



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 PM UTC

PDB ID : 3HA4 / pdb_00003ha4
Title : Crystal structure of the type one membrane protein MIX1 from Leishmania
Authors : Gorman, M.A.; Walsh, P.J.; Parker, M.W.
Deposited on : 2009-05-01
Resolution : 2.40 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:

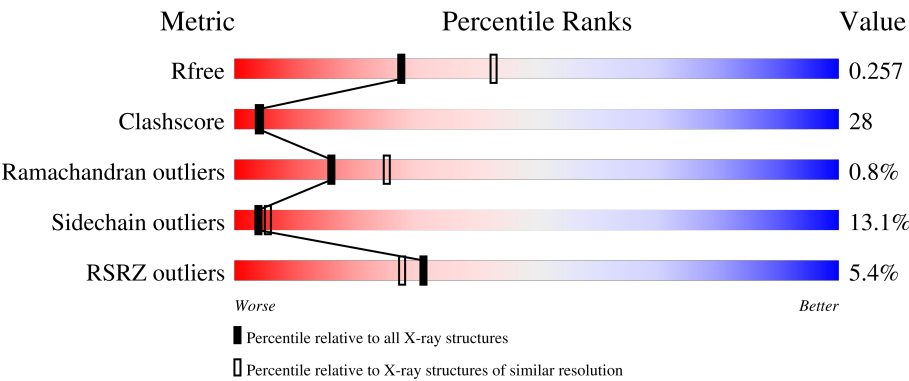
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	154	5% 47% 28% 6% 18%
1	B	154	3% 44% 26% 8% 22%
1	C	154	3% 36% 26% 10% 27%
1	D	154	3% 49% 21% •• 26%
1	E	154	6% 35% 27% 8% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	154	3% 51% 25% 7% 16%
1	G	154	7% 29% 36% 7% 27%
1	H	154	2% 41% 25% 5% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7963 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 MIX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	1	0
			1055	665	187	198	5			
1	B	120	Total	C	N	O	S	0	0	0
			984	624	172	183	5			
1	C	113	Total	C	N	O	S	0	2	0
			939	598	160	176	5			
1	D	114	Total	C	N	O	S	0	1	0
			937	598	159	175	5			
1	E	111	Total	C	N	O	S	0	0	0
			907	580	155	167	5			
1	F	129	Total	C	N	O	S	0	1	0
			1070	675	186	204	5			
1	G	113	Total	C	N	O	S	0	1	0
			932	595	158	174	5			
1	H	109	Total	C	N	O	S	0	0	0
			889	569	150	165	5			

There are 32 discrepancies between the modelled and reference sequences:

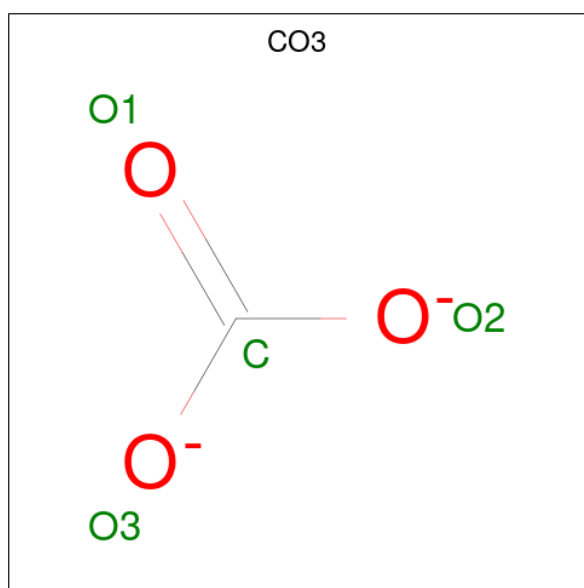
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	expression tag	UNP Q4QI49
A	43	SER	-	expression tag	UNP Q4QI49
A	44	HIS	-	expression tag	UNP Q4QI49
A	45	MET	-	expression tag	UNP Q4QI49
B	42	GLY	-	expression tag	UNP Q4QI49
B	43	SER	-	expression tag	UNP Q4QI49
B	44	HIS	-	expression tag	UNP Q4QI49
B	45	MET	-	expression tag	UNP Q4QI49
C	42	GLY	-	expression tag	UNP Q4QI49
C	43	SER	-	expression tag	UNP Q4QI49
C	44	HIS	-	expression tag	UNP Q4QI49
C	45	MET	-	expression tag	UNP Q4QI49
D	42	GLY	-	expression tag	UNP Q4QI49

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	43	SER	-	expression tag	UNP Q4QI49
D	44	HIS	-	expression tag	UNP Q4QI49
D	45	MET	-	expression tag	UNP Q4QI49
E	42	GLY	-	expression tag	UNP Q4QI49
E	43	SER	-	expression tag	UNP Q4QI49
E	44	HIS	-	expression tag	UNP Q4QI49
E	45	MET	-	expression tag	UNP Q4QI49
F	42	GLY	-	expression tag	UNP Q4QI49
F	43	SER	-	expression tag	UNP Q4QI49
F	44	HIS	-	expression tag	UNP Q4QI49
F	45	MET	-	expression tag	UNP Q4QI49
G	42	GLY	-	expression tag	UNP Q4QI49
G	43	SER	-	expression tag	UNP Q4QI49
G	44	HIS	-	expression tag	UNP Q4QI49
G	45	MET	-	expression tag	UNP Q4QI49
H	42	GLY	-	expression tag	UNP Q4QI49
H	43	SER	-	expression tag	UNP Q4QI49
H	44	HIS	-	expression tag	UNP Q4QI49
H	45	MET	-	expression tag	UNP Q4QI49

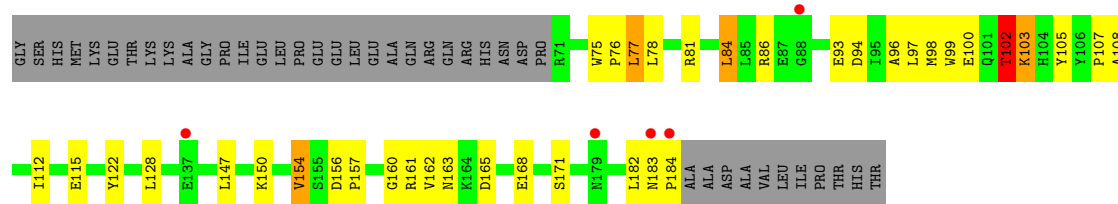
- Molecule 2 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



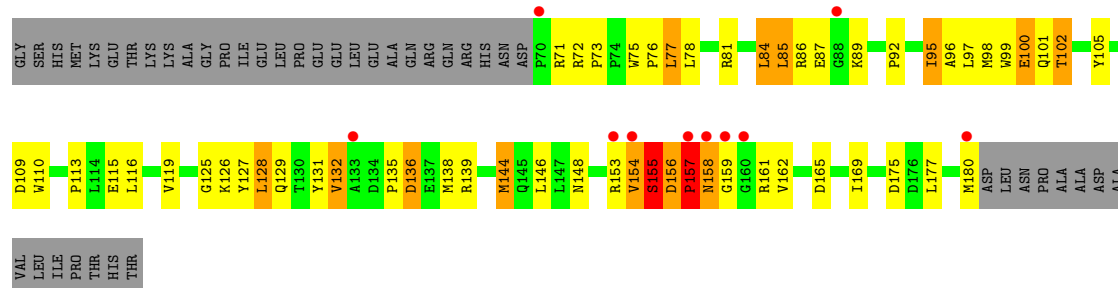
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is water.

