



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:53 PM GMT

PDB ID : 1D1C
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH N-METHYL-O-NITROPHENYL AMINOETHYL
DIPHOSPHATE BERYLLIUM TRIFLUORIDE.
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on : 1999-09-15
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

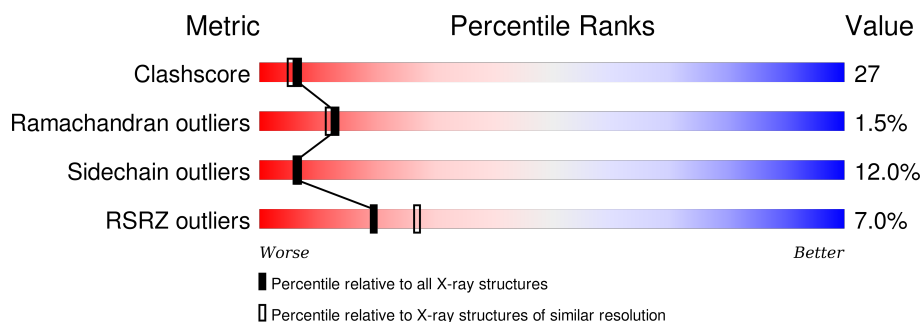
1 Overall quality at a glance

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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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 $\leq 5\%$. 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	761	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6528 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	744	Total	C	N	O	S	0	0	0
			5910	3759	1017	1118	16			

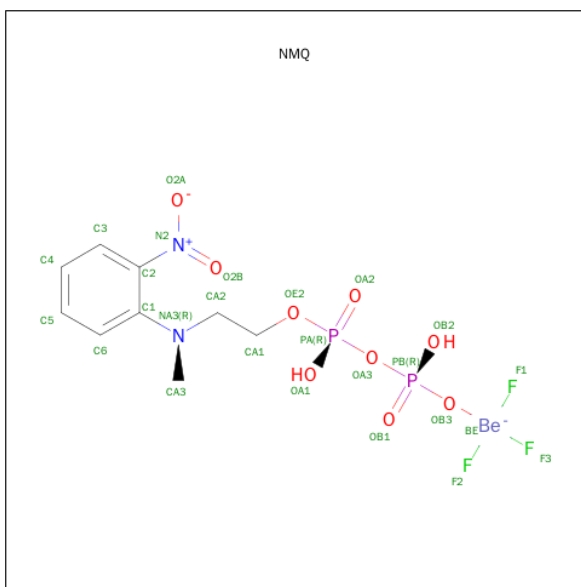
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	SEE REMARK 999	UNP P08799
A	760	PRO	GLN	ENGINEERED	UNP P08799
A	761	ASN	ARG	ENGINEERED	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is N-METHYL O-NITROPHENYL AMINOETHYLDIPHOSPHATE BERYLLIUM TRIFLUORIDE (three-letter code: NMQ) (formula: C₉H₁₃BeF₃N₂O₉P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	26	1	9	3	2	9	2	0	0

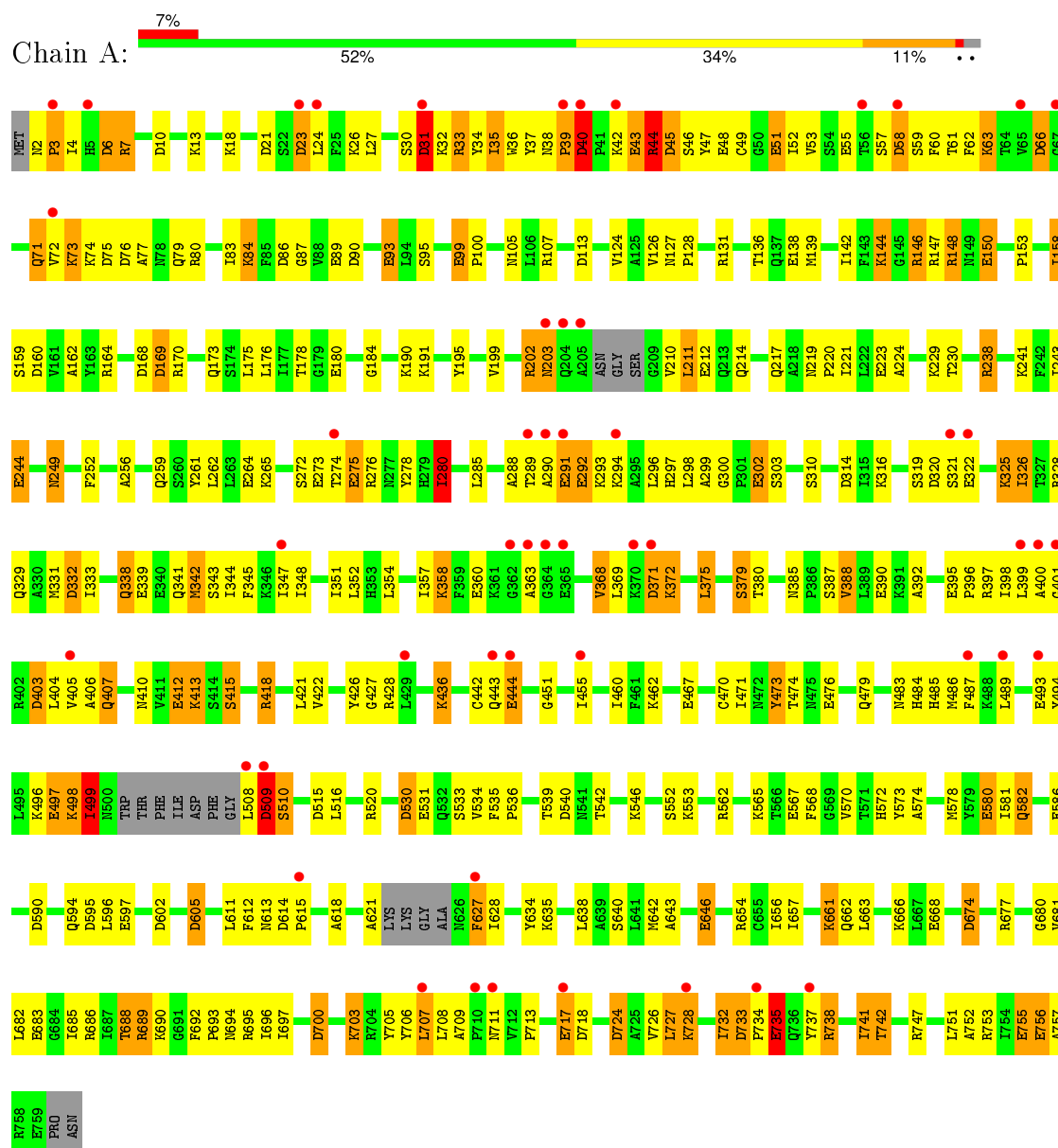
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	591	Total	O	0	0
			591	591		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYOSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.90 Å 180.90 Å 54.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 24.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.9 (25.00-2.30) 87.9 (24.01-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.31 Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.181 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 97.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 40689 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6528	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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, 0.375 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, NMQ

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	0.96	32/6022 (0.5%)	1.27	71/8131 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	580	GLU	CD-OE2	9.46	1.36	1.25
1	A	275	GLU	CD-OE2	6.73	1.33	1.25
1	A	43	GLU	CD-OE2	6.56	1.32	1.25
1	A	497	GLU	CD-OE2	6.56	1.32	1.25
1	A	531	GLU	CD-OE2	6.52	1.32	1.25
1	A	244	GLU	CD-OE2	6.40	1.32	1.25
1	A	717	GLU	CD-OE2	6.30	1.32	1.25
1	A	668	GLU	CD-OE2	6.18	1.32	1.25
1	A	212	GLU	CD-OE2	6.13	1.32	1.25
1	A	586	GLU	CD-OE2	6.07	1.32	1.25
1	A	683	GLU	CD-OE2	6.07	1.32	1.25
1	A	89	GLU	CD-OE2	6.02	1.32	1.25
1	A	444	GLU	CD-OE2	5.97	1.32	1.25
1	A	339	GLU	CD-OE2	5.91	1.32	1.25
1	A	55	GLU	CD-OE2	5.89	1.32	1.25
1	A	93	GLU	CD-OE2	5.89	1.32	1.25
1	A	360	GLU	CD-OE2	5.87	1.32	1.25
1	A	51	GLU	CD-OE2	5.84	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	GLU	CD-OE2	5.75	1.31	1.25
1	A	646	GLU	CD-OE2	5.70	1.31	1.25
1	A	390	GLU	CD-OE2	5.68	1.31	1.25
1	A	412	GLU	CD-OE2	5.64	1.31	1.25
1	A	291	GLU	CD-OE2	5.57	1.31	1.25
1	A	48	GLU	CD-OE2	5.56	1.31	1.25
1	A	138	GLU	CD-OE2	5.50	1.31	1.25
1	A	180	GLU	CD-OE2	5.50	1.31	1.25
1	A	756	GLU	CD-OE2	5.49	1.31	1.25
1	A	735	GLU	CD-OE2	5.47	1.31	1.25
1	A	292	GLU	CD-OE2	5.28	1.31	1.25
1	A	755	GLU	CD-OE2	5.18	1.31	1.25
1	A	150	GLU	CD-OE2	5.09	1.31	1.25
1	A	99	GLU	CD-OE2	5.04	1.31	1.25

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	148	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	320	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	238	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	614	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	590	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	A	320	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	A	418	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	148	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	595	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	A	40	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	737	TYR	O-C-N	6.93	133.78	122.70
