Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:39 AM GMT

PDB ID	:	3MPV
Title	:	Structure of EUTL in the zinc-induced open form
Authors	:	Sagermann, M.; Takenoya, M.; Nikolakakis, K.
Deposited on	:	2010-04-27
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

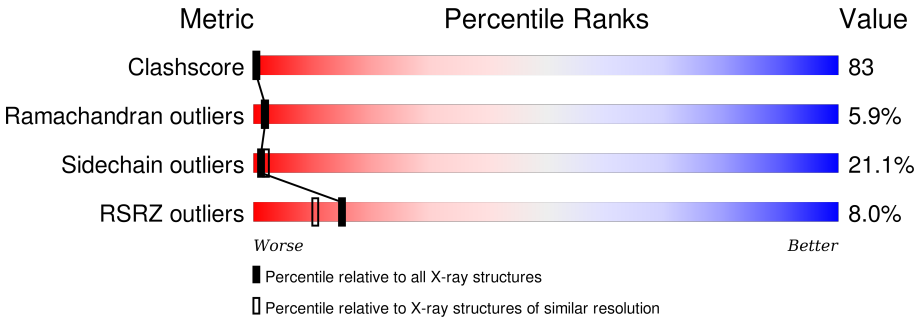
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	225	7% 23% 51% 14% • 11%
1	B	225	8% 22% 50% 15% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2964 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.

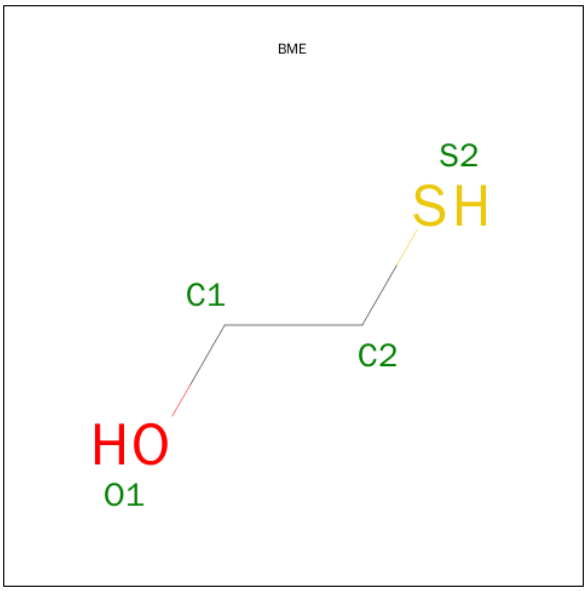
- Molecule 1 is a protein called Ethanolamine utilization protein eutL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1471	931	247	286	7			
1	B	200	Total	C	N	O	S	0	0	0
			1471	931	247	286	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	HIS	-	EXPRESSION TAG	UNP P76541
A	221	HIS	-	EXPRESSION TAG	UNP P76541
A	222	HIS	-	EXPRESSION TAG	UNP P76541
A	223	HIS	-	EXPRESSION TAG	UNP P76541
A	224	HIS	-	EXPRESSION TAG	UNP P76541
A	225	HIS	-	EXPRESSION TAG	UNP P76541
B	220	HIS	-	EXPRESSION TAG	UNP P76541
B	221	HIS	-	EXPRESSION TAG	UNP P76541
B	222	HIS	-	EXPRESSION TAG	UNP P76541
B	223	HIS	-	EXPRESSION TAG	UNP P76541
B	224	HIS	-	EXPRESSION TAG	UNP P76541
B	225	HIS	-	EXPRESSION TAG	UNP P76541

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Zn 2 2	0	0
3	A	3	Total Zn 3 3	0	0

- Molecule 4 is water.

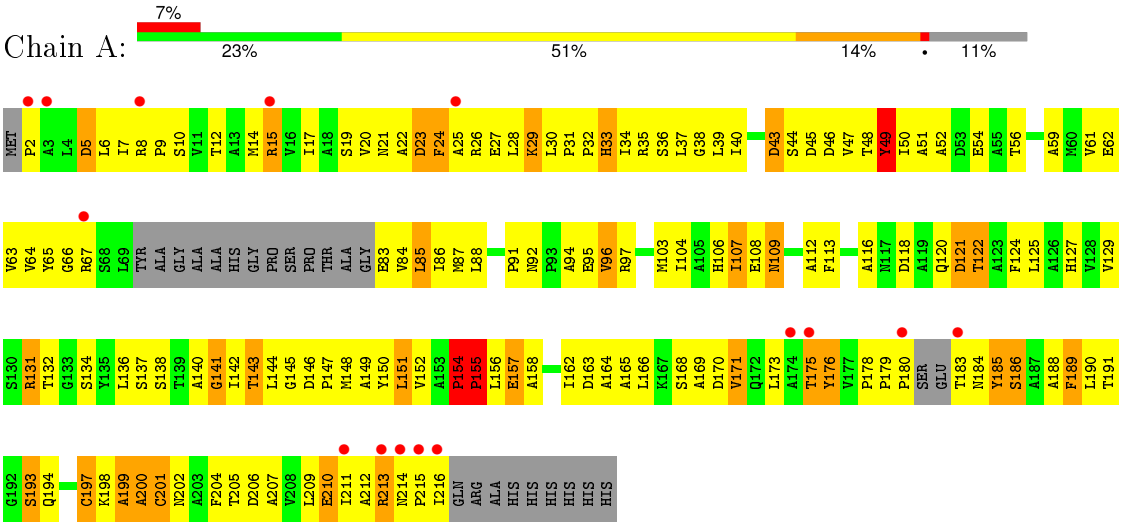
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	6	Total O 6 6	0	0

3 Residue-property plots (i)

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.