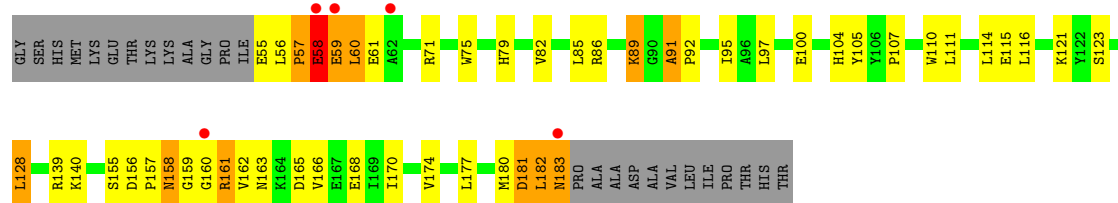
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	53	Total 53	O 53	0	0
3	C	21	Total 21	O 21	0	0
3	D	32	Total 32	O 32	0	0
3	E	10	Total 10	O 10	0	0
3	F	41	Total 41	O 41	0	0
3	G	14	Total 14	O 14	0	0
3	H	18	Total 18	O 18	0	0



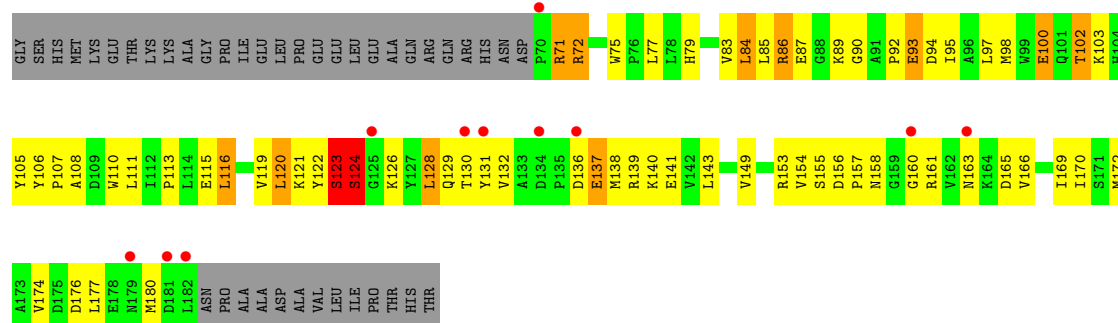
• Molecule 1: MIX1



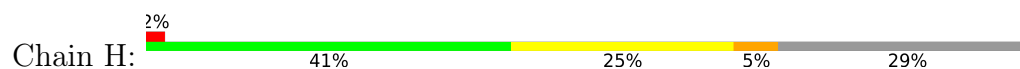
• Molecule 1: MIX1

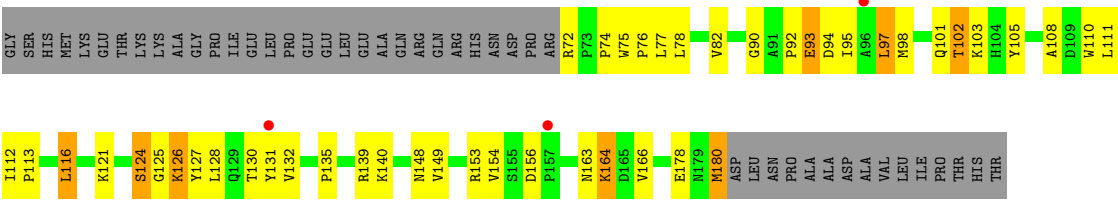


• Molecule 1: MIX1



• Molecule 1: MIX1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.52Å 100.39Å 140.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.40 19.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-2.40) 99.1 (19.96-2.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.212 , 0.261 0.213 , 0.257	Depositor DCC
R_{free} test set	4377 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	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	7963	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: CO3

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	1.54	6/1079 (0.6%)	1.05	5/1464 (0.3%)
1	B	1.28	4/1008 (0.4%)	1.05	5/1370 (0.4%)
1	C	1.46	9/963 (0.9%)	1.11	7/1307 (0.5%)
1	D	1.02	2/959 (0.2%)	0.95	0/1303
1	E	0.96	0/929	1.01	4/1261 (0.3%)
1	F	1.17	1/1094 (0.1%)	1.08	6/1485 (0.4%)
1	G	1.07	0/954	1.00	4/1295 (0.3%)
1	H	0.70	0/910	0.86	1/1236 (0.1%)
All	All	1.19	22/7896 (0.3%)	1.02	32/10721 (0.3%)

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	C	0	1
1	F	0	1
All	All	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	PRO	C-O	-8.48	1.17	1.24
1	A	91	ALA	CA-CB	-8.26	1.43	1.53
1	C	163	ASN	C-O	-6.61	1.19	1.24
1	B	165	ASP	C-O	-6.40	1.16	1.24
1	F	91	ALA	CA-CB	-6.32	1.45	1.53
1	B	91	ALA	CA-CB	-6.25	1.45	1.53
1	A	90	GLY	C-O	-6.12	1.18	1.24
1	B	134	ASP	C-O	-6.04	1.20	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	PRO	C-O	-5.95	1.17	1.24
1	C	73	PRO	CA-C	-5.64	1.48	1.52
1	D	103	LYS	C-O	-5.61	1.17	1.24
1	C	144	MET	C-O	-5.58	1.17	1.24
1	A	138	MET	C-O	-5.52	1.17	1.24
1	A	172	MET	C-O	-5.43	1.17	1.24
1	C	145	GLN	C-O	-5.38	1.17	1.24
1	C	100	GLU	C-O	-5.35	1.17	1.24
1	C	102	THR	C-O	-5.27	1.18	1.24
1	C	74	PRO	C-O	-5.25	1.17	1.23
1	A	91	ALA	C-O	-5.22	1.18	1.24
1	D	102	THR	C-O	-5.08	1.17	1.24
1	B	89	LYS	CA-C	-5.05	1.47	1.53
1	C	101	GLN	C-O	-5.03	1.18	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	89	LYS	N-CA-C	9.62	127.36	113.02
1	A	59	GLU	N-CA-C	-9.52	100.17	114.64
1	C	180	MET	N-CA-C	-7.79	98.73	109.95
1	G	120	LEU	N-CA-C	7.64	119.69	111.36
1	C	160	GLY	N-CA-C	7.46	125.09	115.32
1	E	156	ASP	C-N-CD	-6.62	106.05	120.60
1	E	155	SER	N-CA-C	6.57	120.24	109.06
1	F	181	ASP	N-CA-C	6.54	118.20	111.14
1	B	111	LEU	N-CA-C	6.48	118.14	111.14
1	B	85	LEU	N-CA-C	6.43	119.11	111.33
1	C	96	ALA	N-CA-C	6.10	117.73	111.14
1	A	60	LEU	N-CA-C	-6.09	105.70	113.01
1	G	123	SER	N-CA-C	6.02	117.84	111.28
1	C	106	TYR	CA-C-N	5.94	125.56	119.56
1	C	106	TYR	C-N-CA	5.94	125.56	119.56
1	C	104	HIS	N-CA-C	5.89	117.50	111.14
1	B	89	LYS	N-CA-C	5.84	120.28	109.24
1	F	158	ASN	N-CA-C	5.68	118.79	109.76
1	B	87	GLU	N-CA-C	-5.55	106.48	113.20
1	F	181	ASP	CB-CA-C	-5.42	102.33	110.90
1	A	73	PRO	CA-C-N	-5.41	114.20	119.78
1	A	73	PRO	C-N-CA	-5.41	114.20	119.78
1	G	121	LYS	N-CA-C	5.37	117.21	111.36
1	C	182	LEU	N-CA-C	5.34	118.49	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	136	ASP	N-CA-C	5.32	117.99	111.82
1	E	157	PRO	N-CA-C	5.28	125.82	112.10
1	B	131	TYR	N-CA-C	5.17	119.69	113.17
1	H	130	THR	CB-CA-C	-5.10	102.87	110.88
1	A	163	ASN	N-CA-C	-5.10	99.94	110.80
1	G	137	GLU	N-CA-C	-5.07	105.67	111.14
1	F	57	PRO	CA-C-N	-5.03	111.94	121.54
1	F	57	PRO	C-N-CA	-5.03	111.94	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	180	MET	Peptide
1	F	89	LYS	Peptide