1	A	160	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	168	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	113	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	530	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	6	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	238	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	169	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	10	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	66	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	A	614	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	31	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	75	ASP	CB-CG-OD2	-6.40	112.54	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	A	168	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	160	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	590	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	718	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	31	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	202	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	45	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	A	428	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	602	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	76	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	627	PHE	N-CA-CB	5.98	121.36	110.60
1	A	7	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	605	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	509	ASP	O-C-N	-5.90	113.27	122.70
1	A	737	TYR	CA-C-N	-5.88	104.27	117.20
1	A	23	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	332	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	6	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	371	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	371	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	605	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	602	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	45	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	733	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	595	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	674	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	509	ASP	N-CA-C	5.62	126.18	111.00
1	A	530	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	515	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	58	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	58	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	724	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	169	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	23	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	10	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	21	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	33	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	164	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	674	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	21	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	A	33	ARG	NE-CZ-NH2	-5.25	117.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ILE	CB-CA-C	-5.24	101.13	111.60
1	A	202	ARG	CB-CA-C	5.19	120.79	110.40
1	A	75	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	40	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	700	ASP	CB-CG-OD1	5.04	122.83	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	606	ASN	CA

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	5910	0	5820	318	0
2	A	1	0	0	0	0
3	A	26	0	11	5	0
4	A	591	0	0	30	0
All	All	6528	0	5831	321	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 27.

