



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:43 PM GMT

PDB ID : 1D1A
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH O,P-DINITROPHENYL AMINOETHYLDIPHOSP
HATEBERYLLIUM TRIFLUORIDE.
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on : 1999-09-15
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

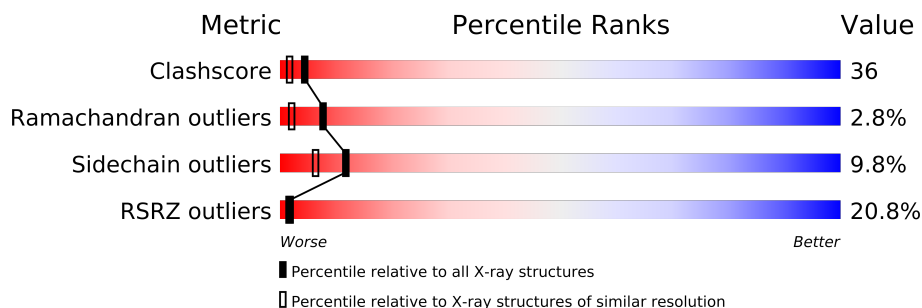
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 6235 atoms, of which 0 are hydrogen and 0 are deuterium.

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	745	Total	C	N	O	S	0	0	0
			5772	3660	994	1102	16			

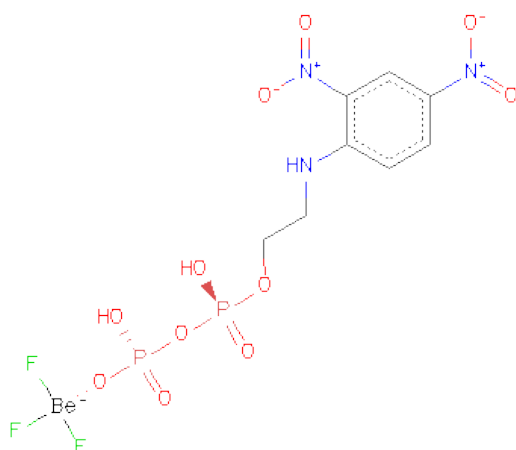
There are 3 discrepancies between the modelled and reference sequences:

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 O,P-DINITROPHENYL AMINOETHYLDIPHOSPHATE-BERYLLIUM TRIFLUORIDE (three-letter code: DAE) (formula: C₈H₁₀BeF₃N₃O₁₁P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	28	1	8	3	3	11	2	0	0

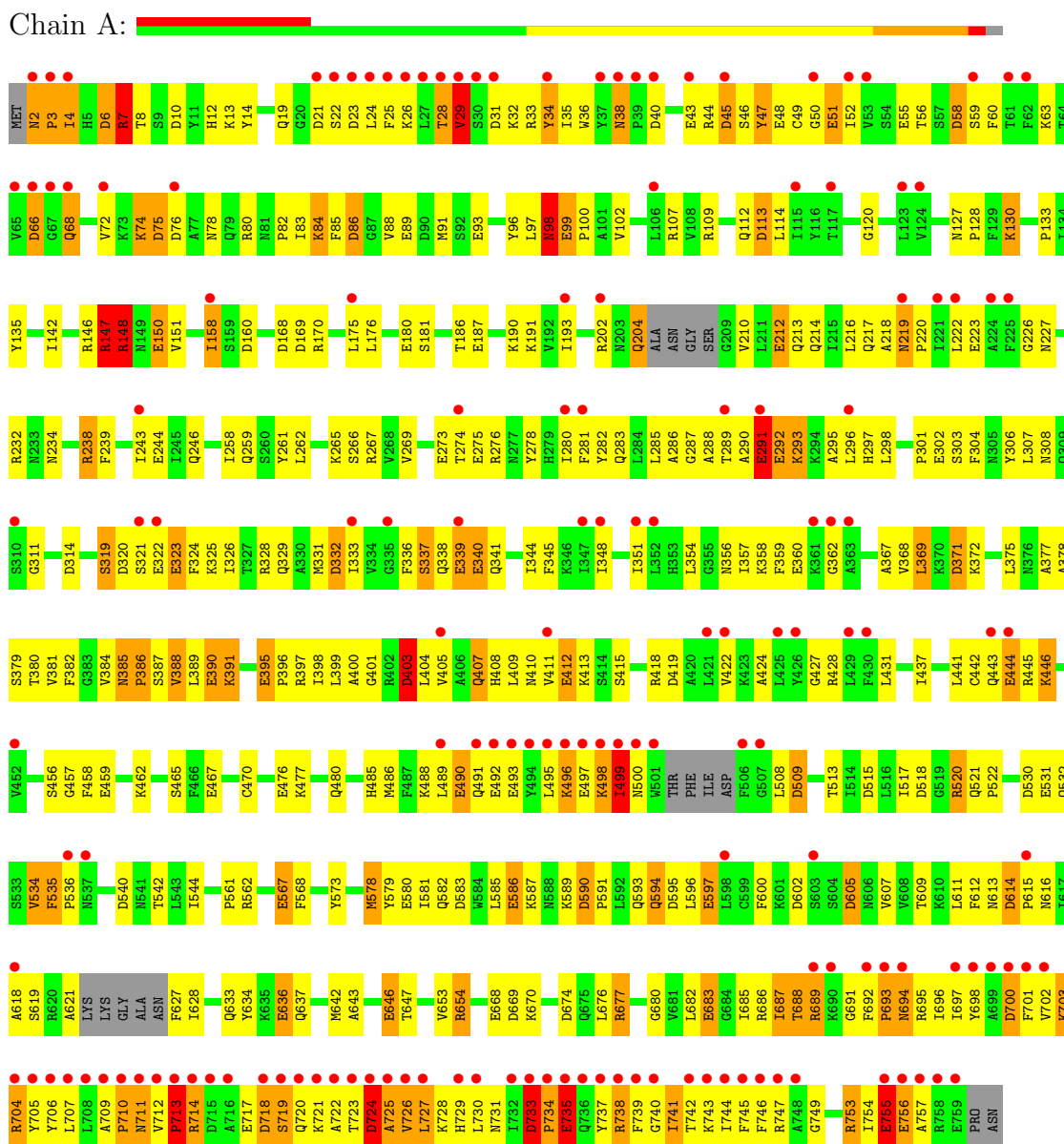
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	434	Total	O	0	0
			434	434		

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	103.73Å 180.00Å 54.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 29.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.00-2.00) 96.8 (29.96-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.00Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.226 , (Not available) 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 127.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66758 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAE, 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	0.93	38/5882 (0.6%)	1.38	74/7967 (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	2	0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	GLU	CD-OE2	7.05	1.33	1.25
1	A	302	GLU	CD-OE2	6.74	1.33	1.25
1	A	89	GLU	CD-OE2	6.57	1.32	1.25
1	A	275	GLU	CD-OE2	6.57	1.32	1.25
1	A	490	GLU	CD-OE2	6.41	1.32	1.25
1	A	756	GLU	CD-OE2	6.27	1.32	1.25
1	A	717	GLU	CD-OE2	6.27	1.32	1.25
1	A	93	GLU	CD-OE2	6.26	1.32	1.25
1	A	48	GLU	CD-OE2	6.21	1.32	1.25
1	A	291	GLU	CD-OE2	6.18	1.32	1.25
1	A	444	GLU	CD-OE2	6.08	1.32	1.25
1	A	99	GLU	CD-OE2	6.04	1.32	1.25
1	A	412	GLU	CD-OE2	6.03	1.32	1.25
1	A	646	GLU	CD-OE2	6.00	1.32	1.25
1	A	150	GLU	CD-OE2	5.98	1.32	1.25
1	A	476	GLU	CD-OE2	5.98	1.32	1.25
1	A	567	GLU	CD-OE2	5.81	1.32	1.25
1	A	51	GLU	CD-OE2	5.80	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	755	GLU	CD-OE2	5.78	1.32	1.25
1	A	55	GLU	CD-OE2	5.72	1.31	1.25
1	A	531	GLU	CD-OE2	5.71	1.31	1.25
1	A	668	GLU	CD-OE2	5.71	1.31	1.25
1	A	586	GLU	CD-OE2	5.68	1.31	1.25
1	A	187	GLU	CD-OE2	5.66	1.31	1.25
1	A	292	GLU	CD-OE2	5.65	1.31	1.25
1	A	323	GLU	CD-OE2	5.63	1.31	1.25
1	A	459	GLU	CD-OE2	5.62	1.31	1.25
1	A	340	GLU	CD-OE2	5.62	1.31	1.25
1	A	597	GLU	CD-OE2	5.58	1.31	1.25
1	A	212	GLU	CD-OE2	5.52	1.31	1.25
1	A	180	GLU	CD-OE2	5.48	1.31	1.25
1	A	390	GLU	CD-OE2	5.47	1.31	1.25
1	A	395	GLU	CD-OE2	5.47	1.31	1.25
1	A	244	GLU	CD-OE2	5.38	1.31	1.25
1	A	636	GLU	CD-OE2	5.35	1.31	1.25
1	A	360	GLU	CD-OE2	5.30	1.31	1.25
1	A	467	GLU	CD-OE2	5.24	1.31	1.25
1	A	735	GLU	CD-OE2	5.18	1.31	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	147	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	689	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	148	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	21	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	605	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	602	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	A	520	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	21	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	A	320	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	168	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	419	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	A	713	PRO	N-CA-CB	7.40	112.18	103.30