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	1055	0	1042	77	1
1	B	984	0	975	52	1
1	C	939	0	936	77	0
1	D	937	0	931	35	0
1	E	907	0	908	85	0
1	F	1070	0	1052	47	0
1	G	932	0	930	78	1
1	H	889	0	889	37	1
2	A	4	0	0	0	0
3	A	57	0	0	11	0
3	B	53	0	0	5	0
3	C	21	0	0	3	0
3	D	32	0	0	4	0
3	E	10	0	0	1	0
3	F	41	0	0	1	0
3	G	14	0	0	3	0
3	H	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7963	0	7663	429	2

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 28.

All (429) 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:C:156:ASP:OD2	3:C:230:HOH:O	1.59	1.16
1:A:100:GLU:OE2	3:A:247:HOH:O	1.64	1.15
1:C:108:ALA:HB3	1:C:156:ASP:HB3	1.27	1.15
1:C:86:ARG:HG3	1:C:86:ARG:HH11	0.94	1.10
1:C:86:ARG:HH11	1:C:86:ARG:CG	1.62	1.10
1:A:61:GLU:OE2	3:A:205:HOH:O	1.68	1.10
1:C:71:ARG:CG	1:C:71:ARG:HH11	1.65	1.10
1:G:86:ARG:HG3	1:G:86:ARG:NH1	1.51	1.09
1:B:81:ARG:HG2	1:B:81:ARG:HH11	1.13	1.09
1:C:71:ARG:HG3	1:C:71:ARG:NH1	1.68	1.09
1:G:86:ARG:HH11	1:G:86:ARG:CG	1.63	1.09
1:A:172:MET:HE1	1:E:76:PRO:HB2	1.35	1.08
1:F:58:GLU:HG2	1:G:161:ARG:NH1	1.66	1.08
1:E:128:LEU:O	1:E:132:VAL:CG1	2.03	1.07
1:A:172:MET:HE1	1:E:76:PRO:CB	1.84	1.06
1:G:123:SER:O	1:G:124:SER:HB3	1.52	1.06
1:C:82:VAL:HB	1:C:98:MET:HE3	1.36	1.06
1:E:161:ARG:HG3	1:E:162:VAL:N	1.73	1.03
1:F:58:GLU:HG2	1:G:161:ARG:HH12	0.87	1.02
1:F:182:LEU:O	1:F:183:ASN:HB3	1.59	1.01
1:A:172:MET:CE	1:E:76:PRO:HB3	1.93	0.99
1:B:89:LYS:HG3	1:B:89:LYS:O	1.63	0.98
1:A:61:GLU:OE1	1:A:64[A]:ARG:NH1	1.99	0.96
1:G:86:ARG:NH1	1:G:115:GLU:OE2	1.98	0.96
1:G:136:ASP:OD1	1:G:139:ARG:NH1	1.99	0.96
1:E:85:LEU:C	1:E:85:LEU:HD22	1.92	0.95
1:E:161:ARG:HG3	1:E:162:VAL:H	1.32	0.95
1:E:85:LEU:HD22	1:E:85:LEU:O	1.68	0.94
1:F:58:GLU:CG	1:G:161:ARG:HH12	1.79	0.94
1:E:128:LEU:O	1:E:132:VAL:HG13	1.68	0.94
1:C:108:ALA:CB	1:C:156:ASP:HB3	1.98	0.93
1:F:86:ARG:HD3	1:F:115:GLU:OE2	1.66	0.93
1:C:180:MET:HB3	1:C:181:ASP:HB3	1.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HG3	1:C:86:ARG:NH1	1.64	0.93
1:A:172:MET:CE	1:E:76:PRO:CB	2.46	0.92
1:A:172:MET:HE3	1:E:76:PRO:HB3	1.47	0.92
1:H:92:PRO:HB2	1:H:131:TYR:CZ	2.05	0.92
1:F:56:LEU:HB3	1:F:57:PRO:CD	1.99	0.91
1:C:180:MET:HA	1:C:181:ASP:HB2	1.52	0.91
1:C:71:ARG:HH11	1:C:71:ARG:HG3	1.24	0.91
1:E:136:ASP:OD1	1:E:139:ARG:NH1	2.04	0.90
1:F:56:LEU:HB3	1:F:57:PRO:HD3	1.52	0.90
1:C:98:MET:HE1	1:C:112:ILE:HG23	1.54	0.89
1:D:86:ARG:HD3	3:D:229:HOH:O	1.72	0.89
1:E:128:LEU:O	1:E:132:VAL:HG12	1.68	0.88
1:C:86:ARG:HH21	1:G:87:GLU:HG2	1.38	0.88
1:C:124:SER:HB2	1:C:126:LYS:HG3	1.56	0.87
1:A:86:ARG:NH1	1:A:115:GLU:OE2	2.08	0.87
1:C:71:ARG:O	3:C:212:HOH:O	1.92	0.85
1:D:81:ARG:NH1	3:D:228:HOH:O	2.09	0.84
1:B:81:ARG:HH11	1:B:81:ARG:CG	1.91	0.84
1:F:156:ASP:O	1:F:161:ARG:NH2	2.11	0.83
1:A:139:ARG:NH2	3:A:206:HOH:O	2.10	0.83
1:H:97:LEU:O	1:H:101:GLN:HG3	1.79	0.81
1:A:87:GLU:HG3	1:A:87:GLU:O	1.79	0.80
1:E:85:LEU:O	1:E:85:LEU:CD2	2.30	0.80
1:E:84:LEU:HD12	1:E:89:LYS:HB2	1.61	0.80
1:F:181:ASP:CG	1:F:182:LEU:N	2.39	0.80
1:E:177:LEU:HA	1:E:180:MET:HE3	1.63	0.79
1:E:75:TRP:HB3	1:E:76:PRO:HD3	1.64	0.79
1:G:86:ARG:HG3	1:G:86:ARG:HH11	0.71	0.79
1:D:160:GLY:C	1:D:161:ARG:HD2	2.08	0.79
1:E:148:ASN:HB3	1:E:154:VAL:CG2	2.12	0.79
1:C:87:GLU:OE2	1:G:86:ARG:CD	2.31	0.79
1:E:85:LEU:C	1:E:85:LEU:CD2	2.56	0.79
1:A:161:ARG:HG3	1:E:161:ARG:CB	2.13	0.78
1:A:161:ARG:HG3	1:E:161:ARG:HB3	1.64	0.78
1:D:183:ASN:HA	1:D:184:PRO:C	2.08	0.78
1:F:58:GLU:O	1:F:60:LEU:N	2.17	0.78
1:E:161:ARG:CG	1:E:162:VAL:H	1.97	0.78
1:C:82:VAL:HB	1:C:98:MET:CE	2.14	0.77
1:F:58:GLU:O	1:F:59:GLU:C	2.26	0.77
1:B:92:PRO:O	1:B:95:ILE:HG13	1.84	0.76
1:A:130:THR:OG1	1:C:139:ARG:NH2	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:PRO:HB2	1:H:131:TYR:CE1	2.20	0.76
1:G:172:MET:HE3	3:G:224:HOH:O	1.84	0.76
1:B:150:LYS:NZ	3:B:235:HOH:O	2.18	0.76
1:C:180:MET:CA	1:C:181:ASP:HB2	2.16	0.75
1:C:87:GLU:OE2	1:G:86:ARG:HD2	1.86	0.75
1:E:155:SER:O	1:E:157:PRO:HG2	1.86	0.75
1:C:87:GLU:HB3	1:C:89:LYS:HG3	1.67	0.74
1:A:67:HIS:HD2	3:A:214:HOH:O	1.70	0.74
1:D:98:MET:HE2	3:D:228:HOH:O	1.86	0.74
1:D:115:GLU:HG2	3:D:2:HOH:O	1.86	0.74
1:E:161:ARG:CG	1:E:162:VAL:N	2.50	0.74
1:F:181:ASP:CG	1:F:182:LEU:H	1.94	0.74
1:A:161:ARG:CG	1:E:161:ARG:HB3	2.18	0.74
1:A:161:ARG:CG	1:E:161:ARG:CB	2.65	0.74
1:E:136:ASP:CG	1:E:139:ARG:NH1	2.45	0.74
1:G:126:LYS:O	1:G:130:THR:N	2.20	0.73
1:C:84:LEU:O	1:C:89:LYS:O	2.07	0.73
1:D:108:ALA:HB2	1:D:154:VAL:HG22	1.70	0.73
1:C:181:ASP:CG	1:C:182:LEU:H	1.95	0.73
1:G:172:MET:CE	3:G:224:HOH:O	2.35	0.73
1:C:89:LYS:HD3	1:G:122:TYR:CD1	2.24	0.72
1:A:163:ASN:C	1:A:163:ASN:OD1	2.30	0.71
1:E:81:ARG:HB3	1:E:98:MET:HE2	1.72	0.71
1:G:123:SER:O	1:G:124:SER:CB	2.32	0.71
1:C:156:ASP:O	1:C:161:ARG:NH2	2.23	0.71
1:F:182:LEU:O	1:F:183:ASN:CB	2.30	0.70