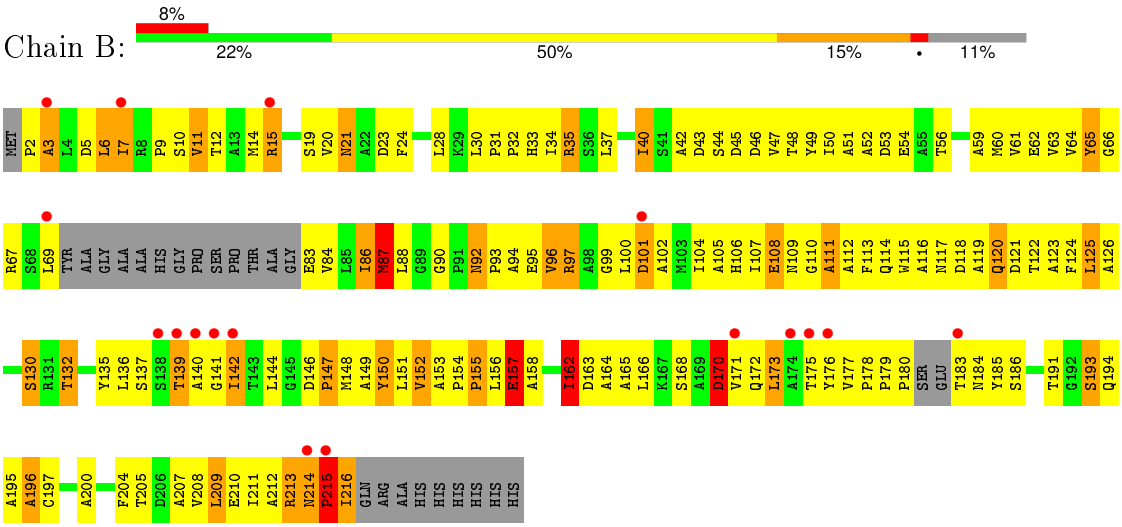
- Molecule 1: Ethanolamine utilization protein eutL

Chain A:



- Molecule 1: Ethanolamine utilization protein eutL

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	67.42Å 67.42Å 79.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.38 – 2.60 58.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (58.38-2.60) 98.4 (58.38-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.222 , 0.267 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.864	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 54.4	EDS
Estimated twinning fraction	0.550 for H, K, L 0.450 for K, H, -L 0.033 for -h,-k,l 0.459 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
Reported twinning fraction	0.550 for H, K, L 0.450 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 12247 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	2964	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: ZN, BME

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	1.05	2/1498 (0.1%)	1.03	2/2047 (0.1%)
1	B	1.10	6/1498 (0.4%)	1.09	3/2047 (0.1%)
All	All	1.08	8/2996 (0.3%)	1.06	5/4094 (0.1%)

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	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	GLU	CB-CG	7.08	1.65	1.52
1	A	157	GLU	CB-CG	5.70	1.62	1.52
1	B	157	GLU	CB-CG	5.60	1.62	1.52
1	B	49	TYR	CE1-CZ	-5.50	1.31	1.38
1	B	62	GLU	CG-CD	5.50	1.60	1.51
1	A	49	TYR	CE2-CZ	-5.42	1.31	1.38
1	B	152	VAL	CA-CB	-5.21	1.43	1.54
1	B	54	GLU	CB-CG	5.05	1.61	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	B	87	MET	CG-SD-CE	5.34	108.75	100.20
1	B	170	ASP	CB-CG-OD2	-5.12	113.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	ILE	CB-CA-C	-5.05	101.50	111.60
1	A	154	PRO	CA-N-CD	-5.04	104.44	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Peptide

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	1471	0	1463	237	1
1	B	1471	0	1464	252	1
2	A	4	0	5	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	7	0	0	3	0
4	B	6	0	0	4	0
All	All	2964	0	2932	489	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 83.