1	A	320	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	6	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	160	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	232	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	45	ASP	CB-CG-OD2	-7.03	111.97	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	674	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	A	168	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	A	530	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	704	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	219	ASN	CB-CA-C	6.55	123.50	110.40
1	A	66	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	509	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	371	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	6	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	160	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	700	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	605	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	520	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	602	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	718	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	385	ASN	C-N-CD	-6.15	107.06	120.60
1	A	238	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	403	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	674	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	518	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	590	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	76	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	45	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	34	TYR	N-CA-C	5.78	126.61	111.00
1	A	614	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	58	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	267	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	669	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	34	TYR	CB-CG-CD2	5.64	124.39	121.00
1	A	535	PHE	CA-CB-CG	-5.62	100.41	113.90
1	A	614	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	314	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	113	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	403	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	47	TYR	CB-CA-C	-5.51	99.38	110.40
1	A	700	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	583	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	515	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	530	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	595	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	562	ARG	NE-CZ-NH2	-5.35	117.62	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASN	N-CA-CB	5.33	120.19	110.60
1	A	733	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	734	PRO	N-CA-CB	5.23	109.57	103.30
1	A	419	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	58	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	75	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	7	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	499	ILE	CB-CA-C	5.11	121.82	111.60
1	A	86	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	724	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	590	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	677	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	332	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	518	ASP	CB-CG-OD1	5.04	122.84	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	219	ASN	CA
1	A	499	ILE	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5772	0	5502	403	0
2	A	1	0	0	0	0
3	A	28	0	8	3	0
4	A	434	0	0	19	0
All	All	6235	0	5510	404	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (404) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.39	1.04