1:C:116:LEU:HD21	1:C:138:MET:HE3	1.74	0.70
1:A:161:ARG:HD2	1:E:161:ARG:HE	1.56	0.70
1:B:81:ARG:HG2	1:B:81:ARG:NH1	1.95	0.70
1:A:165:ASP:OD2	1:E:158:ASN:HB3	1.91	0.70
1:B:163:ASN:ND2	1:D:161:ARG:HD3	2.06	0.70
1:G:139:ARG:HD2	1:G:180:MET:HB3	1.73	0.70
1:A:161:ARG:HE	1:E:161:ARG:HG2	1.56	0.69
1:G:137:GLU:O	1:G:141:GLU:HG3	1.92	0.69
1:G:72:ARG:HH11	1:G:72:ARG:CG	2.05	0.69
1:A:155:SER:O	1:A:156:ASP:HB2	1.91	0.69
1:G:120:LEU:HD11	1:G:138:MET:HE2	1.73	0.69
1:B:139:ARG:HD2	1:B:180:MET:HB3	1.73	0.68
1:C:98:MET:HE1	1:C:112:ILE:CG2	2.21	0.68
1:A:156:ASP:N	1:A:157:PRO:HD3	2.08	0.68
1:D:99:TRP:CE2	1:D:103:LYS:HD2	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ASN:OD1	1:F:183:ASN:C	2.36	0.68
1:C:87:GLU:CB	1:C:89:LYS:HG3	2.24	0.68
1:B:89:LYS:O	1:B:89:LYS:CG	2.30	0.68
1:C:71:ARG:HH11	1:C:71:ARG:HG2	1.59	0.67
1:F:139:ARG:HD2	1:F:180:MET:HB3	1.77	0.67
1:H:98:MET:O	1:H:102:THR:HG22	1.95	0.66
1:C:180:MET:CA	1:C:181:ASP:CB	2.74	0.66
1:C:180:MET:HB3	1:C:181:ASP:CB	2.26	0.65
1:A:103:LYS:NZ	3:A:247:HOH:O	2.28	0.65
1:B:78:LEU:HD21	1:B:102:THR:HG22	1.78	0.65
1:C:75:TRP:CE3	1:G:165:ASP:HB3	2.30	0.65
1:F:181:ASP:OD1	1:F:182:LEU:N	2.30	0.65
1:F:79:HIS:CD2	1:F:111:LEU:HD23	2.32	0.65
1:G:72:ARG:HB2	1:G:105:TYR:CE1	2.31	0.65
1:C:86:ARG:HD2	1:C:86:ARG:C	2.21	0.64
1:A:162:VAL:C	1:A:163:ASN:O	2.30	0.64
1:B:87:GLU:HG2	1:D:86:ARG:HH21	1.62	0.64
1:C:108:ALA:CB	1:C:156:ASP:CB	2.76	0.63
1:F:85:LEU:HD11	1:F:95:ILE:HG12	1.80	0.63
1:E:158:ASN:N	1:E:158:ASN:OD1	2.30	0.63
1:A:161:ARG:HG2	1:E:161:ARG:HG2	1.79	0.63
1:C:89:LYS:HD3	1:G:122:TYR:HD1	1.61	0.63
1:A:161:ARG:CD	1:E:161:ARG:HE	2.11	0.62
1:E:84:LEU:HD12	1:E:89:LYS:CB	2.28	0.62
1:F:160:GLY:C	1:F:161:ARG:HD2	2.24	0.62
1:H:94:ASP:HB2	1:H:98:MET:HE3	1.81	0.62
1:F:161:ARG:HD2	1:F:161:ARG:N	2.14	0.62
1:C:122:TYR:CD2	1:G:87:GLU:HG3	2.35	0.62
1:C:72:ARG:HB2	1:C:105:TYR:CD1	2.33	0.61
1:G:163:ASN:OD1	1:G:166:VAL:HG23	1.99	0.61
1:A:104:HIS:HE1	3:A:210:HOH:O	1.83	0.61
1:F:165:ASP:HB3	1:H:75:TRP:CE3	2.35	0.61
1:H:124:SER:O	1:H:127:TYR:N	2.33	0.61
1:C:86:ARG:HD2	1:C:86:ARG:O	2.01	0.61
1:D:96:ALA:O	1:D:100:GLU:HB2	2.01	0.61
1:A:163:ASN:HB2	1:A:164:LYS:HE2	1.80	0.61
1:D:161:ARG:HD2	1:D:161:ARG:N	2.16	0.61
1:F:58:GLU:O	1:F:61:GLU:N	2.33	0.61
1:B:176:ASP:OD1	3:B:236:HOH:O	2.16	0.61
1:F:58:GLU:CG	1:G:161:ARG:NH1	2.49	0.61
1:C:87:GLU:OE2	1:G:86:ARG:HD3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:PRO:HD2	1:C:156:ASP:OD2	2.01	0.60
1:C:162:VAL:HG22	1:C:163:ASN:N	2.16	0.60
1:B:71:ARG:HA	1:B:71:ARG:NE	2.15	0.60
1:C:162:VAL:CG2	1:C:163:ASN:N	2.64	0.60
1:B:162:VAL:HG13	1:B:166:VAL:HG12	1.82	0.60
1:E:148:ASN:HB3	1:E:154:VAL:HG23	1.82	0.60
1:C:156:ASP:OD1	1:C:157:PRO:HD2	2.01	0.59
1:B:163:ASN:HD22	1:D:161:ARG:HD3	1.67	0.59
1:G:72:ARG:NH1	1:G:72:ARG:HG2	2.18	0.59
1:B:81:ARG:NH1	1:B:98:MET:HE2	2.17	0.58
1:A:98:MET:O	1:A:102:THR:HG23	2.03	0.58
1:D:75:TRP:HB3	1:D:76:PRO:HD3	1.84	0.58
1:F:168:GLU:OE1	1:H:76:PRO:HG2	2.04	0.58
1:C:81:ARG:HD2	1:C:94:ASP:OD1	2.04	0.58
1:B:91:ALA:N	1:B:92:PRO:CD	2.67	0.57
1:C:107:PRO:HD2	1:C:156:ASP:CG	2.29	0.57
1:A:167:GLU:O	1:A:167:GLU:HG3	2.03	0.57
1:G:72:ARG:CG	1:G:72:ARG:NH1	2.64	0.57
1:A:78:LEU:HD21	1:A:102:THR:HG22	1.86	0.57
1:B:91:ALA:N	1:B:92:PRO:HD3	2.19	0.57
1:F:56:LEU:HB3	1:F:57:PRO:HD2	1.84	0.57
1:A:94:ASP:OD2	1:F:71:ARG:HD3	2.05	0.57
1:A:102:THR:HG21	1:A:112:ILE:HG21	1.87	0.57
1:B:67:HIS:O	1:B:67:HIS:CG	2.58	0.57
1:G:94:ASP:HB2	1:G:98:MET:HE3	1.87	0.57
1:C:95:ILE:HD11	1:C:138:MET:HE1	1.86	0.56
1:D:77:LEU:O	1:D:81:ARG:HG3	2.05	0.56
1:H:90:GLY:O	1:H:92:PRO:HD3	2.05	0.56
1:B:65:GLN:N	1:B:68:ASN:OD1	2.39	0.56
1:B:75:TRP:CE3	1:D:165:ASP:HB3	2.41	0.56
1:G:86:ARG:NH1	1:G:86:ARG:CG	2.35	0.55
1:C:145:GLN:O	1:C:149:VAL:HG23	2.07	0.55
1:E:113:PRO:HB2	1:E:146:LEU:HD21	1.88	0.55
1:C:75:TRP:HB3	1:C:76:PRO:HD3	1.87	0.55
1:A:164:LYS:HE2	1:A:164:LYS:H	1.71	0.55
1:E:148:ASN:HA	1:E:153:ARG:HD2	1.89	0.55
1:D:150:LYS:HE3	1:D:171:SER:OG	2.07	0.55
1:B:120:LEU:HB3	1:B:182:LEU:HD21	1.89	0.54
1:C:86:ARG:CG	1:C:86:ARG:NH1	2.34	0.54
1:A:170:ILE:O	1:A:174:VAL:HG23	2.08	0.54
1:E:98:MET:O	1:E:102:THR:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ARG:HB2	1:E:119:VAL:HG22	1.89	0.54
1:E:136:ASP:CG	1:E:139:ARG:HH12	2.16	0.54
1:H:164:LYS:O	1:H:164:LYS:HD3	2.07	0.54
1:A:163:ASN:OD1	1:A:164:LYS:N	2.40	0.54
1:B:92:PRO:HB3	1:B:127:TYR:OH	2.08	0.54
1:B:150:LYS:NZ	3:B:234:HOH:O	2.40	0.53
1:H:124:SER:O	1:H:126:LYS:N	2.42	0.53
1:A:161:ARG:NE	1:E:161:ARG:NE	2.57	0.53
1:G:136:ASP:CG	1:G:139:ARG:NH1	2.67	0.53
1:D:75:TRP:N	1:D:76:PRO:CD	2.72	0.53
1:C:124:SER:CB	1:C:126:LYS:HG3	2.34	0.53
1:G:170:ILE:O	1:G:174:VAL:HG23	2.09	0.53
1:D:99:TRP:NE1	1:D:103:LYS:HD2	2.23	0.53