All (489) 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:15:ARG:NH1	1:A:15:ARG:HB2	1.25	1.43
1:B:157:GLU:OE1	1:B:157:GLU:N	1.59	1.32
1:B:43:ASP:O	1:B:83:GLU:HB2	1.18	1.29
1:A:211:ILE:HA	1:A:215:PRO:CG	1.62	1.28
1:B:207:ALA:O	1:B:211:ILE:CD1	1.80	1.27
1:B:214:ASN:O	1:B:216:ILE:N	1.67	1.27
1:A:106:HIS:HE1	4:A:228:HOH:O	1.08	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLU:O	1:A:215:PRO:HD2	1.33	1.25
1:B:2:PRO:HA	1:B:5:ASP:OD1	1.33	1.24
1:B:106:HIS:HE1	4:B:227:HOH:O	1.17	1.23
1:B:207:ALA:O	1:B:211:ILE:HD12	1.39	1.20
1:A:7:ILE:O	1:A:7:ILE:HG22	1.38	1.14
1:A:211:ILE:CA	1:A:215:PRO:HG2	1.78	1.14
1:A:211:ILE:HA	1:A:215:PRO:HG2	1.11	1.10
1:B:60:MET:HG3	4:B:228:HOH:O	0.94	1.10
1:B:178:PRO:C	1:B:180:PRO:HD2	1.72	1.09
1:A:178:PRO:HB2	1:A:179:PRO:HD2	1.17	1.07
1:A:211:ILE:O	1:A:216:ILE:HG22	1.53	1.07
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.34	1.07
1:A:127:HIS:HB3	4:A:233:HOH:O	1.52	1.06
1:B:15:ARG:HB2	1:B:15:ARG:HH11	1.16	1.06
1:A:2:PRO:HD3	1:A:120:GLN:NE2	1.71	1.06
1:B:7:ILE:O	1:B:7:ILE:HG22	1.56	1.05
1:A:15:ARG:NH1	1:A:15:ARG:CB	2.20	1.05
1:A:15:ARG:CB	1:A:15:ARG:HH11	1.69	1.04
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.21	1.03
1:A:154:PRO:HB2	1:A:157:GLU:OE1	1.58	1.02
1:B:132:THR:HG21	1:B:148:MET:HE2	1.41	1.01
1:B:214:ASN:HB3	1:B:215:PRO:CD	1.90	1.00
1:B:50:ILE:HD11	1:B:150:TYR:CD1	1.96	1.00
1:B:43:ASP:O	1:B:83:GLU:CB	2.09	1.00
1:B:97:ARG:HH11	1:B:97:ARG:HG3	1.25	0.99
1:A:213:ARG:CG	1:A:213:ARG:HH11	1.75	0.99
1:A:2:PRO:CD	1:A:120:GLN:HE21	1.75	0.99
1:B:30:LEU:HD13	1:B:34:ILE:HG21	1.44	0.99
1:A:14:MET:O	1:A:15:ARG:NH1	1.96	0.99
1:A:211:ILE:HG23	1:A:215:PRO:HB2	1.44	0.99
1:B:207:ALA:O	1:B:211:ILE:HD11	1.59	0.99
1:B:30:LEU:HD13	1:B:34:ILE:CG2	1.94	0.97
1:B:213:ARG:HH11	1:B:213:ARG:CG	1.75	0.97
1:A:43:ASP:O	1:A:83:GLU:HB3	1.65	0.97
1:B:14:MET:SD	1:B:104:ILE:HD11	2.05	0.96
1:A:178:PRO:CB	1:A:179:PRO:HD2	1.96	0.96
1:A:50:ILE:O	1:A:50:ILE:HG22	1.63	0.96
1:B:106:HIS:CE1	4:B:227:HOH:O	2.01	0.95
1:B:15:ARG:CB	1:B:15:ARG:HH11	1.78	0.95
1:B:53:ASP:OD2	1:B:136:LEU:HB2	1.66	0.95
1:A:2:PRO:CD	1:A:120:GLN:NE2	2.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASN:O	1:B:216:ILE:HG22	1.69	0.93
1:B:179:PRO:HG3	1:B:186:SER:HB2	1.49	0.93
1:A:151:LEU:HD12	1:A:204:PHE:CD2	2.04	0.93
1:A:7:ILE:O	1:A:7:ILE:CG2	2.14	0.91
1:B:132:THR:CG2	1:B:148:MET:HE2	2.00	0.91
1:B:100:LEU:O	1:B:104:ILE:HD12	1.70	0.91
1:A:211:ILE:HG12	1:A:215:PRO:CG	2.02	0.90
1:A:213:ARG:HH11	1:A:213:ARG:HG3	1.33	0.90
1:A:103:MET:O	1:A:107:ILE:HG13	1.70	0.89
1:A:84:VAL:HG12	1:A:85:LEU:H	1.36	0.88
1:B:23:ASP:OD2	4:B:229:HOH:O	1.89	0.88
1:B:12:THR:HG23	1:B:42:ALA:HA	1.54	0.88
1:A:140:ALA:HA	1:A:175:THR:OG1	1.73	0.88
1:B:179:PRO:O	1:B:180:PRO:C	2.10	0.88
1:B:65:TYR:C	1:B:65:TYR:CD2	2.44	0.88
1:A:15:ARG:CZ	1:A:15:ARG:HB2	2.03	0.87
1:B:65:TYR:HD2	1:B:65:TYR:C	1.78	0.87
1:A:178:PRO:HB2	1:A:179:PRO:CD	2.04	0.86
1:A:122:THR:O	1:A:122:THR:CG2	2.22	0.86
1:A:211:ILE:CG1	1:A:215:PRO:HG2	2.05	0.86
1:A:142:ILE:HG22	1:A:143:THR:O	1.75	0.85
1:A:23:ASP:OD1	1:A:26:ARG:NH2	2.09	0.85
1:A:14:MET:SD	1:A:104:ILE:HD11	2.16	0.85
1:B:157:GLU:H	1:B:157:GLU:CD	1.78	0.85
1:A:2:PRO:HD3	1:A:120:GLN:HE21	1.35	0.85
1:B:179:PRO:HG3	1:B:186:SER:CB	2.08	0.84
1:A:43:ASP:O	1:A:83:GLU:CB	2.26	0.84
