43,45,45	1.07	3 (6%)
5	BEF	A	995	6	0,3,3	-	-	-		
7	GOL	A	998	-	5,5,5	1.50	1 (20%)	5,5,5	1.27	0

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	996	4,5	-	3/16/32/32	0/3/3/3
7	GOL	A	998	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	996	ADP	PA-O5'	-3.81	1.44	1.59
6	A	996	ADP	C4-N3	3.68	1.41	1.34
7	A	998	GOL	C3-C2	2.66	1.61	1.51
6	A	996	ADP	PB-O2B	-2.42	1.45	1.54
6	A	996	ADP	PA-O3A	-2.34	1.57	1.59
6	A	996	ADP	PA-O2A	-2.04	1.45	1.55
6	A	996	ADP	C5'-C4'	-2.02	1.45	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	996	ADP	O3B-PB-O3A	2.87	114.27	104.64
6	A	996	ADP	O3A-PB-O1B	-2.77	96.46	111.04
6	A	996	ADP	O2B-PB-O3A	2.13	111.78	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

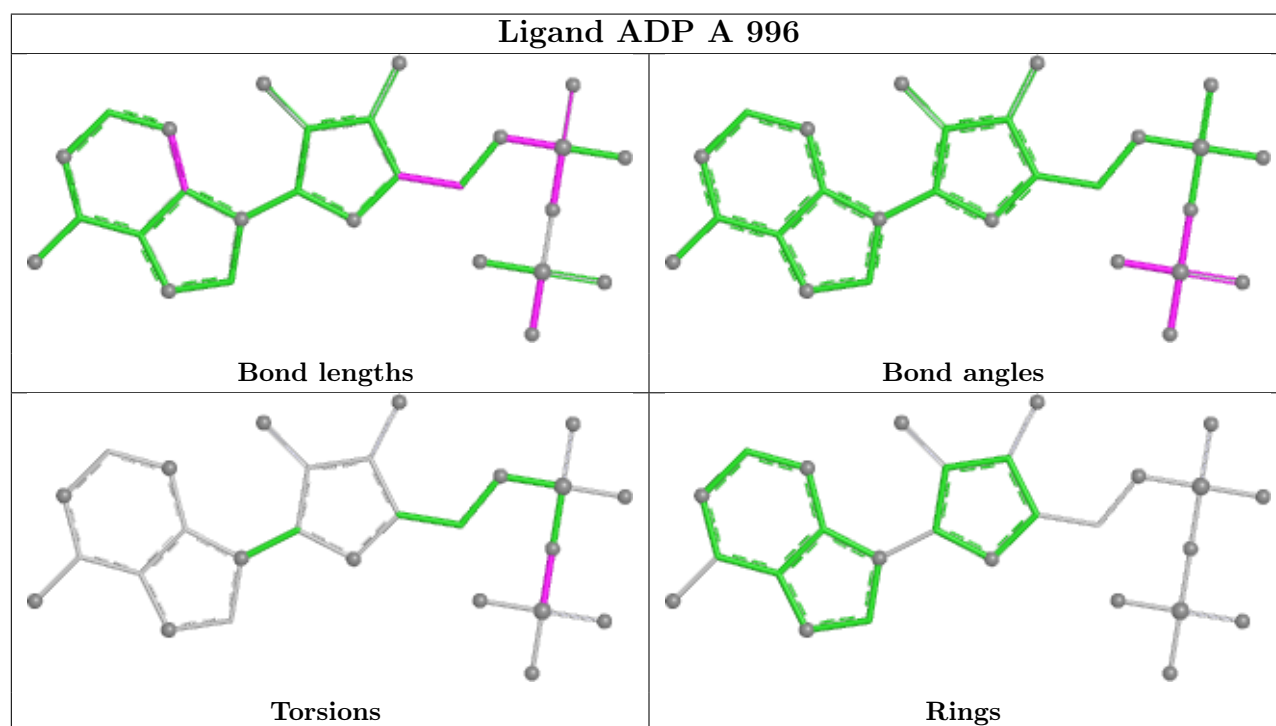
Mol	Chain	Res	Type	Atoms
6	A	996	ADP	PA-O3A-PB-O2B
7	A	998	GOL	O1-C1-C2-C3
7	A	998	GOL	O1-C1-C2-O2
6	A	996	ADP	PA-O3A-PB-O1B
6	A	996	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	998	GOL	9	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 than 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.