1:A:98:ASN:HB2	1:A:100:PRO:HD2	1.41	1.02
1:A:443:GLN:CG	1:A:445:ARG:O	2.07	1.00
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.46	0.97
1:A:709:ALA:HB1	1:A:729:HIS:ND1	1.81	0.96
1:A:4:ILE:HD11	1:A:142:ILE:CG2	1.96	0.93
1:A:34:TYR:HB3	1:A:51:GLU:HA	1.51	0.92
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.05	0.91
1:A:711:ASN:HB2	1:A:729:HIS:CE1	2.08	0.89
1:A:619:SER:HB3	1:A:627:PHE:HE2	1.34	0.88
1:A:45:ASP:HB2	1:A:670:LYS:HG2	1.56	0.87
1:A:737:TYR:HB3	1:A:746:PHE:CE1	2.11	0.84
1:A:723:THR:HG22	1:A:739:PHE:CZ	2.11	0.84
1:A:698:TYR:CD1	1:A:720:GLN:HG2	2.13	0.83
1:A:147:ARG:HG2	1:A:150:GLU:OE1	1.79	0.82
1:A:58:ASP:O	1:A:74:LYS:HB3	1.78	0.82
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.80	0.81
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.45	0.81
1:A:443:GLN:HG2	1:A:445:ARG:O	1.79	0.80
1:A:34:TYR:CB	1:A:51:GLU:HA	2.12	0.80
1:A:723:THR:HG22	1:A:739:PHE:HZ	1.44	0.80
1:A:372:LYS:HE3	1:A:390:GLU:OE1	1.82	0.80
1:A:337:SER:O	1:A:341:GLN:HG3	1.82	0.79
1:A:80:ARG:HH12	1:A:83:ILE:HG12	1.48	0.79
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.62	0.79
1:A:480:GLN:HG3	1:A:508:LEU:HD12	1.66	0.78
1:A:336:PHE:O	1:A:341:GLN:NE2	2.15	0.78
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.66	0.78
1:A:480:GLN:HG3	1:A:508:LEU:CD1	2.14	0.77
1:A:269:VAL:HG12	1:A:306:TYR:CZ	2.20	0.77
1:A:400:ALA:HB3	1:A:403:ASP:HB2	1.67	0.76
1:A:297:HIS:C	1:A:298:LEU:HD23	2.05	0.76
1:A:4:ILE:HD11	1:A:142:ILE:HG21	1.66	0.75
1:A:43:GLU:HB2	1:A:670:LYS:HZ2	1.50	0.75
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.66	0.75
1:A:35:ILE:HG12	1:A:36:TRP:N	2.02	0.75
1:A:702:VAL:HG23	1:A:712:VAL:CG1	2.17	0.75
1:A:735:GLU:HB3	1:A:747:ARG:NH2	2.02	0.74
1:A:485:HIS:NE2	1:A:489:LEU:HD11	2.02	0.74
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.17	0.74
1:A:733:ASP:O	1:A:737:TYR:CE2	2.40	0.74
1:A:158:ILE:HD12	1:A:175:LEU:HD23	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:540:ASP:HB3	1:A:581:ILE:HD13	1.69	0.74
1:A:396:PRO:O	1:A:398:ILE:HD12	1.88	0.73
1:A:395:GLU:HA	1:A:407:GLN:O	1.89	0.72
1:A:107:ARG:HG3	4:A:1192:HOH:O	1.89	0.72
1:A:210:VAL:O	1:A:214:GLN:HG3	1.89	0.72
1:A:377:ALA:O	1:A:380:THR:HG22	1.89	0.72
1:A:7:ARG:HD3	1:A:12:HIS:CE1	2.25	0.71
1:A:709:ALA:HB2	1:A:726:VAL:HG13	1.71	0.70
1:A:443:GLN:HG3	1:A:445:ARG:O	1.92	0.70
1:A:35:ILE:HG12	1:A:36:TRP:H	1.55	0.70
1:A:582:GLN:N	1:A:582:GLN:OE1	2.20	0.70
1:A:98:ASN:CB	1:A:100:PRO:HD2	2.21	0.70
1:A:146:ARG:HD3	1:A:151:VAL:HG13	1.72	0.70
1:A:614:ASP:OD1	1:A:615:PRO:HD2	1.92	0.69
1:A:491:GLN:O	1:A:495:LEU:HD13	1.91	0.69
1:A:687:ILE:HG22	1:A:688:THR:N	2.07	0.69
1:A:735:GLU:CB	1:A:747:ARG:HH21	2.05	0.69
1:A:80:ARG:HH12	1:A:83:ILE:CG1	2.06	0.69
1:A:380:THR:HG23	1:A:381:VAL:N	2.08	0.69
1:A:740:GLY:O	1:A:742:THR:N	2.25	0.68
1:A:38:ASN:OD1	1:A:44:ARG:HA	1.92	0.68
1:A:698:TYR:HH	1:A:739:PHE:HD2	1.41	0.68
1:A:753:ARG:HH21	1:A:757:ALA:HB2	1.58	0.68
1:A:80:ARG:HH12	1:A:83:ILE:CD1	2.06	0.67
1:A:702:VAL:HG23	1:A:712:VAL:HG11	1.75	0.67
1:A:293:LYS:O	1:A:296:LEU:N	2.26	0.67
1:A:738:ARG:O	1:A:744:ILE:HD12	1.95	0.67
1:A:325:LYS:O	1:A:329:GLN:HG3	1.94	0.67
1:A:544:ILE:HB	1:A:581:ILE:HG12	1.77	0.66
1:A:443:GLN:HG3	1:A:445:ARG:C	2.16	0.66
1:A:43:GLU:HB2	1:A:670:LYS:NZ	2.10	0.66
1:A:410:ASN:OD1	1:A:413:LYS:HB2	1.96	0.66
1:A:642:MET:O	1:A:646:GLU:HG2	1.96	0.66
1:A:695:ARG:HA	1:A:745:PHE:HA	1.77	0.66
1:A:686:ARG:O	1:A:689:ARG:HB3	1.95	0.66
1:A:694:ASN:N	1:A:694:ASN:ND2	2.44	0.66
1:A:385:ASN:O	1:A:388:VAL:HG23	1.95	0.66
1:A:34:TYR:CD1	1:A:49:CYS:SG	2.89	0.65
1:A:399:LEU:HG	1:A:401:GLY:H	1.61	0.65
1:A:711:ASN:HB2	1:A:729:HIS:HE1	1.58	0.65
1:A:273:GLU:O	1:A:274:THR:OG1	2.09	0.65
1:A:621:ALA:CB	1:A:628:ILE:HG23	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:586:GLU:HB2	4:A:1399:HOH:O	1.97	0.65