1:B:178:PRO:O	1:B:180:PRO:HD2	1.76	0.83
1:A:211:ILE:O	1:A:216:ILE:CG2	2.26	0.83
1:B:21:ASN:HD22	1:B:24:PHE:H	1.26	0.83
1:A:212:ALA:HA	1:A:216:ILE:CG2	2.09	0.83
1:A:50:ILE:O	1:A:50:ILE:CG2	2.27	0.82
1:B:140:ALA:HB3	1:B:142:ILE:CD1	2.09	0.82
1:A:6:LEU:HD12	1:A:112:ALA:HB3	1.61	0.82
1:B:175:THR:HG22	1:B:175:THR:O	1.79	0.82
1:B:173:LEU:HD22	1:B:176:TYR:HB2	1.62	0.82
1:B:50:ILE:CD1	1:B:150:TYR:CD1	2.63	0.82
1:B:156:LEU:C	1:B:156:LEU:HD23	1.99	0.81
1:B:132:THR:CG2	1:B:148:MET:CE	2.58	0.81
1:A:106:HIS:CE1	4:A:228:HOH:O	1.96	0.81
1:B:97:ARG:HH11	1:B:97:ARG:CG	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:HG12	1:A:215:PRO:HG2	1.63	0.80
1:A:211:ILE:HA	1:A:215:PRO:CD	2.11	0.80
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.47	0.80
1:B:7:ILE:CG2	1:B:7:ILE:O	2.29	0.80
1:B:151:LEU:HD23	1:B:204:PHE:CD1	2.16	0.79
1:A:15:ARG:HB2	1:A:15:ARG:HH11	0.98	0.79
1:A:154:PRO:HD3	1:A:185:TYR:HD2	1.47	0.79
1:B:2:PRO:CA	1:B:5:ASP:OD1	2.26	0.79
1:A:116:ALA:HB3	1:A:122:THR:CG2	2.13	0.79
1:B:9:PRO:HA	1:B:43:ASP:OD1	1.84	0.78
1:B:213:ARG:HG3	1:B:213:ARG:HH11	1.46	0.78
1:B:46:ASP:O	1:B:50:ILE:HG12	1.83	0.78
1:A:122:THR:O	1:A:122:THR:HG23	1.83	0.78
1:A:40:ILE:CG2	1:A:86:ILE:HB	2.14	0.78
1:A:173:LEU:HD23	1:A:190:LEU:HD23	1.66	0.78
1:A:97:ARG:HG3	1:A:97:ARG:NH1	1.98	0.77
1:A:154:PRO:HD3	1:A:185:TYR:CD2	2.19	0.77
1:B:170:ASP:OD2	1:B:170:ASP:N	2.15	0.77
1:B:214:ASN:C	1:B:216:ILE:H	1.88	0.77
1:B:14:MET:CE	1:B:104:ILE:HD11	2.15	0.77
1:B:7:ILE:HD11	1:B:115:TRP:HE1	1.49	0.76
1:B:101:ASP:CG	1:B:102:ALA:N	2.39	0.76
1:B:213:ARG:HG2	1:B:213:ARG:HH11	1.49	0.76
1:A:162:ILE:HG22	1:A:166:LEU:HD11	1.66	0.76
1:B:65:TYR:CD2	1:B:66:GLY:N	2.54	0.76
1:B:60:MET:N	1:B:95:GLU:OE2	2.13	0.76
1:B:140:ALA:O	1:B:142:ILE:N	2.17	0.75
1:B:139:THR:O	1:B:139:THR:CG2	2.35	0.75
1:A:155:PRO:O	1:A:158:ALA:HB3	1.86	0.74
1:A:210:GLU:O	1:A:215:PRO:CD	2.26	0.74
1:A:14:MET:C	1:A:15:ARG:HH11	1.91	0.73
1:B:37:LEU:HD11	1:B:87:MET:HG2	1.68	0.73
1:A:162:ILE:O	1:A:163:ASP:C	2.20	0.73
1:B:97:ARG:C	1:B:99:GLY:H	1.90	0.73
1:B:156:LEU:C	1:B:156:LEU:CD2	2.56	0.73
1:B:140:ALA:C	1:B:142:ILE:H	1.89	0.73
1:A:30:LEU:HD13	1:A:34:ILE:HG22	1.70	0.73
1:B:179:PRO:CG	1:B:186:SER:HB2	2.19	0.72
1:B:171:VAL:HG12	1:B:196:ALA:HB1	1.72	0.72
1:A:142:ILE:CG2	1:A:143:THR:O	2.38	0.72
1:A:14:MET:C	1:A:15:ARG:NH1	2.42	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:O	1:A:180:PRO:C	2.28	0.71
1:B:34:ILE:O	1:B:34:ILE:HG22	1.88	0.71
1:B:21:ASN:ND2	1:B:24:PHE:H	1.87	0.71
1:B:155:PRO:O	1:B:156:LEU:C	2.25	0.71
1:A:39:LEU:CD2	1:A:87:MET:HG2	2.20	0.71
1:A:199:ALA:O	1:A:200:ALA:C	2.28	0.71
1:A:97:ARG:HH11	1:A:97:ARG:CG	2.02	0.70
1:A:162:ILE:O	1:A:165:ALA:HB3	1.91	0.70
1:B:213:ARG:NH1	1:B:213:ARG:HG2	2.06	0.70
1:A:17:ILE:HG22	1:A:17:ILE:O	1.90	0.70
1:A:144:LEU:C	1:A:144:LEU:HD23	2.12	0.70
1:B:30:LEU:HD13	1:B:34:ILE:HG22	1.74	0.70
1:B:193:SER:OG	1:B:196:ALA:HB2	1.90	0.70
1:B:158:ALA:O	1:B:162:ILE:HG12	1.92	0.70
1:A:188:ALA:C	1:A:189:PHE:HD2	1.95	0.70
1:A:211:ILE:C	1:A:216:ILE:HG22	2.13	0.69
1:A:188:ALA:C	1:A:189:PHE:CD2	2.66	0.69
1:A:199:ALA:O	1:A:201:CYS:N	2.26	0.69
1:B:124:PHE:HE1	1:B:205:THR:HG22	1.58	0.69
1:A:40:ILE:HG23	1:A:86:ILE:HB	1.74	0.68
1:A:66:GLY:HA2	1:A:85:LEU:O	1.91	0.68
1:A:26:ARG:O	1:A:27:GLU:C	2.31	0.68
1:B:35:ARG:NE	1:B:35:ARG:HA	2.07	0.68