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	793/837 (94%)	0.55	48 (6%)	27 29	29, 51, 87, 99	3 (0%)
2	B	139/139 (100%)	0.62	5 (3%)	46 48	39, 62, 89, 96	0
3	C	154/154 (100%)	0.50	3 (1%)	66 68	33, 54, 79, 88	1 (0%)
All	All	1086/1130 (96%)	0.55	56 (5%)	33 34	29, 53, 86, 99	4 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	LEU	5.0
1	A	21	MET	4.7
1	A	568	PRO	3.9
1	A	3	ILE	3.7
1	A	198	CYS	3.7
1	A	17	ARG	3.7
1	A	755	LEU	3.6
2	B	16	GLN	3.2
2	B	151	SER	3.2
1	A	252	GLY	3.1
1	A	696	VAL	3.1
1	A	583	TYR	3.0
1	A	370	GLU	2.9
1	A	5	PHE	2.9
1	A	1	MET	2.8
1	A	410	VAL	2.8
1	A	512	PHE	2.8
1	A	22	LYS	2.7
1	A	750	PRO	2.7
1	A	172	CYS	2.7
2	B	13	PRO	2.6
1	A	122	ALA	2.6
1	A	477	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	399	LEU	2.6
1	A	510	ILE	2.6
1	A	201	LYS	2.5
1	A	538	MET	2.5
1	A	706	GLY	2.5
1	A	697	LEU	2.4
1	A	62	ALA	2.4
1	A	2	ASN	2.4
1	A	211	LYS	2.4
1	A	537	CYS	2.4
1	A	403	VAL	2.3
1	A	25	THR	2.3
1	A	591	ILE	2.3
1	A	321	ASN	2.3
1	A	830	TYR	2.3
1	A	527	MET	2.3
1	A	38	ASP	2.2
3	C	9	ASP	2.2
3	C	122	VAL	2.2
1	A	619	ALA	2.2
1	A	724	ALA	2.2
1	A	210	LYS	2.2
1	A	398	LEU	2.1
1	A	595	LEU	2.1
1	A	705	LYS	2.1
1	A	571	PRO	2.1
2	B	66	PRO	2.1
1	A	532	ILE	2.1
2	B	14	GLN	2.1
1	A	26	ALA	2.0
1	A	489	ASN	2.0
1	A	16	ASP	2.0
3	C	12	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

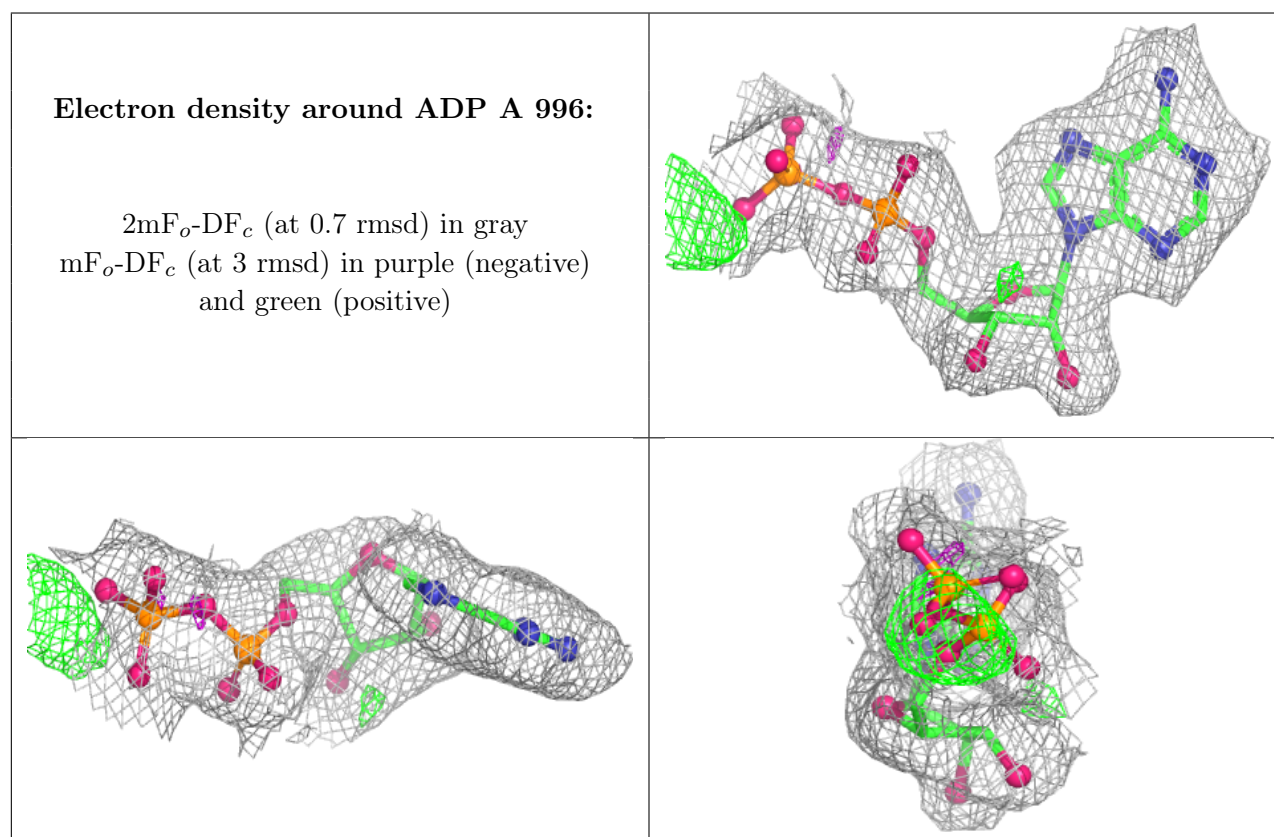
There are no oligosaccharides in this entry.

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
7	GOL	A	998	6/6	0.81	0.15	55,56,58,59	0
5	BEF	A	995	4/4	0.88	0.19	33,35,36,39	0
6	ADP	A	996	27/27	0.96	0.06	32,34,36,39	0
4	MG	A	997	1/1	0.97	0.04	29,29,29,29	0
4	MG	B	998	1/1	0.98	0.03	61,61,61,61	0
8	CA	C	999	1/1	0.99	0.02	44,44,44,44	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.