1:A:283:GLN:HB3	1:A:324:PHE:HB2	1.79	0.65
1:A:12:HIS:ND1	4:A:1198:HOH:O	2.28	0.65
1:A:753:ARG:NE	1:A:753:ARG:O	2.30	0.65
1:A:246:GLN:OE1	1:A:443:GLN:HB3	1.97	0.64
1:A:580:GLU:HG3	1:A:580:GLU:O	1.96	0.64
1:A:158:ILE:CD1	1:A:175:LEU:HD23	2.26	0.64
1:A:298:LEU:HD23	1:A:298:LEU:N	2.12	0.64
1:A:753:ARG:HH11	1:A:753:ARG:HG3	1.63	0.64
1:A:222:LEU:HD11	1:A:258:ILE:HD13	1.80	0.64
1:A:43:GLU:HA	1:A:670:LYS:HZ1	1.64	0.63
1:A:293:LYS:O	1:A:297:HIS:N	2.31	0.63
1:A:753:ARG:HA	1:A:756:GLU:OE2	1.99	0.63
1:A:621:ALA:HB3	1:A:628:ILE:H	1.64	0.63
1:A:753:ARG:O	1:A:756:GLU:HB2	1.98	0.63
1:A:697:ILE:HG22	1:A:700:ASP:H	1.64	0.63
1:A:35:ILE:HG22	1:A:50:GLY:O	1.99	0.62
1:A:498:LYS:CB	1:A:741:ILE:HG13	2.29	0.62
1:A:698:TYR:HE2	1:A:739:PHE:CE2	2.17	0.62
1:A:338:GLN:HB3	1:A:339:GLU:OE1	2.00	0.62
1:A:698:TYR:CG	1:A:720:GLN:HG2	2.35	0.62
1:A:686:ARG:HA	1:A:689:ARG:HB2	1.82	0.62
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.30	0.62
1:A:382:PHE:HB2	1:A:384:VAL:HG22	1.82	0.62
1:A:490:GLU:HA	1:A:490:GLU:OE1	1.98	0.61
1:A:534:VAL:O	1:A:536:PRO:HD3	2.00	0.61
1:A:698:TYR:O	1:A:702:VAL:HG12	1.99	0.61
1:A:380:THR:HG23	1:A:381:VAL:H	1.66	0.61
1:A:296:LEU:CB	1:A:298:LEU:HG	2.27	0.61
1:A:7:ARG:NH1	1:A:12:HIS:HE1	1.99	0.61
1:A:2:ASN:ND2	1:A:4:ILE:H	1.99	0.60
1:A:495:LEU:N	1:A:495:LEU:HD12	2.17	0.60
1:A:443:GLN:CD	1:A:445:ARG:O	2.40	0.60
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.36	0.60
1:A:33:ARG:O	1:A:52:ILE:HB	2.01	0.60
1:A:34:TYR:HD1	1:A:49:CYS:SG	2.25	0.60
1:A:80:ARG:NH1	1:A:83:ILE:HG12	2.16	0.60
1:A:158:ILE:HD12	1:A:175:LEU:CD2	2.31	0.60
1:A:387:SER:O	1:A:391:LYS:HB2	2.01	0.60
1:A:130:LYS:HA	3:A:999:DAE:O4A	2.01	0.59
1:A:380:THR:CG2	1:A:381:VAL:H	2.15	0.59
1:A:713:PRO:O	1:A:714:ARG:O	2.21	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:24:LEU:HB3	1:A:26:LYS:CB	2.33	0.59
1:A:694:ASN:N	1:A:694:ASN:HD22	1.99	0.59
1:A:24:LEU:HD13	1:A:26:LYS:CB	2.32	0.59
1:A:219:ASN:N	1:A:220:PRO:HD2	2.16	0.59
1:A:611:LEU:O	1:A:618:ALA:HB2	2.02	0.59
1:A:399:LEU:HG	1:A:401:GLY:N	2.16	0.59
1:A:25:PHE:HA	1:A:704:ARG:NH2	2.18	0.59
1:A:289:THR:HB	1:A:291:GLU:OE1	2.03	0.58
1:A:706:TYR:CB	1:A:712:VAL:HG12	2.33	0.58
1:A:409:LEU:HD22	1:A:413:LYS:HB3	1.84	0.58
1:A:698:TYR:HE2	1:A:739:PHE:HE2	1.50	0.58
1:A:412:GLU:HG2	4:A:1375:HOH:O	2.02	0.58
1:A:304:PHE:O	1:A:308:ASN:ND2	2.35	0.58
1:A:499:ILE:HD11	1:A:745:PHE:CD1	2.39	0.58
1:A:585:LEU:O	1:A:589:LYS:HG3	2.03	0.57
1:A:213:GLN:O	1:A:217:GLN:HG2	2.04	0.57
1:A:619:SER:CB	1:A:627:PHE:HE2	2.14	0.57
1:A:685:ILE:HG22	1:A:686:ARG:N	2.18	0.57
1:A:534:VAL:HG22	1:A:535:PHE:CE2	2.39	0.57
1:A:276:ARG:NH1	1:A:282:TYR:CG	2.72	0.57
1:A:589:LYS:HB2	1:A:591:PRO:HD3	1.87	0.57
1:A:509:ASP:O	4:A:1254:HOH:O	2.18	0.57
1:A:709:ALA:HB1	1:A:729:HIS:CE1	2.39	0.56
1:A:26:LYS:O	1:A:29:VAL:HG22	2.05	0.56
1:A:534:VAL:CG2	1:A:535:PHE:CE2	2.88	0.56
1:A:375:LEU:HD23	1:A:375:LEU:C	2.25	0.56
1:A:686:ARG:HA	1:A:689:ARG:CB	2.36	0.56
1:A:465:SER:OG	1:A:587:LYS:NZ	2.38	0.56
1:A:358:LYS:NZ	4:A:1236:HOH:O	2.39	0.56
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.10	0.56
1:A:725:ALA:O	1:A:728:LYS:N	2.39	0.56
1:A:99:GLU:H	1:A:100:PRO:CD	2.18	0.55
1:A:492:GLU:O	1:A:495:LEU:HB2	2.06	0.55
1:A:698:TYR:OH	1:A:739:PHE:HD2	1.90	0.55
1:A:43:GLU:CB	1:A:670:LYS:HZ2	2.18	0.55
1:A:621:ALA:HB2	1:A:628:ILE:CG1	2.36	0.55
1:A:380:THR:CG2	1:A:381:VAL:N	2.68	0.55
1:A:234:ASN:ND2	4:A:1220:HOH:O	2.40	0.55
1:A:705:TYR:O	1:A:726:VAL:HG21	2.07	0.55
1:A:377:ALA:O	1:A:381:VAL:HG22	2.07	0.54
1:A:721:LYS:O	1:A:724:ASP:HB2	2.07	0.54
1:A:486:MET:CE	1:A:687:ILE:HG21	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:719:SER:O	1:A:722:ALA:N	2.41	0.54
1:A:704:ARG:HB3	1:A:705:TYR:CE2	2.42	0.54
1:A:223:GLU:O	1:A:227:ASN:HB2	2.07	0.54
1:A:480:GLN:HG3	1:A:508:LEU:HD13	1.89	0.54