1:B:100:LEU:C	1:B:104:ILE:HD12	2.13	0.68
1:A:65:TYR:CD2	1:A:66:GLY:N	2.61	0.68
1:A:62:GLU:OE1	1:A:134:SER:OG	2.12	0.68
1:B:105:ALA:O	1:B:109:ASN:HB2	1.93	0.68
1:A:193:SER:OG	1:A:194:GLN:N	2.27	0.68
1:B:165:ALA:O	1:B:168:SER:OG	2.11	0.67
1:B:140:ALA:HB3	1:B:142:ILE:HD11	1.77	0.67
1:A:31:PRO:HB3	1:A:33:HIS:NE2	2.10	0.67
1:B:7:ILE:CG1	1:B:115:TRP:NE1	2.57	0.67
1:B:2:PRO:HB3	1:B:120:GLN:HE21	1.60	0.67
1:B:15:ARG:NH1	1:B:15:ARG:HB2	2.01	0.67
1:A:211:ILE:HA	1:A:215:PRO:CB	2.26	0.66
1:B:213:ARG:NH1	1:B:213:ARG:CG	2.46	0.66
1:A:178:PRO:CB	1:A:179:PRO:CD	2.70	0.66
1:B:208:VAL:HA	1:B:211:ILE:HD13	1.78	0.66
1:A:103:MET:O	1:A:107:ILE:CG1	2.42	0.66
1:A:151:LEU:HB3	1:A:204:PHE:CZ	2.31	0.66
1:B:142:ILE:HG22	1:B:146:ASP:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD23	1:A:145:GLY:N	2.10	0.66
1:B:7:ILE:CD1	1:B:115:TRP:HE1	2.09	0.65
1:A:116:ALA:HB3	1:A:122:THR:HG23	1.78	0.65
1:B:165:ALA:HB1	1:B:200:ALA:HB1	1.78	0.65
1:B:2:PRO:HB2	1:B:118:ASP:HA	1.77	0.65
1:B:214:ASN:O	1:B:216:ILE:CG2	2.43	0.65
1:A:47:VAL:O	1:A:47:VAL:HG12	1.97	0.65
1:A:34:ILE:O	1:A:34:ILE:HG22	1.96	0.65
1:A:173:LEU:HD23	1:A:190:LEU:CD2	2.26	0.65
1:A:162:ILE:HG22	1:A:166:LEU:CD1	2.25	0.65
1:B:92:ASN:ND2	1:B:95:GLU:H	1.93	0.65
1:B:63:VAL:HG11	1:B:135:TYR:CE1	2.32	0.65
1:A:2:PRO:N	1:A:120:GLN:HE21	1.93	0.64
1:B:114:GLN:O	1:B:123:ALA:HA	1.98	0.64
1:A:154:PRO:CB	1:A:157:GLU:OE1	2.39	0.64
1:A:46:ASP:OD2	1:A:152:VAL:HG21	1.97	0.64
1:A:151:LEU:HB3	1:A:204:PHE:CE2	2.32	0.64
1:B:65:TYR:HB3	1:B:87:MET:CE	2.27	0.64
1:A:212:ALA:HA	1:A:216:ILE:HG21	1.78	0.64
1:A:109:ASN:CG	1:A:109:ASN:O	2.35	0.64
1:A:45:ASP:OD1	1:A:84:VAL:HG22	1.98	0.64
1:A:211:ILE:CG2	1:A:215:PRO:HB2	2.24	0.64
1:A:211:ILE:CB	1:A:215:PRO:HG2	2.27	0.64
1:B:140:ALA:HB3	1:B:142:ILE:HD12	1.79	0.64
1:B:34:ILE:O	1:B:35:ARG:CZ	2.47	0.63
1:A:46:ASP:CG	1:A:152:VAL:HG21	2.19	0.63
1:A:143:THR:OG1	1:A:146:ASP:OD2	2.16	0.63
1:A:158:ALA:HB1	1:A:186:SER:HB3	1.79	0.63
1:B:45:ASP:HA	1:B:84:VAL:CG2	2.28	0.63
1:B:204:PHE:O	1:B:205:THR:C	2.35	0.63
1:A:132:THR:HG22	1:A:148:MET:HE2	1.81	0.63
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.00	0.62
1:B:7:ILE:CG1	1:B:115:TRP:HE1	2.12	0.62
1:B:171:VAL:CG1	1:B:196:ALA:HB1	2.29	0.62
1:A:156:LEU:C	1:A:156:LEU:HD23	2.19	0.62
1:B:30:LEU:HD22	1:B:64:VAL:HG21	1.79	0.62
1:B:65:TYR:CZ	1:B:67:ARG:HB2	2.35	0.62
1:A:131:ARG:NH1	1:A:131:ARG:HG2	2.13	0.62
1:B:61:VAL:HB	1:B:88:LEU:HD22	1.79	0.62
1:A:151:LEU:CD1	1:A:204:PHE:CD2	2.82	0.61
1:B:155:PRO:O	1:B:158:ALA:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:MET:CE	1:B:104:ILE:CD1	2.77	0.61
1:A:142:ILE:HG23	1:A:146:ASP:HB2	1.81	0.61
1:B:209:LEU:HD23	1:B:209:LEU:N	2.16	0.61
1:A:179:PRO:N	1:A:180:PRO:HD2	2.14	0.61
1:B:65:TYR:OH	1:B:67:ARG:HB2	1.99	0.61
1:A:158:ALA:CB	1:A:186:SER:HB3	2.30	0.61
1:B:65:TYR:CE2	1:B:67:ARG:HB2	2.35	0.61
1:A:124:PHE:CE1	1:A:205:THR:HG22	2.36	0.61
1:A:188:ALA:O	1:A:189:PHE:HD2	1.83	0.60
1:A:84:VAL:HG12	1:A:85:LEU:N	2.11	0.60
1:B:92:ASN:ND2	1:B:94:ALA:HB3	2.16	0.60
1:A:26:ARG:O	1:A:29:LYS:N	2.27	0.60
1:A:162:ILE:O	1:A:165:ALA:N	2.34	0.60
1:B:214:ASN:C	1:B:216:ILE:N	2.46	0.60
1:B:30:LEU:HD21	1:B:64:VAL:HG11	1.83	0.60
1:A:205:THR:O	1:A:209:LEU:HG	2.00	0.60
1:B:50:ILE:CD1	1:B:150:TYR:HD1	2.11	0.60
1:A:59:ALA:HB1	1:A:95:GLU:OE2	2.02	0.59
1:B:97:ARG:C	1:B:99:GLY:N	2.48	0.59