All (321) 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:147:ARG:HB2	1:A:150:GLU:HG3	1.30	1.12
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.19	1.12
1:A:707:LEU:HD23	1:A:707:LEU:H	1.17	1.08
1:A:385:ASN:HB3	1:A:388:VAL:HG21	1.38	1.04
1:A:686:ARG:HA	1:A:689:ARG:HH12	1.25	0.98
1:A:385:ASN:HB3	1:A:388:VAL:CG2	1.94	0.97
1:A:707:LEU:CD2	1:A:707:LEU:H	1.81	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HH11	1:A:252:PHE:HB2	1.31	0.93
1:A:741:ILE:HG22	1:A:742:THR:CG2	1.99	0.93
1:A:410:ASN:H	1:A:413:LYS:HZ3	1.01	0.92
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.52	0.90
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.53	0.90
1:A:707:LEU:HD23	1:A:707:LEU:N	1.89	0.88
1:A:410:ASN:H	1:A:413:LYS:NZ	1.74	0.86
1:A:40:ASP:OD2	1:A:42:LYS:HB2	1.76	0.86
1:A:273:GLU:O	1:A:274:THR:OG1	1.95	0.85
1:A:249:ASN:H	1:A:249:ASN:ND2	1.71	0.84
1:A:59:SER:HB2	1:A:72:VAL:O	1.77	0.84
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.60	0.84
1:A:202:ARG:HH11	1:A:252:PHE:CB	1.89	0.84
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.61	0.82
1:A:686:ARG:HA	1:A:689:ARG:NH1	1.95	0.82
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.10	0.82
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.79	0.81
1:A:735:GLU:HA	1:A:738:ARG:HH22	1.46	0.81
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.07	0.81
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.83	0.81
1:A:43:GLU:HA	4:A:1110:HOH:O	1.81	0.80
1:A:84:LYS:HE3	4:A:1251:HOH:O	1.83	0.78
1:A:44:ARG:HH21	1:A:677:ARG:CZ	1.96	0.78
1:A:62:PHE:HE2	1:A:72:VAL:HG23	1.50	0.77
1:A:158:ILE:HD13	1:A:159:SER:N	1.99	0.77
1:A:689:ARG:HB3	1:A:689:ARG:HH11	1.50	0.77
1:A:497:GLU:O	1:A:741:ILE:HD12	1.85	0.76
1:A:176:LEU:HD12	1:A:176:LEU:N	2.01	0.76
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.68	0.76
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.66	0.75
1:A:289:THR:HB	1:A:291:GLU:OE2	1.87	0.75
1:A:290:ALA:HA	1:A:293:LYS:CD	2.17	0.75
1:A:510:SER:HB2	4:A:1438:HOH:O	1.88	0.74
1:A:497:GLU:C	1:A:741:ILE:HD12	2.08	0.74
1:A:241:LYS:HD2	1:A:243:ILE:HD11	1.69	0.74
1:A:397:ARG:HD2	1:A:404:LEU:CD1	2.17	0.73
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.68	0.73
1:A:62:PHE:HE2	1:A:72:VAL:CG2	2.02	0.72
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.71	0.71
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.71	0.71
1:A:344:ILE:O	1:A:348:ILE:HG12	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HG11	1:A:63:LYS:CG	2.20	0.71
1:A:735:GLU:OE2	1:A:747:ARG:NH2	2.22	0.71
1:A:682:LEU:O	1:A:686:ARG:HG3	1.91	0.71
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.09	0.71
1:A:202:ARG:NH1	1:A:252:PHE:HB2	2.06	0.71
1:A:396:PRO:HG2	1:A:398:ILE:HD11	1.72	0.70
1:A:24:LEU:HD23	1:A:24:LEU:N	2.05	0.70
1:A:289:THR:HG23	1:A:292:GLU:OE2	1.91	0.69
1:A:302:GLU:H	1:A:302:GLU:CD	1.94	0.69
1:A:574:ALA:HA	4:A:1258:HOH:O	1.93	0.69
1:A:407:GLN:HA	1:A:407:GLN:HE21	1.56	0.69
1:A:321:SER:O	1:A:325:LYS:HE3	1.93	0.69
1:A:343:SER:HB3	1:A:605:ASP:OD1	1.92	0.69