1:B:66:ARG:HG2	1:B:104:HIS:CE1	2.44	0.52
1:A:167:GLU:HG2	3:A:209:HOH:O	2.10	0.52
1:A:161:ARG:HG3	1:E:161:ARG:HB2	1.90	0.52
1:H:92:PRO:C	1:H:131:TYR:CE1	2.88	0.52
1:H:124:SER:C	1:H:126:LYS:N	2.62	0.52
1:E:177:LEU:HD23	1:E:180:MET:HE1	1.90	0.52
1:H:139:ARG:NH1	1:H:140:LYS:HG3	2.25	0.52
1:D:98:MET:O	1:D:102:THR:HG23	2.09	0.52
1:H:108:ALA:HB2	1:H:154:VAL:HG22	1.90	0.52
1:G:119:VAL:O	1:G:123:SER:HB2	2.08	0.52
1:G:158:ASN:ND2	1:G:158:ASN:H	2.07	0.52
1:A:87:GLU:HB2	1:E:86:ARG:NH2	2.25	0.52
1:C:116:LEU:HD11	1:C:138:MET:CE	2.40	0.52
1:B:98:MET:O	1:B:102:THR:CG2	2.58	0.51
1:E:136:ASP:OD2	1:E:139:ARG:NH1	2.42	0.51
1:A:161:ARG:HG2	1:E:161:ARG:HB3	1.92	0.51
1:B:87:GLU:HG3	1:D:122:TYR:CD2	2.45	0.51
1:C:116:LEU:HD11	1:C:138:MET:HE1	1.93	0.51
1:A:72:ARG:HB2	1:A:105:TYR:CE1	2.45	0.51
1:G:156:ASP:O	1:G:156:ASP:OD1	2.29	0.51
1:F:170:ILE:O	1:F:174:VAL:HG23	2.11	0.51
1:G:128:LEU:HD13	1:G:132:VAL:CG2	2.41	0.51
1:H:92:PRO:O	1:H:95:ILE:HG13	2.11	0.51
1:A:97:LEU:O	1:A:101:GLN:HG3	2.11	0.50
1:B:72:ARG:HB2	1:B:105:TYR:CE1	2.47	0.50
1:A:86:ARG:NH2	1:E:115:GLU:OE2	2.44	0.50
1:E:127:TYR:C	1:E:127:TYR:CD2	2.90	0.50
1:G:166:VAL:O	1:G:169:ILE:HG22	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:CD2	1:E:87:GLU:HG3	2.47	0.50
1:H:112:ILE:HB	1:H:113:PRO:HD3	1.94	0.50
1:B:94:ASP:HB2	1:B:98:MET:HE3	1.94	0.50
1:E:95:ILE:CD1	1:E:138:MET:HE1	2.41	0.50
1:F:92:PRO:O	1:F:95:ILE:HG13	2.11	0.50
1:A:161:ARG:NE	1:E:161:ARG:HE	2.10	0.50
1:C:72:ARG:O	1:C:72:ARG:CG	2.57	0.50
1:C:182:LEU:O	1:C:183:ASN:O	2.30	0.50
1:F:82:VAL:O	1:F:85:LEU:HB2	2.11	0.50
1:E:156:ASP:HA	1:E:157:PRO:HB2	1.93	0.50
1:G:158:ASN:C	1:G:160:GLY:H	2.20	0.50
1:C:120:LEU:HD21	1:C:138:MET:HE2	1.94	0.49
1:C:143:LEU:HD11	1:C:174:VAL:HG13	1.93	0.49
1:E:136:ASP:OD2	1:E:136:ASP:O	2.30	0.49
1:E:158:ASN:CB	1:E:159:GLY:HA2	2.39	0.49
1:G:176:ASP:O	1:G:180:MET:HE3	2.12	0.49
1:G:155:SER:O	1:G:156:ASP:OD1	2.30	0.49
1:F:162:VAL:HG12	1:F:163:ASN:N	2.27	0.49
1:C:180:MET:CB	1:C:181:ASP:CB	2.90	0.49
1:D:93:GLU:O	1:D:94:ASP:C	2.54	0.49
1:H:90:GLY:C	1:H:92:PRO:HD3	2.38	0.49
1:E:109:ASP:HB2	1:E:159:GLY:H	1.76	0.49
1:H:124:SER:C	1:H:126:LYS:H	2.20	0.49
1:G:72:ARG:O	1:G:72:ARG:HG3	1.99	0.49
3:C:205:HOH:O	1:F:104:HIS:HE1	1.96	0.49
1:A:167:GLU:O	1:A:167:GLU:CG	2.56	0.49
1:H:121:LYS:HA	1:H:180:MET:HE2	1.94	0.49
1:A:103:LYS:CE	3:A:247:HOH:O	2.60	0.48
1:C:108:ALA:HA	1:C:154:VAL:HG11	1.95	0.48
1:C:72:ARG:O	1:C:72:ARG:HG2	2.13	0.48
1:C:86:ARG:NH2	1:G:87:GLU:HG2	2.18	0.48
1:E:132:VAL:HG21	1:E:135:PRO:HA	1.94	0.48
1:E:73:PRO:HG3	1:E:101:GLN:NE2	2.28	0.48
1:A:161:ARG:NE	1:E:161:ARG:HG2	2.27	0.48
1:C:80[B]:GLN:OE1	1:G:172:MET:HE1	2.14	0.48
1:E:77:LEU:O	1:E:81:ARG:HG3	2.13	0.48
1:F:155:SER:HA	3:F:216:HOH:O	2.14	0.48
1:F:182:LEU:N	1:F:182:LEU:CD1	2.76	0.48
1:A:87:GLU:O	1:A:87:GLU:CG	2.56	0.48
1:D:98:MET:O	1:D:102:THR:CG2	2.61	0.48
1:G:90:GLY:O	1:G:92:PRO:HD3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100[B]:GLU:OE2	1:G:103:LYS:NZ	2.26	0.48
1:A:61:GLU:CD	1:A:64[A]:ARG:NH1	2.72	0.48
1:A:64[B]:ARG:CZ	1:A:68:ASN:HD21	2.26	0.48
1:B:112:ILE:N	1:B:113:PRO:CD	2.76	0.48
1:H:164:LYS:HD3	1:H:164:LYS:C	2.38	0.48
1:B:79:HIS:O	1:B:83:VAL:HG23	2.14	0.48
1:E:98:MET:O	1:E:102:THR:CG2	2.62	0.48
1:G:79:HIS:O	1:G:83:VAL:HG23	2.14	0.48
1:D:102:THR:HG21	1:D:112:ILE:HG21	1.95	0.47
1:G:108:ALA:HA	1:G:154:VAL:HG21	1.96	0.47
1:H:124:SER:O	1:H:125:GLY:C	2.55	0.47
1:F:75:TRP:CE2	1:F:159:GLY:HA2	2.49	0.47
1:A:86:ARG:HD3	3:A:246:HOH:O	2.14	0.47
1:A:161:ARG:HG2	1:E:161:ARG:CB	2.43	0.47
1:B:87:GLU:HG2	1:D:86:ARG:NH2	2.28	0.47
1:A:156:ASP:H	1:A:157:PRO:HD3	1.79	0.47
1:B:109:ASP:O	1:B:113:PRO:HG2	2.15	0.47
1:G:92:PRO:HB2	1:G:131:TYR:CE2	2.50	0.47
1:A:156:ASP:N	1:A:157:PRO:CD	2.78	0.47
1:G:75:TRP:CH2	1:G:111:LEU:HD23	2.50	0.47
1:B:92:PRO:O	1:B:95:ILE:CG1	2.59	0.47
1:E:125:GLY:O	1:E:129:GLN:HG3	2.14	0.47
1:A:75:TRP:CE3	1:E:165:ASP:HB3	2.50	0.46
1:B:158:ASN:H	1:B:158:ASN:HD22	1.63	0.46
1:G:84:LEU:HD12	1:G:84:LEU:HA	1.41	0.46
1:H:74:PRO:HD2	1:H:77:LEU:HD12	1.96	0.46
1:B:81:ARG:CG	1:B:81:ARG:NH1	2.59	0.46
1:G:103:LYS:O	1:G:107:PRO:HG3	2.15	0.46
1:G:72:ARG:HD3	1:G:105:TYR:CD1	2.50	0.46
1:D:107:PRO:HB2	1:D:154:VAL:HG21	1.98	0.46
1:E:95:ILE:HD11	1:E:138:MET:HE1	1.98	0.46
1:D:160:GLY:O	1:D:161:ARG:HD2	2.14	0.46
1:E:92:PRO:HB2	1:E:131:TYR:CD1	2.50	0.46
1:G:139:ARG:NH1	1:G:139:ARG:HB3	2.31	0.46
1:B:65:GLN:CA	1:B:68:ASN:OD1	2.64	0.45
1:B:98:MET:O	1:B:102:THR:HG23	2.16	0.45
1:E:95:ILE:CG2	1:E:96:ALA:N	2.79	0.45
1:A:162:VAL:O	1:A:163:ASN:O	2.35	0.45
1:A:161:ARG:HG2	1:E:161:ARG:CG	2.45	0.45
1:F:123:SER:HB2	1:F:128:LEU:HD13	1.98	0.45
1:G:128:LEU:CD1	1:G:132:VAL:HG21	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TRP:CZ3	1:D:165:ASP:HB3	2.51	0.45