1:B:92:ASN:HD22	1:B:94:ALA:H	1.50	0.59
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.62	0.59
1:A:155:PRO:HD3	1:A:185:TYR:HA	1.84	0.59
1:B:151:LEU:N	1:B:151:LEU:HD12	2.16	0.59
1:A:154:PRO:O	1:A:158:ALA:N	2.35	0.59
1:B:179:PRO:O	1:B:180:PRO:O	2.19	0.59
1:A:178:PRO:C	1:A:180:PRO:HD2	2.23	0.59
1:B:31:PRO:HG2	1:B:34:ILE:HG12	1.85	0.59
1:B:65:TYR:HB3	1:B:87:MET:HE2	1.84	0.59
1:B:178:PRO:C	1:B:180:PRO:CD	2.62	0.59
1:B:139:THR:O	1:B:139:THR:HG22	2.02	0.59
1:A:198:LYS:O	1:A:201:CYS:HB2	2.02	0.59
1:B:132:THR:HB	1:B:137:SER:HB3	1.84	0.59
1:A:92:ASN:HD22	1:A:94:ALA:N	2.01	0.58
1:A:149:ALA:O	1:A:189:PHE:HA	2.04	0.58
1:A:122:THR:O	1:A:122:THR:HG22	2.01	0.58
1:A:61:VAL:HG21	1:A:88:LEU:HD22	1.85	0.58
1:B:45:ASP:HA	1:B:84:VAL:HG21	1.86	0.58
1:A:137:SER:O	1:A:140:ALA:O	2.21	0.58
1:B:156:LEU:O	1:B:157:GLU:C	2.42	0.57
1:A:20:VAL:CG1	1:A:37:LEU:HD22	2.34	0.57
1:A:20:VAL:HG11	1:A:37:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:O	1:A:156:LEU:HD23	2.05	0.57
1:A:136:LEU:O	1:A:137:SER:C	2.42	0.57
1:A:24:PHE:O	1:A:28:LEU:HB2	2.04	0.57
1:B:6:LEU:HD12	1:B:112:ALA:HB3	1.86	0.57
1:A:189:PHE:N	1:A:189:PHE:CD2	2.69	0.56
1:A:45:ASP:HA	1:A:84:VAL:HG21	1.87	0.56
1:B:32:PRO:C	1:B:35:ARG:HH11	2.09	0.56
1:B:53:ASP:HB2	1:B:136:LEU:HG	1.87	0.56
1:B:52:ALA:O	1:B:53:ASP:C	2.41	0.56
1:B:15:ARG:NH1	1:B:15:ARG:CB	2.60	0.56
1:B:173:LEU:CD2	1:B:176:TYR:HB2	2.35	0.56
1:A:52:ALA:O	1:A:56:THR:HG23	2.05	0.56
1:B:117:ASN:O	1:B:117:ASN:OD1	2.23	0.56
1:B:214:ASN:O	1:B:216:ILE:CA	2.53	0.56
1:B:92:ASN:HD21	1:B:94:ALA:HB3	1.71	0.56
1:B:96:VAL:O	1:B:99:GLY:HA3	2.06	0.56
1:B:113:PHE:CE2	1:B:125:LEU:HB2	2.40	0.56
1:B:211:ILE:HA	1:B:215:PRO:HB2	1.87	0.56
1:A:151:LEU:HD12	1:A:204:PHE:HD2	1.67	0.56
1:B:65:TYR:CB	1:B:87:MET:CE	2.84	0.56
1:B:63:VAL:HB	1:B:135:TYR:CD1	2.41	0.55
1:A:21:ASN:HB3	1:A:24:PHE:H	1.71	0.55
1:A:211:ILE:CA	1:A:215:PRO:CG	2.52	0.55
1:A:61:VAL:CG2	1:A:88:LEU:HD22	2.35	0.55
1:A:211:ILE:HG12	1:A:215:PRO:CB	2.36	0.55
1:A:125:LEU:HD13	1:A:125:LEU:O	2.06	0.55
1:A:49:TYR:N	1:A:49:TYR:CD2	2.71	0.55
1:A:136:LEU:C	1:A:138:SER:N	2.55	0.55
1:A:143:THR:OG1	1:A:146:ASP:CG	2.45	0.55
1:A:124:PHE:HE1	1:A:205:THR:HG22	1.71	0.55
1:A:51:ALA:O	1:A:54:GLU:N	2.40	0.55
1:B:179:PRO:CB	1:B:186:SER:HB2	2.37	0.55
1:B:179:PRO:HG3	1:B:186:SER:OG	2.07	0.55
1:A:213:ARG:HG3	1:A:213:ARG:NH1	2.13	0.55
1:B:93:PRO:O	1:B:97:ARG:HG3	2.06	0.54
1:B:146:ASP:HB3	1:B:147:PRO:HD2	1.89	0.54
1:B:119:ALA:O	1:B:121:ASP:N	2.40	0.54
1:A:125:LEU:HD13	1:A:125:LEU:C	2.28	0.54
1:A:97:ARG:CG	1:A:97:ARG:NH1	2.64	0.54
1:A:84:VAL:CG1	1:A:85:LEU:H	2.13	0.54
1:A:9:PRO:HG2	1:A:47:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ALA:C	1:B:197:CYS:N	2.58	0.54
1:B:9:PRO:HG2	1:B:47:VAL:HG11	1.90	0.54
1:A:194:GLN:HA	1:A:197:CYS:HB2	1.89	0.54
1:B:61:VAL:CB	1:B:88:LEU:HD22	2.38	0.54
1:B:32:PRO:HA	1:B:35:ARG:NH1	2.23	0.54
1:B:10:SER:O	1:B:12:THR:HG22	2.08	0.54
1:A:213:ARG:CG	1:A:213:ARG:NH1	2.47	0.54
1:A:132:THR:CG2	1:A:148:MET:HE2	2.39	0.53
1:B:156:LEU:HD23	1:B:156:LEU:O	2.08	0.53
1:B:111:ALA:O	1:B:112:ALA:HB2	2.08	0.53
1:A:83:GLU:C	1:A:84:VAL:CG2	2.77	0.53
1:B:19:SER:HA	1:B:35:ARG:O	2.09	0.53
1:B:171:VAL:HG11	1:B:196:ALA:O	2.08	0.53
1:B:92:ASN:HB2	1:B:93:PRO:CD	2.39	0.53
1:B:155:PRO:HG3	1:B:179:PRO:HB3	1.89	0.52