1:A:706:TYR:CE2	1:A:707:LEU:HD22	2.28	0.68
1:A:395:GLU:HA	1:A:407:GLN:O	1.93	0.68
1:A:399:LEU:HD13	1:A:401:GLY:H	1.59	0.68
1:A:689:ARG:CB	1:A:689:ARG:HH11	2.06	0.68
1:A:224:ALA:O	1:A:280:ILE:HG13	1.92	0.68
1:A:642:MET:O	1:A:646:GLU:HG2	1.92	0.67
1:A:509:ASP:O	1:A:509:ASP:OD2	2.12	0.67
1:A:44:ARG:NH2	1:A:677:ARG:NE	2.43	0.67
1:A:689:ARG:HH11	1:A:689:ARG:CG	2.08	0.67
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.25	0.67
1:A:415:SER:OG	1:A:418:ARG:NH2	2.27	0.67
1:A:582:GLN:NE2	4:A:1057:HOH:O	2.29	0.66
1:A:396:PRO:O	1:A:398:ILE:HD12	1.94	0.66
3:A:999:NMQ:OE2	3:A:999:NMQ:HA33	1.96	0.66
1:A:23:ASP:OD2	1:A:23:ASP:N	2.28	0.66
1:A:2:ASN:ND2	4:A:1336:HOH:O	2.30	0.65
1:A:238:ARG:HD3	1:A:264:GLU:OE2	1.96	0.65
1:A:392:ALA:HB1	1:A:596:LEU:HD23	1.79	0.65
1:A:735:GLU:HA	1:A:738:ARG:NH2	2.10	0.65
1:A:385:ASN:O	1:A:388:VAL:HG23	1.97	0.65
1:A:219:ASN:N	1:A:220:PRO:HD2	2.12	0.65
1:A:316:LYS:NZ	4:A:1428:HOH:O	2.30	0.64
1:A:296:LEU:HB3	1:A:298:LEU:HD21	1.80	0.64
1:A:44:ARG:NH1	4:A:1311:HOH:O	2.30	0.63
1:A:397:ARG:HA	1:A:406:ALA:HA	1.81	0.63
1:A:508:LEU:HG	1:A:509:ASP:H	1.64	0.62
1:A:398:ILE:HD13	1:A:407:GLN:HG2	1.81	0.62
1:A:485:HIS:NE2	1:A:489:LEU:HD11	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:CB	1:A:150:GLU:HG3	2.20	0.62
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.81	0.62
1:A:329:GLN:O	1:A:332:ASP:HB2	1.99	0.62
1:A:436:LYS:HB3	1:A:436:LYS:HZ3	1.63	0.62
1:A:38:ASN:ND2	1:A:46:SER:O	2.31	0.62
1:A:410:ASN:OD1	1:A:413:LYS:HB2	2.01	0.61
1:A:53:VAL:HG11	1:A:63:LYS:HG2	1.81	0.61
1:A:436:LYS:HB3	1:A:436:LYS:NZ	2.16	0.61
1:A:498:LYS:C	1:A:499:ILE:HG12	2.20	0.61
1:A:44:ARG:HH21	1:A:677:ARG:NE	1.99	0.60
1:A:407:GLN:CA	1:A:407:GLN:HE21	2.14	0.60
1:A:661:LYS:HD3	1:A:663:LEU:HD12	1.83	0.60
1:A:399:LEU:HD22	1:A:403:ASP:O	2.02	0.60
1:A:399:LEU:HD22	1:A:400:ALA:N	2.16	0.60
1:A:43:GLU:O	1:A:44:ARG:HB3	2.02	0.59
1:A:621:ALA:CB	1:A:628:ILE:HG12	2.29	0.59
1:A:191:LYS:CA	1:A:191:LYS:HE2	2.32	0.59
1:A:62:PHE:CE2	1:A:72:VAL:HG23	2.34	0.59
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.03	0.59
1:A:44:ARG:NH2	1:A:677:ARG:CZ	2.66	0.58
1:A:280:ILE:HD11	1:A:426:TYR:OH	2.02	0.58
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.04	0.58
1:A:436:LYS:HE2	4:A:1494:HOH:O	2.03	0.58
1:A:243:ILE:O	1:A:451:GLY:HA2	2.04	0.58
1:A:635:LYS:NZ	4:A:1195:HOH:O	2.35	0.58
1:A:706:TYR:CD2	1:A:707:LEU:HD22	2.38	0.58
1:A:144:LYS:HE2	4:A:1134:HOH:O	2.03	0.58
1:A:347:ILE:O	1:A:351:ILE:HG13	2.04	0.57
1:A:184:GLY:HA2	3:A:999:NMQ:PA	2.45	0.57
1:A:83:ILE:HD12	1:A:86:ASP:OD1	2.04	0.57
1:A:375:LEU:O	1:A:379:SER:OG	2.21	0.57
1:A:293:LYS:O	1:A:297:HIS:N	2.37	0.57
1:A:37:TYR:O	1:A:47:TYR:HA	2.05	0.56
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.86	0.56
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.40	0.56
1:A:202:ARG:NH1	1:A:252:PHE:CB	2.64	0.56
1:A:368:VAL:HG22	1:A:369:LEU:H	1.70	0.56
1:A:289:THR:HB	1:A:291:GLU:CD	2.26	0.56
1:A:328:ARG:HA	1:A:331:MET:HE2	1.87	0.56
1:A:124:VAL:HG13	1:A:656:ILE:CD1	2.36	0.56