1:F:110:TRP:CZ3	1:F:111:LEU:HD12	2.52	0.45
1:A:111:LEU:HD22	1:E:110:TRP:HH2	1.82	0.45
1:E:81:ARG:NH1	1:E:98:MET:HE2	2.31	0.45
1:G:93:GLU:CD	1:G:93:GLU:H	2.24	0.45
1:C:71:ARG:CG	1:C:71:ARG:NH1	2.30	0.45
1:C:92:PRO:O	1:C:95:ILE:HG22	2.17	0.45
1:G:136:ASP:CG	1:G:139:ARG:HH12	2.24	0.45
1:A:115:GLU:HG3	3:A:246:HOH:O	2.17	0.44
1:A:161:ARG:CG	1:E:161:ARG:HG2	2.47	0.44
1:B:83:VAL:O	1:B:83:VAL:HG12	2.18	0.44
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.77	0.44
1:A:58:GLU:HB3	1:A:59:GLU:H	1.45	0.44
1:A:124:SER:OG	1:C:179:ASN:ND2	2.51	0.44
1:B:71:ARG:HA	1:B:71:ARG:HE	1.79	0.44
1:H:75:TRP:CH2	1:H:111:LEU:HD23	2.52	0.44
1:A:172:MET:CE	1:E:76:PRO:HB2	2.18	0.44
1:C:72:ARG:HA	1:C:73:PRO:HD3	1.73	0.44
1:C:177:LEU:C	1:C:179:ASN:H	2.24	0.44
1:E:100:GLU:OE1	3:E:215:HOH:O	2.21	0.44
1:A:69:ASP:HA	1:A:70:PRO:HD3	1.85	0.44
1:A:83:VAL:O	1:A:83:VAL:HG12	2.17	0.44
1:B:153:ARG:NH1	3:B:24:HOH:O	2.49	0.44
1:B:162:VAL:HG13	1:B:166:VAL:CG1	2.47	0.44
1:F:123:SER:CB	1:F:128:LEU:HD13	2.48	0.44
1:H:82:VAL:HG13	1:H:116:LEU:HD13	1.99	0.44
1:H:92:PRO:O	1:H:131:TYR:CD1	2.70	0.44
1:G:128:LEU:HD13	1:G:132:VAL:HG21	1.99	0.44
1:C:181:ASP:CG	1:C:182:LEU:N	2.62	0.44
1:E:72:ARG:HG3	1:E:105:TYR:HB3	1.98	0.44
1:A:164:LYS:HE2	1:A:164:LYS:N	2.32	0.43
1:B:172:MET:HE1	1:D:77:LEU:HD12	2.00	0.43
1:E:95:ILE:HG23	1:E:96:ALA:N	2.33	0.43
1:E:161:ARG:CD	1:E:162:VAL:H	2.31	0.43
1:C:82:VAL:O	1:C:85:LEU:HB2	2.18	0.43
1:C:108:ALA:HB2	1:C:156:ASP:CB	2.49	0.43
1:F:156:ASP:OD2	1:F:158:ASN:ND2	2.50	0.43
1:E:99:TRP:HB2	1:E:138:MET:HE3	2.00	0.43
1:G:102:THR:O	1:G:106:TYR:C	2.61	0.43
1:A:83:VAL:O	1:A:83:VAL:CG1	2.66	0.43
1:B:158:ASN:H	1:B:158:ASN:ND2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:TRP:HB3	1:H:76:PRO:HD3	2.00	0.43
1:B:72:ARG:HA	1:B:73:PRO:HD3	1.89	0.43
1:C:164:LYS:O	1:C:164:LYS:HG3	2.18	0.43
1:F:56:LEU:N	1:F:57:PRO:HD2	2.34	0.43
1:F:163:ASN:H	1:F:166:VAL:HB	1.84	0.43
1:F:105:TYR:C	1:F:107:PRO:HD3	2.44	0.43
1:F:121:LYS:HA	1:F:180:MET:HE2	2.00	0.43
1:G:139:ARG:NE	1:G:177:LEU:O	2.36	0.43
1:H:126:LYS:HE3	1:H:126:LYS:HB2	1.37	0.42
1:A:90:GLY:N	3:A:221:HOH:O	2.01	0.42
1:C:98:MET:CE	1:C:112:ILE:HG23	2.36	0.42
1:C:128:LEU:HD12	1:C:128:LEU:HA	1.75	0.42
1:H:116:LEU:HA	1:H:116:LEU:HD12	1.73	0.42
1:A:161:ARG:HE	1:E:161:ARG:CG	2.28	0.42
1:H:78:LEU:O	1:H:82:VAL:HG23	2.20	0.42
1:C:177:LEU:C	1:C:179:ASN:N	2.77	0.42
1:E:78:LEU:HD21	1:E:102:THR:HG22	2.01	0.42
1:C:77:LEU:HD12	1:C:77:LEU:HA	1.82	0.42
1:C:180:MET:CB	1:C:181:ASP:HB3	2.35	0.42
1:D:163:ASN:OD1	1:D:163:ASN:C	2.63	0.42
1:E:128:LEU:HD12	1:E:128:LEU:HA	1.80	0.42
1:F:86:ARG:HE	1:F:86:ARG:HB3	1.31	0.42
1:H:72:ARG:HB2	1:H:105:TYR:CE1	2.54	0.42
1:G:128:LEU:CD1	1:G:132:VAL:CG2	2.98	0.42
1:G:136:ASP:O	1:G:140:LYS:HG3	2.20	0.42
1:H:92:PRO:HB2	1:H:131:TYR:CE2	2.51	0.42
1:B:165:ASP:HB3	1:D:75:TRP:CE3	2.55	0.42
1:A:71:ARG:HE	1:A:71:ARG:HB3	1.49	0.42
1:E:132:VAL:HG13	1:E:135:PRO:HG3	2.02	0.42
1:F:182:LEU:HA	1:F:182:LEU:HD12	1.45	0.42
1:G:94:ASP:O	1:G:95:ILE:C	2.62	0.42
1:D:84:LEU:HD13	1:D:84:LEU:HA	1.85	0.41
1:G:110:TRP:C	1:G:113:PRO:HD2	2.45	0.41
1:G:85:LEU:HD13	1:G:95:ILE:HG12	2.02	0.41
1:G:90:GLY:C	1:G:92:PRO:HD3	2.44	0.41
1:G:156:ASP:N	1:G:157:PRO:HD3	2.35	0.41
1:G:176:ASP:O	1:G:180:MET:HB2	2.19	0.41
1:B:125:GLY:O	1:B:129:GLN:HG2	2.20	0.41
1:E:110:TRP:C	1:E:113:PRO:HD2	2.46	0.41
1:H:110:TRP:HB3	1:H:149:VAL:HG11	2.02	0.41
1:F:139:ARG:CD	1:F:180:MET:HB3	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLU:CD	1:A:64[A]:ARG:HH12	2.18	0.41
1:H:148:ASN:O	1:H:153:ARG:N	2.52	0.41
1:A:59:GLU:O	1:A:63:GLN:HG3	2.21	0.41
1:B:158:ASN:ND2	3:B:207:HOH:O	2.43	0.41
1:G:92:PRO:HA	1:G:95:ILE:HG13	2.01	0.41
1:G:106:TYR:N	1:G:107:PRO:HD3	2.35	0.41
1:C:84:LEU:CD2	1:C:89:LYS:HB2	2.51	0.41
1:D:156:ASP:HA	1:D:157:PRO:HD3	1.82	0.41
1:E:144:MET:HE2	1:E:144:MET:HA	2.02	0.41
1:F:156:ASP:HA	1:F:157:PRO:HD3	1.84	0.41
1:G:71:ARG:HD3	1:G:71:ARG:HA	1.17	0.41
1:G:105:TYR:C	1:G:107:PRO:HD3	2.46	0.41
1:G:139:ARG:HB3	1:G:139:ARG:HH11	1.86	0.41
1:G:116:LEU:HD12	1:G:116:LEU:HA	1.79	0.41
1:H:93:GLU:N	1:H:131:TYR:CE1	2.89	0.41
1:H:163:ASN:OD1	1:H:166:VAL:HG23	2.20	0.41
1:B:90:GLY:C	1:B:92:PRO:HD3	2.46	0.40
1:B:98:MET:O	1:B:102:THR:HG22	2.21	0.40
1:G:110:TRP:HB3	1:G:149:VAL:HG11	2.01	0.40
1:G:172:MET:HE2	3:G:224:HOH:O	2.12	0.40
1:H:132:VAL:HG11	1:H:135:PRO:HA	2.02	0.40
1:A:70:PRO:HB2	1:F:91:ALA:HB2	2.02	0.40
1:A:75:TRP:CH2	1:E:169:ILE:HD13	2.57	0.40
1:D:105:TYR:C	1:D:107:PRO:HD3	2.46	0.40
1:E:75:TRP:HB3	1:E:76:PRO:CD	2.43	0.40
1:G:158:ASN:C	1:G:160:GLY:N	2.79	0.40
1:D:78:LEU:HD21	1:D:102:THR:HG22	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLU:OE1	1:B:153:ARG:NH2[2_654]	1.96	0.24
1:G:153:ARG:NH1	1:H:178:GLU:OE2[3_655]	2.05	0.15