1:A:324:PHE:CE2	1:A:328:ARG:HD2	2.43	0.54
1:A:594:GLN:NE2	1:A:594:GLN:HA	2.17	0.53
1:A:688:THR:O	1:A:691:GLY:N	2.40	0.53
1:A:443:GLN:HG2	1:A:446:LYS:HB3	1.90	0.53
1:A:97:LEU:O	1:A:98:ASN:O	2.27	0.53
1:A:296:LEU:O	1:A:297:HIS:HB2	2.09	0.53
1:A:292:GLU:O	1:A:295:ALA:HB3	2.09	0.53
1:A:735:GLU:HB2	1:A:747:ARG:HH21	1.72	0.53
1:A:380:THR:HG23	1:A:381:VAL:HG13	1.91	0.53
1:A:24:LEU:HB3	1:A:26:LYS:H	1.74	0.53
1:A:695:ARG:CB	1:A:745:PHE:CE2	2.92	0.53
1:A:63:LYS:HG3	1:A:68:GLN:O	2.09	0.53
1:A:45:ASP:CG	1:A:677:ARG:HH22	2.13	0.52
1:A:693:PRO:HD2	1:A:746:PHE:O	2.09	0.52
1:A:26:LYS:HA	1:A:29:VAL:HG13	1.90	0.52
1:A:98:ASN:O	1:A:102:VAL:HG23	2.09	0.52
1:A:513:THR:O	1:A:517:ILE:HD12	2.10	0.52
1:A:344:ILE:O	1:A:348:ILE:HG12	2.10	0.52
1:A:99:GLU:N	1:A:100:PRO:CD	2.72	0.52
1:A:694:ASN:ND2	1:A:694:ASN:H	2.05	0.52
1:A:219:ASN:N	1:A:220:PRO:CD	2.73	0.52
1:A:319:SER:OG	1:A:322:GLU:HB2	2.10	0.52
1:A:4:ILE:CD1	1:A:4:ILE:N	2.72	0.51
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.75	0.51
1:A:99:GLU:HG2	1:A:682:LEU:HD13	1.91	0.51
1:A:379:SER:HA	1:A:384:VAL:HG23	1.93	0.51
1:A:653:VAL:C	1:A:654:ARG:HE	2.14	0.51
1:A:99:GLU:H	1:A:100:PRO:HD2	1.75	0.51
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.93	0.51
1:A:437:ILE:O	1:A:441:LEU:HG	2.11	0.51
1:A:43:GLU:HG3	1:A:43:GLU:O	2.12	0.50
1:A:692:PHE:CZ	1:A:747:ARG:NH1	2.80	0.50
1:A:408:HIS:HD2	1:A:409:LEU:N	2.09	0.50
1:A:135:TYR:CD1	1:A:191:LYS:HD2	2.46	0.50
1:A:290:ALA:N	1:A:291:GLU:OE2	2.45	0.50
1:A:696:ILE:O	1:A:743:LYS:HA	2.12	0.50
1:A:354:LEU:O	1:A:418:ARG:HD3	2.12	0.50
1:A:609:THR:CG2	1:A:613:ASN:ND2	2.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:THR:HG22	1:A:190:LYS:HE3	1.93	0.50
1:A:710:PRO:O	1:A:711:ASN:OD1	2.30	0.50
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.93	0.49
1:A:367:ALA:O	1:A:408:HIS:NE2	2.44	0.49
1:A:458:PHE:CZ	1:A:573:TYR:HB3	2.47	0.49
1:A:147:ARG:NH1	4:A:1215:HOH:O	2.23	0.49
1:A:102:VAL:HG21	1:A:685:ILE:HD13	1.95	0.49
1:A:737:TYR:HB3	1:A:746:PHE:HE1	1.70	0.49
1:A:47:TYR:CE1	1:A:100:PRO:HG3	2.47	0.49
1:A:594:GLN:O	1:A:597:GLU:HB2	2.12	0.49
1:A:280:ILE:HD11	1:A:345:PHE:HE1	1.77	0.49
1:A:582:GLN:NE2	4:A:1245:HOH:O	2.27	0.49
1:A:753:ARG:NH1	1:A:753:ARG:HG3	2.27	0.49
1:A:621:ALA:CB	1:A:628:ILE:HG12	2.37	0.49
1:A:594:GLN:NE2	1:A:594:GLN:CA	2.74	0.48
1:A:28:THR:HG21	1:A:84:LYS:HB2	1.96	0.48
1:A:738:ARG:HB3	1:A:745:PHE:HB2	1.95	0.48
1:A:470:CYS:HB3	1:A:634:TYR:CZ	2.48	0.48
1:A:442:CYS:SG	1:A:443:GLN:N	2.86	0.48
1:A:609:THR:HG23	1:A:613:ASN:ND2	2.28	0.48
1:A:85:PHE:O	1:A:88:VAL:HG13	2.14	0.48
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.49	0.48
1:A:191:LYS:NZ	4:A:1365:HOH:O	2.25	0.48
1:A:286:ALA:HB1	1:A:321:SER:OG	2.13	0.48
1:A:428:ARG:O	1:A:431:LEU:HB2	2.14	0.48
1:A:99:GLU:N	1:A:100:PRO:HD2	2.29	0.48
1:A:723:THR:CG2	1:A:739:PHE:CZ	2.91	0.48
1:A:331:MET:CE	1:A:345:PHE:CZ	2.96	0.48
1:A:702:VAL:O	1:A:706:TYR:HB3	2.14	0.48
1:A:597:GLU:OE1	1:A:612:PHE:HD2	1.97	0.48
1:A:722:ALA:O	1:A:725:ALA:HB3	2.13	0.48
1:A:96:TYR:CE2	1:A:749:GLY:HA2	2.49	0.47
1:A:701:PHE:O	1:A:705:TYR:HD2	1.97	0.47
1:A:217:GLN:HG3	1:A:333:ILE:HD13	1.95	0.47
1:A:84:LYS:HD2	1:A:755:GLU:OE2	2.15	0.47
1:A:499:ILE:CD1	1:A:745:PHE:CD1	2.98	0.47
1:A:24:LEU:CD1	1:A:26:LYS:CB	2.92	0.47
1:A:288:ALA:HB1	1:A:292:GLU:HB2	1.97	0.47
1:A:311:GLY:N	4:A:1144:HOH:O	2.36	0.47
1:A:680:GLY:N	4:A:1099:HOH:O	2.45	0.47
1:A:695:ARG:CB	1:A:745:PHE:CD2	2.98	0.47
1:A:324:PHE:O	1:A:328:ARG:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:GLN:HG3	1:A:333:ILE:CD1	2.45	0.47
1:A:683:GLU:HG3	1:A:686:ARG:NH2	2.30	0.47
1:A:614:ASP:O	1:A:616:ASN:N	2.48	0.46
1:A:96:TYR:CE2	1:A:749:GLY:CA	2.97	0.46
1:A:696:ILE:O	1:A:743:LYS:CA	2.64	0.46
1:A:31:ASP:O	1:A:32:LYS:HG2	2.14	0.46
1:A:297:HIS:O	1:A:298:LEU:HD23	2.15	0.46
1:A:371:ASP:OD2	1:A:372:LYS:N	2.48	0.46