1:A:399:LEU:HD21	1:A:401:GLY:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:GLU:CA	1:A:738:ARG:HH22	2.17	0.55
1:A:398:ILE:CD1	1:A:407:GLN:HG2	2.35	0.55
1:A:176:LEU:CD1	1:A:176:LEU:N	2.69	0.55
1:A:685:ILE:HA	1:A:688:THR:OG1	2.07	0.55
1:A:535:PHE:N	1:A:535:PHE:CD2	2.74	0.55
1:A:61:THR:HA	1:A:71:GLN:HG2	1.88	0.55
1:A:285:LEU:HD22	1:A:299:ALA:O	2.06	0.55
1:A:338:GLN:HB2	4:A:1279:HOH:O	2.07	0.55
1:A:195:TYR:CE2	1:A:199:VAL:HG11	2.41	0.55
1:A:697:ILE:HB	1:A:700:ASP:OD1	2.06	0.55
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.43	0.55
1:A:407:GLN:HA	1:A:407:GLN:NE2	2.22	0.54
1:A:732:ILE:N	1:A:732:ILE:HD13	2.21	0.54
1:A:392:ALA:CB	1:A:596:LEU:HD23	2.37	0.54
1:A:289:THR:C	1:A:293:LYS:HD2	2.28	0.54
1:A:486:MET:CE	1:A:688:THR:HG23	2.37	0.54
1:A:288:ALA:O	1:A:293:LYS:NZ	2.34	0.54
1:A:611:LEU:O	1:A:618:ALA:HB2	2.07	0.54
1:A:60:PHE:CE1	1:A:74:LYS:HG2	2.43	0.54
1:A:38:ASN:C	1:A:40:ASP:H	2.10	0.53
1:A:61:THR:OG1	1:A:71:GLN:OE1	2.27	0.53
1:A:87:GLY:H	1:A:105:ASN:ND2	2.06	0.53
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.56	0.53
1:A:689:ARG:NH2	4:A:1282:HOH:O	2.42	0.53
1:A:397:ARG:HD2	1:A:404:LEU:HD11	1.90	0.53
1:A:153:PRO:HD3	4:A:1037:HOH:O	2.09	0.53
1:A:83:ILE:HD11	4:A:1397:HOH:O	2.08	0.52
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.90	0.52
1:A:368:VAL:HG22	1:A:369:LEU:N	2.25	0.52
1:A:124:VAL:HG13	1:A:656:ILE:HD12	1.92	0.52
1:A:2:ASN:HD21	1:A:146:ARG:HH22	1.56	0.52
1:A:474:THR:HG23	1:A:638:LEU:HD13	1.92	0.52
1:A:708:LEU:HD13	1:A:757:ALA:HB3	1.93	0.51
1:A:753:ARG:O	1:A:756:GLU:HB2	2.10	0.51
1:A:703:LYS:O	1:A:703:LYS:HG3	2.09	0.51
1:A:38:ASN:O	1:A:40:ASP:N	2.43	0.51
1:A:534:VAL:O	1:A:536:PRO:HD3	2.11	0.51
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.30	0.51
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.91	0.51
1:A:184:GLY:HA2	3:A:999:NMQ:OA1	2.10	0.51
1:A:39:PRO:O	1:A:40:ASP:HB3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HD13	1:A:158:ILE:C	2.29	0.51
1:A:238:ARG:HB2	1:A:278:TYR:HE1	1.75	0.51
1:A:484:HIS:O	1:A:487:PHE:HB3	2.11	0.51
1:A:689:ARG:HH11	1:A:689:ARG:HG2	1.76	0.50
1:A:689:ARG:HG2	1:A:689:ARG:NH1	2.27	0.50
1:A:53:VAL:HG11	1:A:63:LYS:HG3	1.92	0.50
1:A:210:VAL:O	1:A:214:GLN:HG3	2.11	0.50
1:A:265:LYS:HD3	1:A:427:GLY:HA3	1.93	0.50
1:A:30:SER:O	4:A:1462:HOH:O	2.19	0.50
1:A:493:GLU:HA	1:A:493:GLU:OE1	2.11	0.50
1:A:392:ALA:N	4:A:1566:HOH:O	2.43	0.50
1:A:2:ASN:O	1:A:4:ILE:N	2.45	0.50
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.46	0.50
1:A:692:PHE:CE1	1:A:747:ARG:HG2	2.46	0.50
1:A:147:ARG:HG3	1:A:150:GLU:OE1	2.11	0.50
1:A:38:ASN:C	1:A:40:ASP:N	2.65	0.50
1:A:643:ALA:O	1:A:646:GLU:HB2	2.12	0.50
1:A:338:GLN:O	1:A:342:MET:SD	2.70	0.49
1:A:44:ARG:HG2	1:A:45:ASP:OD2	2.12	0.49
1:A:202:ARG:HH11	1:A:252:PHE:HB3	1.76	0.49
3:A:999:NMQ:CA2	3:A:999:NMQ:O2B	2.60	0.49
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.42	0.49
1:A:244:GLU:O	1:A:256:ALA:HA	2.12	0.49
1:A:18:LYS:HB2	4:A:1375:HOH:O	2.12	0.49
1:A:341:GLN:O	1:A:345:PHE:CD2	2.65	0.49
1:A:662:GLN:NE2	4:A:1070:HOH:O	2.45	0.49