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	126/154 (82%)	122 (97%)	2 (2%)	2 (2%)	7	11
1	B	118/154 (77%)	113 (96%)	5 (4%)	0	100	100
1	C	113/154 (73%)	105 (93%)	7 (6%)	1 (1%)	14	22
1	D	113/154 (73%)	112 (99%)	1 (1%)	0	100	100
1	E	109/154 (71%)	100 (92%)	8 (7%)	1 (1%)	14	22
1	F	128/154 (83%)	122 (95%)	4 (3%)	2 (2%)	7	11
1	G	112/154 (73%)	105 (94%)	6 (5%)	1 (1%)	14	22
1	H	107/154 (70%)	101 (94%)	6 (6%)	0	100	100
All	All	926/1232 (75%)	880 (95%)	39 (4%)	7 (1%)	16	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	C	181	ASP
1	E	157	PRO
1	F	59	GLU
1	G	124	SER
1	F	58	GLU
1	A	156	ASP

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	116/136 (85%)	103 (89%)	13 (11%)	6	9
1	B	109/136 (80%)	93 (85%)	16 (15%)	3	4
1	C	104/136 (76%)	89 (86%)	15 (14%)	3	4
1	D	103/136 (76%)	93 (90%)	10 (10%)	8	12
1	E	100/136 (74%)	83 (83%)	17 (17%)	2	2
1	F	118/136 (87%)	105 (89%)	13 (11%)	6	9
1	G	103/136 (76%)	86 (84%)	17 (16%)	2	3
1	H	98/136 (72%)	87 (89%)	11 (11%)	6	9
All	All	851/1088 (78%)	739 (87%)	112 (13%)	4	5