1:A:218:ALA:C	1:A:220:PRO:HD2	2.36	0.46
1:A:643:ALA:O	1:A:647:THR:HG23	2.15	0.46
1:A:296:LEU:O	1:A:298:LEU:HD23	2.16	0.46
1:A:582:GLN:H	1:A:582:GLN:CD	2.16	0.46
1:A:219:ASN:ND2	4:A:1426:HOH:O	2.38	0.46
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.30	0.46
1:A:176:LEU:HD12	1:A:176:LEU:N	2.31	0.46
1:A:567:GLU:HA	1:A:579:TYR:O	2.15	0.46
1:A:726:VAL:HG12	1:A:730:LEU:CD1	2.45	0.46
1:A:219:ASN:HD21	1:A:243:ILE:HD11	1.80	0.46
1:A:735:GLU:CB	1:A:747:ARG:NH2	2.68	0.46
1:A:6:ASP:O	1:A:8:THR:N	2.48	0.46
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.98	0.46
1:A:340:GLU:O	1:A:344:ILE:HG13	2.16	0.46
1:A:59:SER:CB	1:A:72:VAL:O	2.64	0.46
1:A:534:VAL:HG22	1:A:535:PHE:CD2	2.51	0.45
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.68	0.45
1:A:456:SER:OG	1:A:457:GLY:N	2.49	0.45
1:A:568:PHE:O	1:A:578:MET:HE3	2.17	0.45
1:A:686:ARG:CB	1:A:689:ARG:CZ	2.94	0.45
1:A:495:LEU:N	1:A:495:LEU:CD1	2.79	0.45
1:A:728:LYS:O	1:A:731:ASN:N	2.46	0.45
1:A:654:ARG:NH1	4:A:1349:HOH:O	2.49	0.45
1:A:578:MET:HA	1:A:578:MET:HE3	1.98	0.45
1:A:697:ILE:HD12	1:A:743:LYS:HG2	1.99	0.45
1:A:82:PRO:HG2	1:A:85:PHE:HE1	1.81	0.45
1:A:685:ILE:HG22	1:A:689:ARG:HH11	1.82	0.45
1:A:147:ARG:O	1:A:150:GLU:HB2	2.15	0.45
1:A:287:GLY:HA3	1:A:324:PHE:CD2	2.51	0.45
1:A:590:ASP:N	1:A:591:PRO:CD	2.79	0.45
1:A:238:ARG:HB2	1:A:278:TYR:HE1	1.82	0.45
1:A:259:GLN:HG3	1:A:261:TYR:CZ	2.52	0.45
1:A:709:ALA:CB	1:A:729:HIS:ND1	2.68	0.45
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:PRO:O	1:A:12:HIS:HD2	2.00	0.45
1:A:633:GLN:O	1:A:637:GLN:HG3	2.17	0.45
1:A:38:ASN:N	1:A:38:ASN:HD22	2.15	0.44
1:A:497:GLU:C	1:A:741:ILE:HD12	2.38	0.44
1:A:219:ASN:HD21	1:A:243:ILE:CD1	2.30	0.44
1:A:222:LEU:CD1	1:A:258:ILE:HD13	2.47	0.44
1:A:521:GLN:HA	1:A:522:PRO:C	2.38	0.44
1:A:415:SER:O	1:A:418:ARG:HB3	2.16	0.44
1:A:493:GLU:C	1:A:495:LEU:N	2.68	0.44
1:A:120:GLY:O	1:A:148:ARG:NH2	2.46	0.44
1:A:2:ASN:ND2	4:A:1196:HOH:O	2.51	0.44
1:A:4:ILE:HD12	1:A:4:ILE:N	2.32	0.44
1:A:696:ILE:O	1:A:744:ILE:N	2.45	0.44
1:A:297:HIS:N	1:A:297:HIS:ND1	2.66	0.43
1:A:723:THR:CG2	1:A:739:PHE:CE2	3.00	0.43
1:A:289:THR:C	1:A:291:GLU:N	2.69	0.43
1:A:375:LEU:HD22	1:A:386:PRO:HB3	2.00	0.43
1:A:424:ALA:O	1:A:428:ARG:HG3	2.18	0.43
1:A:605:ASP:OD1	1:A:607:VAL:N	2.49	0.43
1:A:686:ARG:HB3	1:A:689:ARG:CZ	2.49	0.43
1:A:359:PHE:HB3	1:A:411:VAL:HG12	1.99	0.43
1:A:462:LYS:HG3	4:A:1243:HOH:O	2.17	0.43
1:A:686:ARG:HB3	1:A:689:ARG:NH2	2.33	0.43
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.17	0.43
1:A:351:ILE:HG23	1:A:422:VAL:HG13	2.01	0.43
1:A:692:PHE:HB3	1:A:745:PHE:HB3	2.00	0.43
1:A:375:LEU:HD23	1:A:375:LEU:O	2.19	0.43
1:A:698:TYR:CD2	1:A:720:GLN:HA	2.54	0.43
1:A:488:LYS:C	1:A:490:GLU:H	2.21	0.43
1:A:341:GLN:O	1:A:345:PHE:CD2	2.72	0.43
1:A:499:ILE:HG22	1:A:500:ASN:H	1.84	0.43
1:A:369:LEU:O	1:A:372:LYS:NZ	2.45	0.43
1:A:614:ASP:C	1:A:616:ASN:N	2.72	0.43
1:A:493:GLU:C	1:A:495:LEU:H	2.20	0.43
1:A:36:TRP:HB2	1:A:78:ASN:HB3	2.00	0.43
1:A:609:THR:O	1:A:613:ASN:N	2.47	0.43
1:A:49:CYS:SG	1:A:80:ARG:HD2	2.59	0.43
1:A:670:LYS:HG3	4:A:1199:HOH:O	2.19	0.43
1:A:535:PHE:CD2	1:A:535:PHE:N	2.86	0.43
1:A:532:GLN:NE2	1:A:542:THR:OG1	2.47	0.42
1:A:698:TYR:CE2	1:A:739:PHE:CE2	3.04	0.42
1:A:707:LEU:C	1:A:709:ALA:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:697:ILE:HG22	1:A:700:ASP:N	2.31	0.42
1:A:614:ASP:C	1:A:616:ASN:H	2.21	0.42
1:A:590:ASP:N	1:A:591:PRO:HD3	2.34	0.42
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.54	0.42
1:A:368:VAL:HG22	1:A:369:LEU:N	2.35	0.42
1:A:326:ILE:O	1:A:329:GLN:HB2	2.19	0.42
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.20	0.42
1:A:281:PHE:O	1:A:285:LEU:HG	2.20	0.42
1:A:443:GLN:CG	1:A:445:ARG:C	2.75	0.42
1:A:701:PHE:O	1:A:705:TYR:N	2.53	0.42
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.49	0.42
1:A:409:LEU:HA	1:A:409:LEU:HD23	1.79	0.42