1:A:59:SER:HB3	1:A:73:LYS:HD3	1.95	0.49
1:A:18:LYS:HG3	4:A:1086:HOH:O	2.12	0.49
1:A:735:GLU:CD	1:A:747:ARG:HH21	2.16	0.49
1:A:259:GLN:CG	1:A:261:TYR:CZ	2.97	0.48
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.22	0.48
1:A:35:ILE:HD11	1:A:77:ALA:CB	2.33	0.48
1:A:535:PHE:HA	1:A:536:PRO:HD2	1.78	0.48
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.14	0.48
1:A:7:ARG:NH2	4:A:1576:HOH:O	2.34	0.48
1:A:621:ALA:HB3	1:A:628:ILE:H	1.77	0.48
1:A:175:LEU:C	1:A:176:LEU:HD12	2.35	0.47
1:A:486:MET:HE3	1:A:688:THR:HG23	1.96	0.47
1:A:371:ASP:OD2	1:A:372:LYS:N	2.47	0.47
1:A:661:LYS:HB2	1:A:663:LEU:HG	1.96	0.47
1:A:58:ASP:OD1	1:A:73:LYS:NZ	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLN:HE21	1:A:483:ASN:ND2	2.13	0.47
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.97	0.47
1:A:707:LEU:HA	4:A:1525:HOH:O	2.14	0.47
1:A:190:LYS:HE3	1:A:223:GLU:OE2	2.15	0.47
1:A:568:PHE:N	1:A:578:MET:HE1	2.30	0.47
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.55	0.47
1:A:724:ASP:O	1:A:728:LYS:HB2	2.14	0.47
1:A:202:ARG:O	1:A:203:ASN:O	2.33	0.47
1:A:442:CYS:SG	1:A:443:GLN:N	2.88	0.46
1:A:229:LYS:HE2	1:A:274:THR:O	2.16	0.46
1:A:162:ALA:O	1:A:173:GLN:HG3	2.15	0.46
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.30	0.46
1:A:552:SER:O	1:A:553:LYS:HB2	2.16	0.46
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.50	0.46
1:A:568:PHE:O	1:A:578:MET:HE3	2.16	0.46
1:A:72:VAL:HG12	1:A:73:LYS:O	2.16	0.46
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.80	0.46
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.75	0.46
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.48	0.46
1:A:520:ARG:HD3	4:A:1561:HOH:O	2.16	0.46
1:A:407:GLN:CA	1:A:407:GLN:NE2	2.79	0.45
1:A:302:GLU:N	1:A:302:GLU:CD	2.67	0.45
1:A:126:VAL:HG13	1:A:656:ILE:HG22	1.98	0.45
1:A:72:VAL:HG12	1:A:73:LYS:N	2.31	0.45
1:A:342:MET:SD	1:A:342:MET:N	2.89	0.45
1:A:467:GLU:H	1:A:467:GLU:CD	2.19	0.45
1:A:83:ILE:CD1	1:A:86:ASP:OD1	2.64	0.45
1:A:568:PHE:CA	1:A:578:MET:HE1	2.46	0.45
1:A:24:LEU:HD11	4:A:1523:HOH:O	2.16	0.45
1:A:696:ILE:HG22	1:A:697:ILE:N	2.30	0.45
1:A:35:ILE:HG12	1:A:79:GLN:HA	1.99	0.45
1:A:328:ARG:HA	1:A:331:MET:CE	2.46	0.45
1:A:358:LYS:HA	1:A:358:LYS:HZ2	1.82	0.45
1:A:689:ARG:HA	1:A:693:PRO:HG3	1.98	0.45
1:A:290:ALA:N	1:A:293:LYS:HD2	2.31	0.45
1:A:689:ARG:CG	1:A:689:ARG:NH1	2.71	0.45
1:A:219:ASN:N	1:A:220:PRO:CD	2.80	0.44
1:A:272:SER:O	1:A:310:SER:HB2	2.18	0.44
1:A:99:GLU:HB2	1:A:100:PRO:HD3	1.99	0.44
1:A:289:THR:O	1:A:293:LYS:HD2	2.17	0.44
1:A:388:VAL:HG23	1:A:388:VAL:H	1.29	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.61	0.44
1:A:158:ILE:HD13	1:A:159:SER:H	1.78	0.44
1:A:338:GLN:NE2	4:A:1496:HOH:O	2.27	0.44
1:A:372:LYS:HB2	1:A:372:LYS:HE3	1.70	0.44
1:A:573:TYR:OH	1:A:680:GLY:HA2	2.17	0.44
1:A:530:ASP:O	1:A:533:SER:HB2	2.18	0.44
1:A:296:LEU:HB2	1:A:298:LEU:CG	2.46	0.44
1:A:567:GLU:HB3	1:A:578:MET:HE2	2.00	0.44
1:A:494:TYR:HE2	1:A:695:ARG:NH2	2.16	0.44
1:A:290:ALA:HA	1:A:293:LYS:HD3	1.95	0.43
1:A:399:LEU:HD13	1:A:399:LEU:C	2.38	0.43