1:B:5:ASP:C	1:B:6:LEU:O	2.44	0.52
1:B:92:ASN:O	1:B:96:VAL:HG13	2.09	0.52
1:A:132:THR:HG22	1:A:148:MET:CE	2.39	0.52
1:A:113:PHE:CD2	1:A:124:PHE:O	2.63	0.52
1:B:211:ILE:H	1:B:211:ILE:HD12	1.75	0.52
1:B:2:PRO:O	1:B:3:ALA:C	2.48	0.52
1:A:47:VAL:O	1:A:47:VAL:CG1	2.58	0.52
1:A:162:ILE:CG2	1:A:166:LEU:HD11	2.36	0.52
1:A:201:CYS:O	1:A:202:ASN:C	2.48	0.52
1:A:15:ARG:CA	1:A:15:ARG:HH11	2.21	0.52
1:A:125:LEU:HD21	1:A:127:HIS:HD2	1.73	0.52
1:A:59:ALA:HB1	1:A:95:GLU:O	2.10	0.52
1:A:183:THR:HB	1:A:185:TYR:HD1	1.75	0.52
1:B:65:TYR:HD2	1:B:66:GLY:N	2.01	0.52
1:B:96:VAL:O	1:B:99:GLY:CA	2.58	0.52
1:A:199:ALA:C	1:A:201:CYS:N	2.62	0.52
1:A:116:ALA:HB3	1:A:122:THR:O	2.10	0.51
1:A:92:ASN:ND2	1:A:95:GLU:H	2.09	0.51
1:A:142:ILE:HG22	1:A:143:THR:C	2.30	0.51
1:B:101:ASP:C	1:B:101:ASP:OD1	2.47	0.51
1:A:92:ASN:HD22	1:A:94:ALA:H	1.58	0.51
1:A:138:SER:C	1:A:140:ALA:H	2.13	0.51
1:B:65:TYR:CB	1:B:87:MET:HE1	2.40	0.51
1:A:140:ALA:CA	1:A:175:THR:OG1	2.54	0.51
1:B:193:SER:OG	1:B:196:ALA:CB	2.57	0.51
1:A:49:TYR:OH	1:A:67:ARG:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:VAL:O	1:B:153:ALA:HB2	2.11	0.51
1:B:154:PRO:O	1:B:155:PRO:C	2.50	0.50
1:B:117:ASN:C	1:B:117:ASN:OD1	2.48	0.50
1:B:40:ILE:HB	1:B:100:LEU:CD2	2.41	0.50
1:A:175:THR:O	1:A:176:TYR:HB2	2.11	0.50
1:B:24:PHE:O	1:B:28:LEU:HG	2.12	0.50
1:A:109:ASN:OD1	1:A:109:ASN:O	2.30	0.50
1:B:21:ASN:HD22	1:B:24:PHE:N	2.02	0.50
1:B:175:THR:CG2	1:B:175:THR:O	2.53	0.50
1:B:114:GLN:HB2	1:B:124:PHE:CE2	2.47	0.50
1:A:184:ASN:O	1:A:184:ASN:OD1	2.30	0.50
1:B:115:TRP:CZ3	1:B:120:GLN:O	2.65	0.50
1:B:107:ILE:HG22	1:B:108:GLU:N	2.27	0.50
1:A:43:ASP:O	1:A:83:GLU:HB2	2.08	0.50
1:B:92:ASN:HD22	1:B:94:ALA:N	2.10	0.50
1:A:116:ALA:HB3	1:A:122:THR:HG22	1.90	0.50
1:B:7:ILE:HG12	1:B:115:TRP:NE1	2.26	0.49
1:A:65:TYR:CG	1:A:66:GLY:N	2.80	0.49
1:B:60:MET:CB	1:B:95:GLU:OE2	2.61	0.49
1:A:10:SER:N	1:A:43:ASP:OD1	2.45	0.49
1:B:3:ALA:N	1:B:118:ASP:OD1	2.45	0.49
1:B:171:VAL:HG12	1:B:196:ALA:CB	2.42	0.49
1:B:125:LEU:HD22	1:B:126:ALA:H	1.77	0.49
1:A:38:GLY:O	1:A:87:MET:HA	2.13	0.49
1:A:140:ALA:O	1:A:141:GLY:C	2.51	0.49
1:B:156:LEU:HB3	1:B:157:GLU:OE1	2.12	0.49
1:B:149:ALA:HB1	1:B:151:LEU:HD11	1.95	0.49
1:A:156:LEU:CD2	1:A:156:LEU:C	2.80	0.49
1:A:198:LYS:O	1:A:201:CYS:CB	2.60	0.49
1:A:144:LEU:C	1:A:144:LEU:CD2	2.80	0.49
1:A:166:LEU:C	1:A:168:SER:H	2.15	0.48
1:B:195:ALA:C	1:B:197:CYS:H	2.17	0.48
1:B:148:MET:HE3	1:B:148:MET:HB3	1.53	0.48
1:B:14:MET:HE3	1:B:104:ILE:HD11	1.95	0.48
1:B:11:VAL:HG21	1:B:104:ILE:HG12	1.94	0.48
1:B:50:ILE:HD13	1:B:136:LEU:HD11	1.95	0.48
1:A:30:LEU:O	1:A:31:PRO:C	2.47	0.48
1:B:48:THR:HG22	1:B:48:THR:O	2.13	0.48
1:A:198:LYS:O	1:A:201:CYS:N	2.46	0.48
1:A:184:ASN:CG	1:A:184:ASN:O	2.52	0.48
1:A:54:GLU:HG2	1:A:106:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:HG23	1:A:107:ILE:HD11	1.96	0.48
1:A:2:PRO:HD2	1:A:5:ASP:OD1	2.13	0.47
1:A:151:LEU:HG	1:A:204:PHE:CG	2.49	0.47
1:A:158:ALA:CB	1:A:186:SER:CB	2.92	0.47
1:A:125:LEU:CD2	1:A:127:HIS:HD2	2.28	0.47
1:A:2:PRO:HG2	1:A:5:ASP:OD1	2.15	0.47
1:B:178:PRO:HB2	1:B:180:PRO:CD	2.44	0.47
1:A:7:ILE:O	1:A:8:ARG:C	2.51	0.47
1:B:195:ALA:O	1:B:196:ALA:C	2.53	0.47
1:B:12:THR:CG2	1:B:42:ALA:HA	2.37	0.47
1:B:110:GLY:O	1:B:111:ALA:O	2.32	0.47
1:A:136:LEU:C	1:A:138:SER:H	2.17	0.47
1:A:64:VAL:HG12	1:A:64:VAL:O	2.14	0.47