1:A:181:SER:HA	3:A:999:DAE:F1	2.10	0.42
1:A:169:ASP:C	1:A:170:ARG:HG2	2.40	0.42
1:A:265:LYS:HD3	1:A:427:GLY:HA3	2.01	0.42
1:A:112:GLN:O	1:A:113:ASP:HB2	2.19	0.42
1:A:628:ILE:HD13	1:A:628:ILE:HG21	1.86	0.42
1:A:7:ARG:NH1	1:A:19:GLN:OE1	2.53	0.42
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.85	0.42
1:A:477:LYS:NZ	4:A:1093:HOH:O	2.46	0.42
1:A:685:ILE:HG22	1:A:689:ARG:NH1	2.35	0.41
1:A:493:GLU:O	1:A:496:LYS:HB2	2.19	0.41
1:A:319:SER:OG	1:A:322:GLU:CB	2.68	0.41
1:A:96:TYR:HE2	1:A:749:GLY:HA3	1.85	0.41
1:A:96:TYR:CE2	1:A:749:GLY:HA3	2.55	0.41
1:A:43:GLU:HA	1:A:670:LYS:NZ	2.33	0.41
1:A:698:TYR:CE2	1:A:739:PHE:HE2	2.34	0.41
1:A:488:LYS:HE2	1:A:488:LYS:HB2	1.83	0.41
1:A:593:GLN:HB2	1:A:596:LEU:HD12	2.02	0.41
1:A:43:GLU:CB	1:A:670:LYS:NZ	2.79	0.41
1:A:289:THR:C	1:A:291:GLU:H	2.24	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.86	0.41
1:A:488:LYS:C	1:A:490:GLU:N	2.73	0.41
1:A:609:THR:O	1:A:613:ASN:ND2	2.48	0.41
1:A:212:GLU:O	1:A:216:LEU:HG	2.21	0.41
1:A:581:ILE:N	1:A:582:GLN:OE1	2.54	0.41
1:A:593:GLN:O	1:A:596:LEU:HB2	2.20	0.41
1:A:193:ILE:HG21	1:A:193:ILE:HD13	1.81	0.41
1:A:397:ARG:HB3	1:A:404:LEU:HG	2.03	0.41
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.55	0.41
1:A:34:TYR:HB2	1:A:51:GLU:HA	2.00	0.41
1:A:614:ASP:HA	1:A:615:PRO:HD3	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:676:LEU:HB3	1:A:682:LEU:HG	2.03	0.41
1:A:323:GLU:O	1:A:326:ILE:HB	2.21	0.41
3:A:999:DAE:HA21	3:A:999:DAE:H6	1.62	0.41
1:A:680:GLY:CA	4:A:1099:HOH:O	2.68	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.85	0.41
1:A:686:ARG:CB	1:A:689:ARG:NH2	2.84	0.41
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.53	0.41
1:A:703:LYS:O	1:A:706:TYR:HD2	2.04	0.41
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.82	0.41
1:A:497:GLU:O	1:A:741:ILE:HB	2.20	0.41
1:A:202:ARG:N	1:A:212:GLU:OE2	2.51	0.41
1:A:293:LYS:HA	1:A:298:LEU:HB2	2.02	0.41
1:A:683:GLU:CG	1:A:686:ARG:NH2	2.84	0.40
1:A:280:ILE:O	1:A:280:ILE:HG13	2.21	0.40
1:A:399:LEU:HA	1:A:403:ASP:O	2.21	0.40
1:A:727:LEU:O	1:A:731:ASN:N	2.54	0.40
1:A:204:GLN:H	1:A:204:GLN:HG3	1.72	0.40
1:A:710:PRO:HD2	1:A:729:HIS:CG	2.56	0.40
1:A:341:GLN:O	1:A:345:PHE:HD2	2.04	0.40
1:A:339:GLU:CD	1:A:339:GLU:N	2.75	0.40
1:A:329:GLN:O	1:A:332:ASP:HB2	2.21	0.40
1:A:212:GLU:O	1:A:216:LEU:HD12	2.22	0.40
1:A:10:ASP:O	1:A:13:LYS:HB3	2.21	0.40
1:A:600:PHE:HB3	1:A:612:PHE:CE1	2.56	0.40
1:A:378:ALA:O	1:A:381:VAL:HG22	2.22	0.40
1:A:379:SER:HB3	1:A:384:VAL: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	737/761 (97%)	654 (89%)	62 (8%)	21 (3%)	8 2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	714	ARG
1	A	741	ILE
1	A	7	ARG
1	A	29	VAL
1	A	60	PHE
1	A	68	GLN
1	A	293	LYS
1	A	498	LYS
1	A	719	SER
1	A	386	PRO
1	A	693	PRO
1	A	711	ASN
1	A	713	PRO
1	A	725	ALA
1	A	86	ASP
1	A	718	ASP
1	A	754	ILE
1	A	703	LYS
1	A	362	GLY
1	A	3	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	594/665 (89%)	536 (90%)	58 (10%)	12 6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	ILE
1	A	22	SER
1	A	28	THR
1	A	29	VAL
1	A	38	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	ASP
1	A	46	SER
1	A	56	THR
1	A	66	ASP
1	A	74	LYS
1	A	75	ASP
1	A	84	LYS
1	A	91	MET
1	A	98	ASN
1	A	130	LYS
1	A	147	ARG
1	A	148	ARG
1	A	158	ILE
1	A	204	GLN
1	A	266	SER
1	A	291	GLU
1	A	301	PRO
1	A	303	SER
1	A	307	LEU
1	A	319	SER
1	A	337	SER
1	A	369	LEU
1	A	388	VAL
1	A	389	LEU
1	A	391	LYS
1	A	403	ASP
1	A	405	VAL
1	A	407	GLN
1	A	444	GLU
1	A	446	LYS
1	A	496	LYS
1	A	499	ILE
1	A	520	ARG
1	A	534	VAL
1	A	561	PRO
1	A	578	MET
1	A	594	GLN
1	A	636	GLU
1	A	654	ARG
1	A	683	GLU
1	A	687	ILE
1	A	688	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	694	ASN
1	A	710	PRO
1	A	724	ASP
1	A	726	VAL
1	A	727	LEU
1	A	733	ASP
1	A	735	GLU
1	A	738	ARG
1	A	753	ARG
1	A	755	GLU