1:A:596:LEU:HA	1:A:596:LEU:HD23	1.77	0.43
1:A:474:THR:OG1	1:A:634:TYR:OH	2.34	0.43
1:A:60:PHE:N	1:A:72:VAL:O	2.41	0.43
1:A:273:GLU:O	1:A:274:THR:CB	2.65	0.43
1:A:508:LEU:O	1:A:509:ASP:CB	2.67	0.43
1:A:326:ILE:O	1:A:329:GLN:HB3	2.18	0.43
1:A:259:GLN:HG3	1:A:261:TYR:CZ	2.53	0.43
1:A:567:GLU:HB3	1:A:578:MET:CE	2.49	0.43
1:A:249:ASN:OD1	4:A:1146:HOH:O	2.21	0.43
1:A:298:LEU:HD23	1:A:298:LEU:N	2.33	0.43
1:A:705:TYR:O	1:A:706:TYR:C	2.57	0.43
3:A:999:NMQ:HA22	3:A:999:NMQ:O2B	2.19	0.43
1:A:178:THR:HG22	1:A:455:ILE:O	2.19	0.43
1:A:169:ASP:C	1:A:170:ARG:HG2	2.38	0.43
1:A:299:ALA:HB3	1:A:303:SER:OG	2.19	0.42
1:A:329:GLN:O	1:A:333:ILE:CD1	2.68	0.42
1:A:421:LEU:HB2	1:A:596:LEU:HD13	2.01	0.42
1:A:436:LYS:CB	1:A:436:LYS:NZ	2.78	0.42
1:A:697:ILE:O	1:A:700:ASP:HB2	2.20	0.42
1:A:230:THR:HB	1:A:275:GLU:OE2	2.19	0.42
1:A:217:GLN:O	1:A:221:ILE:HG13	2.19	0.42
1:A:399:LEU:CD2	1:A:403:ASP:O	2.66	0.42
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.67	0.42
1:A:752:ALA:O	1:A:755:GLU:HB3	2.20	0.42
1:A:139:MET:HA	1:A:142:ILE:HD12	2.02	0.42
1:A:485:HIS:NE2	1:A:489:LEU:CD1	2.81	0.41
1:A:31:ASP:OD2	1:A:31:ASP:N	2.53	0.41
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.19	0.41
1:A:107:ARG:NE	4:A:1409:HOH:O	2.39	0.41
1:A:319:SER:OG	1:A:322:GLU:CG	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD13	1:A:421:LEU:HD23	2.02	0.41
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.50	0.41
1:A:733:ASP:OD2	1:A:734:PRO:CD	2.68	0.41
1:A:520:ARG:HB2	4:A:1227:HOH:O	2.19	0.41
1:A:144:LYS:HD3	4:A:1134:HOH:O	2.20	0.41
1:A:470:CYS:O	1:A:473:TYR:HB3	2.21	0.41
1:A:681:VAL:HG13	4:A:1130:HOH:O	2.18	0.41
1:A:570:VAL:HG22	1:A:572:HIS:CD2	2.55	0.41
1:A:90:ASP:O	1:A:93:GLU:HB2	2.20	0.41
1:A:709:ALA:HB2	1:A:726:VAL:HA	2.02	0.41
1:A:276:ARG:HH11	1:A:314:ASP:HA	1.86	0.41
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.37	0.41
1:A:33:ARG:HB3	1:A:52:ILE:HD12	2.03	0.41
1:A:597:GLU:OE1	1:A:612:PHE:HD2	2.03	0.41
1:A:539:THR:OG1	1:A:542:THR:HG23	2.21	0.41
1:A:190:LYS:CE	1:A:223:GLU:OE2	2.69	0.41
1:A:694:ASN:C	1:A:695:ARG:HG3	2.39	0.41
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.65	0.40
1:A:136:THR:OG1	1:A:139:MET:HG2	2.22	0.40
1:A:568:PHE:C	1:A:578:MET:CE	2.90	0.40
1:A:613:ASN:O	1:A:615:PRO:HD3	2.21	0.40
1:A:296:LEU:CB	1:A:298:LEU:HG	2.52	0.40
1:A:471:ILE:HD12	1:A:471:ILE:HA	1.78	0.40
1:A:59:SER:CB	1:A:72:VAL:O	2.60	0.40
1:A:296:LEU:O	1:A:297:HIS:HB2	2.21	0.40
1:A:580:GLU:OE1	1:A:582:GLN:HB3	2.21	0.40
1:A:195:TYR:CZ	1:A:199:VAL:HG11	2.55	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	736/761 (97%)	692 (94%)	33 (4%)	11 (2%)	13 12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	363	ALA
1	A	44	ARG
1	A	509	ASP
1	A	711	ASN
1	A	498	LYS
1	A	499	ILE
1	A	713	PRO
1	A	3	PRO
1	A	40	ASP
1	A	39	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	634/665 (95%)	558 (88%)	76 (12%)	6 6

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	26	LYS
1	A	27	LEU
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	44	ARG