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	60	LEU
1	A	71	ARG
1	A	84	LEU
1	A	97	LEU
1	A	102	THR
1	A	116	LEU
1	A	126	LYS
1	A	129	GLN
1	A	139	ARG
1	A	156	ASP
1	A	161	ARG
1	A	164	LYS
1	B	65	GLN
1	B	66	ARG
1	B	68	ASN
1	B	77	LEU
1	B	81	ARG
1	B	85	LEU
1	B	89	LYS
1	B	93	GLU
1	B	102	THR
1	B	111	LEU
1	B	116	LEU
1	B	128	LEU
1	B	132	VAL
1	B	156	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	ILE
1	B	182	LEU
1	C	71	ARG
1	C	72	ARG
1	C	77	LEU
1	C	85	LEU
1	C	86	ARG
1	C	89	LYS
1	C	114	LEU
1	C	128	LEU
1	C	144	MET
1	C	155	SER
1	C	161	ARG
1	C	162	VAL
1	C	164	LYS
1	C	182	LEU
1	C	183	ASN
1	D	77	LEU
1	D	84	LEU
1	D	97	LEU
1	D	102	THR
1	D	128	LEU
1	D	147	LEU
1	D	154	VAL
1	D	162	VAL
1	D	168	GLU
1	D	182	LEU
1	E	71	ARG
1	E	77	LEU
1	E	84	LEU
1	E	85	LEU
1	E	95	ILE
1	E	97	LEU
1	E	100	GLU
1	E	102	THR
1	E	116	LEU
1	E	126	LYS
1	E	128	LEU
1	E	132	VAL
1	E	144	MET
1	E	154	VAL
1	E	155	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	158	ASN
1	E	175	ASP
1	F	55	GLU
1	F	58	GLU
1	F	60	LEU
1	F	97	LEU
1	F	100	GLU
1	F	114	LEU
1	F	116	LEU
1	F	128	LEU
1	F	140	LYS
1	F	161	ARG
1	F	177	LEU
1	F	182	LEU
1	F	183	ASN
1	G	71	ARG
1	G	72	ARG
1	G	77	LEU
1	G	84	LEU
1	G	86	ARG
1	G	89	LYS
1	G	93	GLU
1	G	97	LEU
1	G	100[A]	GLU
1	G	100[B]	GLU
1	G	102	THR
1	G	116	LEU
1	G	123	SER
1	G	124	SER
1	G	128	LEU
1	G	129	GLN
1	G	143	LEU
1	H	93	GLU
1	H	97	LEU
1	H	102	THR
1	H	103	LYS
1	H	116	LEU
1	H	124	SER
1	H	126	LYS
1	H	128	LEU
1	H	156	ASP
1	H	164	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	180	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	67	HIS
1	A	68	ASN
1	A	104	HIS
1	A	129	GLN
1	B	104	HIS
1	B	118	GLN
1	B	129	GLN
1	B	158	ASN
1	C	129	GLN
1	C	179	ASN
1	D	80	GLN
1	D	118	GLN
1	D	129	GLN
1	D	158	ASN
1	E	118	GLN
1	F	63	GLN
1	F	65	GLN
1	F	104	HIS
1	G	158	ASN
1	H	79	HIS
1	H	118	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 oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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	$\# Z > 2$
2	CO3	A	1	-	3,3,3	0.76	0	2,3,3	1.01	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	127/154 (82%)	-0.10	7 (5%)	30	27	24, 37, 79, 143	1 (0%)
1	B	120/154 (77%)	-0.02	5 (4%)	40	36	24, 43, 101, 128	0
1	C	113/154 (73%)	0.13	5 (4%)	39	34	17, 43, 83, 100	2 (1%)
1	D	114/154 (74%)	-0.05	5 (4%)	39	34	20, 37, 75, 128	1 (0%)
1	E	111/154 (72%)	0.65	10 (9%)	15	12	34, 66, 108, 144	0
1	F	129/154 (83%)	-0.02	5 (3%)	43	39	24, 41, 90, 126	1 (0%)
1	G	113/154 (73%)	0.84	11 (9%)	13	10	31, 62, 101, 132	1 (0%)
1	H	109/154 (70%)	0.26	3 (2%)	55	51	32, 62, 94, 114	0
All	All	936/1232 (75%)	0.20	51 (5%)	31	28	17, 48, 95, 144	6 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	ASP	4.9
1	D	184	PRO	4.5
1	D	183	ASN	4.1
1	E	158	ASN	4.1
1	F	58	GLU	3.9
1	G	70	PRO	3.8
1	E	70	PRO	3.7
1	B	66	ARG	3.7
1	A	64[A]	ARG	3.5
1	C	88	GLY	3.0
1	A	61	GLU	3.0
1	F	59	GLU	2.9
1	A	159	GLY	2.9
1	G	136	ASP	2.9
1	E	160	GLY	2.9
1	H	96	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	182	LEU	2.8
1	D	88	GLY	2.7
1	F	160	GLY	2.7
1	A	161	ARG	2.7
1	C	125	GLY	2.7
1	E	153	ARG	2.6
1	G	125	GLY	2.6
1	E	133	ALA	2.5
1	B	71	ARG	2.5
1	C	160	GLY	2.5
1	G	181	ASP	2.5
1	A	88	GLY	2.5
1	G	179	ASN	2.4
1	B	65	GLN	2.4
1	E	154	VAL	2.4
1	A	60	LEU	2.3
1	F	62	ALA	2.3
1	B	131	TYR	2.3
1	E	157	PRO	2.3
1	F	183	ASN	2.3
1	G	160	GLY	2.2
1	E	180	MET	2.2
1	G	134	ASP	2.2
1	E	88	GLY	2.1
1	A	58	GLU	2.1
1	D	179	ASN	2.1
1	B	129	GLN	2.1
1	G	130	THR	2.1
1	D	137[A]	GLU	2.1
1	H	131	TYR	2.1
1	G	163	ASN	2.1
1	G	131	TYR	2.1
1	C	159	GLY	2.0
1	E	159	GLY	2.0
1	H	157	PRO	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 [i](#)

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($\text{\AA}^2$)	Q<0.9
2	CO3	A	1	4/4	0.87	0.13	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.