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	2	ASN
1	A	188	ASN
1	A	219	ASN
1	A	234	ASN
1	A	259	GLN
1	A	283	GLN
1	A	329	GLN
1	A	407	GLN
1	A	439	ASN
1	A	479	GLN
1	A	532	GLN
1	A	594	GLN
1	A	613	ASN
1	A	694	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	DAE	A	999	2	27,28,28	1.36	4 (14%)	35,42,42	1.46	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAE	A	999	2	-	0/22/28/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	DAE	PB-OB3	4.58	1.61	1.51
3	A	999	DAE	C2-N2	2.49	1.50	1.46
3	A	999	DAE	C1-NA3	2.48	1.45	1.38
3	A	999	DAE	C4-N4	2.05	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	DAE	O4B-N4-C4	4.05	122.21	114.42
3	A	999	DAE	C3-C2-N2	3.56	119.39	115.82
3	A	999	DAE	CA2-NA3-C1	-3.42	113.89	122.95
3	A	999	DAE	C5-C4-N4	2.50	121.28	118.96
3	A	999	DAE	C3-C2-C1	-2.10	119.77	121.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	745/761 (97%)	1.09	155 (20%) 1 2	17, 46, 97, 100	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	10.8
1	A	494	TYR	8.5
1	A	744	ILE	8.0
1	A	712	VAL	7.8
1	A	27	LEU	7.6
1	A	24	LEU	7.6
1	A	710	PRO	6.9
1	A	498	LYS	6.7
1	A	723	THR	6.2
1	A	698	TYR	6.2
1	A	25	PHE	6.2
1	A	495	LEU	6.2
1	A	362	GLY	6.1
1	A	497	GLU	6.1
1	A	725	ALA	6.0
1	A	536	PRO	5.6
1	A	65	VAL	5.6
1	A	443	GLN	5.5
1	A	22	SER	5.4
1	A	702	VAL	5.2
1	A	348	ILE	5.1
1	A	537	ASN	5.1
1	A	29	VAL	5.0
1	A	713	PRO	4.9
1	A	745	PHE	4.8
1	A	711	ASN	4.7
1	A	53	VAL	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	492	GLU	4.6
1	A	699	ALA	4.6
1	A	39	PRO	4.6
1	A	707	LEU	4.6
1	A	499	ILE	4.5
1	A	429	LEU	4.5
1	A	708	LEU	4.4
1	A	31	ASP	4.3
1	A	709	ALA	4.3
1	A	722	ALA	4.3
1	A	706	TYR	4.2
1	A	718	ASP	4.2
1	A	496	LYS	4.1
1	A	225	PHE	4.1
1	A	705	TYR	4.1
1	A	715	ASP	4.0
1	A	727	LEU	4.0
1	A	30	SER	4.0
1	A	738	ARG	4.0
1	A	693	PRO	3.9
1	A	740	GLY	3.9
1	A	701	PHE	3.8
1	A	739	PHE	3.8
1	A	426	TYR	3.7
1	A	716	ALA	3.7
1	A	500	ASN	3.7
1	A	748	ALA	3.7
1	A	742	THR	3.6
1	A	23	ASP	3.6
1	A	734	PRO	3.6
1	A	62	PHE	3.5
1	A	43	GLU	3.5
1	A	743	LYS	3.5
1	A	746	PHE	3.5
1	A	757	ALA	3.5
1	A	26	LYS	3.5
1	A	351	ILE	3.4
1	A	714	ARG	3.4
1	A	59	SER	3.4
1	A	507	GLY	3.3
1	A	68	GLN	3.3
1	A	66	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	430	PHE	3.3
1	A	40	ASP	3.3
1	A	733	ASP	3.3
1	A	280	ILE	3.3
1	A	491	GLN	3.2
1	A	729	HIS	3.2
1	A	730	LEU	3.2
1	A	274	THR	3.2
1	A	724	ASP	3.1
1	A	281	PHE	3.0
1	A	732	ILE	3.0
1	A	61	THR	2.9
1	A	704	ARG	2.9
1	A	4	ILE	2.9
1	A	222	LEU	2.9
1	A	296	LEU	2.9
1	A	758	ARG	2.9
1	A	352	LEU	2.9
1	A	291	GLU	2.9
1	A	3	PRO	2.9
1	A	361	LYS	2.8
1	A	45	ASP	2.8
1	A	425	LEU	2.8
1	A	615	PRO	2.8
1	A	28	THR	2.8
1	A	697	ILE	2.8
1	A	690	LYS	2.8
1	A	721	LYS	2.8
1	A	759	GLU	2.7
1	A	700	ASP	2.7
1	A	726	VAL	2.7
1	A	736	GLN	2.7
1	A	444	GLU	2.7
1	A	506	PHE	2.7
1	A	34	TYR	2.6
1	A	37	TYR	2.6
1	A	2	ASN	2.6
1	A	106	LEU	2.6
1	A	720	GLN	2.6
1	A	243	ILE	2.6
1	A	603	SER	2.6
1	A	72	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	452	VAL	2.5
1	A	489	LEU	2.5
1	A	67	GLY	2.5
1	A	123	LEU	2.5
1	A	175	LEU	2.5
1	A	363	ALA	2.5
1	A	735	GLU	2.5
1	A	289	THR	2.5
1	A	692	PHE	2.4
1	A	501	TRP	2.4
1	A	38	ASN	2.4
1	A	405	VAL	2.4
1	A	339	GLU	2.4
1	A	124	VAL	2.4
1	A	411	VAL	2.4
1	A	221	ILE	2.4
1	A	421	LEU	2.3
1	A	322	GLU	2.3
1	A	52	ILE	2.3
1	A	493	GLU	2.3
1	A	310	SER	2.3
1	A	347	ILE	2.3
1	A	219	ASN	2.3
1	A	335	GLY	2.3
1	A	719	SER	2.2
1	A	756	GLU	2.2
1	A	158	ILE	2.2
1	A	21	ASP	2.2
1	A	755	GLU	2.2
1	A	422	VAL	2.2
1	A	115	ILE	2.1
1	A	747	ARG	2.1
1	A	117	THR	2.1
1	A	76	ASP	2.1
1	A	694	ASN	2.1
1	A	598	LEU	2.1
1	A	618	ALA	2.1
1	A	321	SER	2.1
1	A	202	ARG	2.1
1	A	224	ALA	2.0
1	A	689	ARG	2.0
1	A	333	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	50	GLY	2.0
1	A	193	ILE	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	DAE	A	999	28/28	0.14	0.84	19,54,100,100	0
2	MG	A	998	1/1	0.06	-7.01	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.