1	A	57	SER
1	A	63	LYS
1	A	66	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	71	GLN
1	A	73	LYS
1	A	84	LYS
1	A	95	SER
1	A	131	ARG
1	A	144	LYS
1	A	146	ARG
1	A	148	ARG
1	A	158	ILE
1	A	211	LEU
1	A	249	ASN
1	A	262	LEU
1	A	280	ILE
1	A	294	LYS
1	A	302	GLU
1	A	325	LYS
1	A	326	ILE
1	A	338	GLN
1	A	342	MET
1	A	358	LYS
1	A	368	VAL
1	A	372	LYS
1	A	375	LEU
1	A	379	SER
1	A	380	THR
1	A	387	SER
1	A	388	VAL
1	A	403	ASP
1	A	405	VAL
1	A	407	GLN
1	A	412	GLU
1	A	413	LYS
1	A	415	SER
1	A	436	LYS
1	A	444	GLU
1	A	460	ILE
1	A	462	LYS
1	A	496	LYS
1	A	499	ILE
1	A	510	SER
1	A	516	LEU
1	A	546	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	562	ARG
1	A	565	LYS
1	A	582	GLN
1	A	594	GLN
1	A	627	PHE
1	A	640	SER
1	A	657	ILE
1	A	661	LYS
1	A	666	LYS
1	A	674	ASP
1	A	688	THR
1	A	689	ARG
1	A	690	LYS
1	A	703	LYS
1	A	707	LEU
1	A	717	GLU
1	A	727	LEU
1	A	728	LYS
1	A	732	ILE
1	A	735	GLU
1	A	738	ARG
1	A	741	ILE
1	A	742	THR
1	A	751	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	105	ASN
1	A	217	GLN
1	A	234	ASN
1	A	249	ASN
1	A	259	GLN
1	A	283	GLN
1	A	407	GLN
1	A	439	ASN
1	A	483	ASN
1	A	582	GLN
1	A	594	GLN
1	A	662	GLN
1	A	720	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NMQ	A	999	2	22,26,26	1.52	3 (13%)	24,39,39	1.68	4 (16%)

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
3	NMQ	A	999	2	-	0/20/27/27	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NMQ	C1-NA3	-3.64	1.33	1.41
3	A	999	NMQ	CA3-NA3	-3.39	1.40	1.46
3	A	999	NMQ	C4-C5	2.28	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NMQ	C6-C1-NA3	-4.89	114.69	122.13
3	A	999	NMQ	OA1-PA-OA2	-3.17	109.26	118.70
3	A	999	NMQ	CA2-NA3-C1	-2.91	107.54	116.11
3	A	999	NMQ	CA3-NA3-C1	-2.79	107.59	115.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	NMQ	5	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

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	744/761 (97%)	0.24	52 (6%)	19 27	9, 31, 75, 100	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	GLY	6.9
1	A	362	GLY	6.3
1	A	204	GLN	6.0
1	A	508	LEU	5.4
1	A	443	GLN	5.2
1	A	364	GLY	4.8
1	A	509	ASP	4.6
1	A	710	PRO	4.6
1	A	405	VAL	4.6
1	A	42	LYS	4.6
1	A	205	ALA	4.3
1	A	23	ASP	4.1
1	A	707	LEU	4.0
1	A	65	VAL	3.6
1	A	444	GLU	3.5
1	A	365	GLU	3.5
1	A	40	ASP	3.4
1	A	371	ASP	3.4
1	A	5	HIS	3.3
1	A	56	THR	3.2
1	A	322	GLU	3.2
1	A	290	ALA	3.1
1	A	72	VAL	3.1
1	A	58	ASP	3.0
1	A	294	LYS	3.0
1	A	289	THR	3.0
1	A	31	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	291	GLU	2.8
1	A	363	ALA	2.8
1	A	370	LYS	2.8
1	A	489	LEU	2.7
1	A	737	TYR	2.6
1	A	399	LEU	2.6
1	A	39	PRO	2.5
1	A	711	ASN	2.5
1	A	347	ILE	2.5
1	A	734	PRO	2.5
1	A	67	GLY	2.5
1	A	429	LEU	2.4
1	A	493	GLU	2.4
1	A	455	ILE	2.3
1	A	728	LYS	2.3
1	A	203	ASN	2.3
1	A	274	THR	2.3
1	A	24	LEU	2.2
1	A	615	PRO	2.2
1	A	3	PRO	2.1
1	A	487	PHE	2.1
1	A	717	GLU	2.1
1	A	627	PHE	2.0
1	A	400	ALA	2.0
1	A	321	SER	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
3	NMQ	A	999	26/26	0.96	0.13	0.83	8,24,52,100	0
2	MG	A	998	1/1	0.86	0.12	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.