1:B:65:TYR:CB	1:B:87:MET:HE2	2.44	0.46
1:B:65:TYR:CG	1:B:87:MET:HE1	2.50	0.46
1:B:151:LEU:HD23	1:B:204:PHE:CG	2.50	0.46
1:A:125:LEU:HB3	1:A:152:VAL:HB	1.96	0.46
1:B:21:ASN:ND2	1:B:24:PHE:N	2.59	0.46
1:B:214:ASN:CB	1:B:215:PRO:CD	2.76	0.46
1:A:162:ILE:O	1:A:165:ALA:CB	2.61	0.46
1:A:25:ALA:O	1:A:30:LEU:HB2	2.15	0.46
1:A:169:ALA:O	1:A:171:VAL:HG22	2.16	0.46
1:B:139:THR:O	1:B:139:THR:HG23	2.11	0.46
1:A:104:ILE:O	1:A:107:ILE:N	2.39	0.46
1:A:147:PRO:O	1:A:191:THR:HG22	2.16	0.46
1:A:164:ALA:O	1:A:165:ALA:C	2.54	0.46
1:B:21:ASN:C	1:B:21:ASN:ND2	2.69	0.46
1:B:210:GLU:O	1:B:211:ILE:C	2.53	0.45
1:B:96:VAL:O	1:B:99:GLY:N	2.48	0.45
1:A:85:LEU:CD2	1:A:86:ILE:N	2.79	0.45
1:A:140:ALA:O	1:A:142:ILE:N	2.49	0.45
1:B:66:GLY:HA2	1:B:86:ILE:HD12	1.98	0.45
1:B:177:VAL:HG22	1:B:178:PRO:N	2.31	0.45
1:B:110:GLY:O	1:B:111:ALA:C	2.54	0.45
1:A:63:VAL:HG12	1:A:65:TYR:O	2.16	0.45
1:B:90:GLY:HA3	1:B:96:VAL:HG12	1.99	0.45
1:A:213:ARG:HG2	1:A:213:ARG:NH1	2.23	0.45
1:A:83:GLU:C	1:A:84:VAL:HG23	2.38	0.45
1:B:151:LEU:CD1	1:B:151:LEU:N	2.80	0.45
1:B:162:ILE:O	1:B:163:ASP:C	2.54	0.45
1:A:185:TYR:CD1	1:A:185:TYR:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:TYR:HB3	1:B:87:MET:HB2	1.99	0.45
1:B:130:SER:HB3	1:B:194:GLN:HE21	1.83	0.44
1:B:14:MET:HE3	1:B:104:ILE:CD1	2.47	0.44
1:A:206:ASP:O	1:A:207:ALA:C	2.55	0.44
1:B:142:ILE:CG2	1:B:146:ASP:HB2	2.47	0.44
1:A:40:ILE:HG21	1:A:103:MET:SD	2.57	0.44
1:B:140:ALA:C	1:B:142:ILE:N	2.60	0.44
1:B:7:ILE:HG13	1:B:115:TRP:NE1	2.32	0.44
1:B:92:ASN:HD21	1:B:95:GLU:H	1.63	0.44
1:A:49:TYR:N	1:A:49:TYR:HD2	2.15	0.44
1:B:162:ILE:HD13	1:B:162:ILE:H	1.83	0.43
1:B:179:PRO:HB3	1:B:186:SER:HB2	2.00	0.43
1:B:152:VAL:HG12	1:B:153:ALA:N	2.33	0.43
1:A:31:PRO:HB3	1:A:33:HIS:CD2	2.54	0.43
1:B:116:ALA:CB	1:B:122:THR:O	2.66	0.43
1:A:136:LEU:O	1:A:138:SER:N	2.52	0.43
1:A:129:VAL:HG21	1:A:148:MET:HE3	1.99	0.43
1:B:56:THR:O	1:B:59:ALA:O	2.35	0.43
1:B:42:ALA:O	1:B:83:GLU:N	2.51	0.43
1:B:140:ALA:CB	1:B:142:ILE:HD11	2.47	0.43
1:A:45:ASP:O	1:A:48:THR:N	2.42	0.43
1:A:96:VAL:CG2	1:A:97:ARG:N	2.77	0.43
1:A:113:PHE:HD2	1:A:124:PHE:O	2.01	0.43
1:A:85:LEU:HD23	1:A:86:ILE:H	1.84	0.42
1:B:178:PRO:HA	1:B:179:PRO:HD2	1.88	0.42
1:B:65:TYR:CZ	1:B:67:ARG:HD2	2.54	0.42
1:B:60:MET:HB3	1:B:95:GLU:OE2	2.20	0.42
1:B:124:PHE:CE1	1:B:205:THR:HG22	2.47	0.42
1:A:121:ASP:OD1	1:A:121:ASP:C	2.58	0.42
1:B:162:ILE:N	1:B:162:ILE:HD13	2.34	0.42
1:A:157:GLU:HG3	1:A:211:ILE:HG21	2.01	0.42
1:A:36:SER:O	1:A:37:LEU:HD12	2.18	0.42
1:B:45:ASP:OD2	1:B:46:ASP:OD2	2.37	0.42
1:A:142:ILE:CG2	1:A:143:THR:N	2.82	0.42
1:B:61:VAL:CG2	1:B:88:LEU:HD22	2.49	0.42
1:B:172:GLN:N	1:B:191:THR:O	2.47	0.42
1:B:136:LEU:HA	1:B:136:LEU:HD23	1.62	0.42
1:A:212:ALA:HA	1:A:216:ILE:HG23	1.98	0.42
1:B:208:VAL:HA	1:B:211:ILE:CD1	2.46	0.42
1:B:216:ILE:HD13	1:B:216:ILE:C	2.40	0.42
1:A:15:ARG:N	1:A:15:ARG:HH11	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:TYR:CD1	1:B:87:MET:HE1	2.54	0.41
1:A:64:VAL:CG1	1:A:64:VAL:O	2.68	0.41
1:B:164:ALA:O	1:B:165:ALA:C	2.53	0.41
1:B:183:THR:C	1:B:185:TYR:N	2.73	0.41
1:A:118:ASP:C	1:A:120:GLN:H	2.23	0.41
1:A:2:PRO:CD	1:A:5:ASP:OD1	2.68	0.41
1:B:30:LEU:HD22	1:B:64:VAL:CG2	2.48	0.41
1:B:34:ILE:O	1:B:35:ARG:NH2	2.53	0.41
1:B:14:MET:HB3	1:B:40:ILE:HG13	2.03	0.41
1:B:40:ILE:HB	1:B:100:LEU:HD22	2.02	0.41
1:B:210:GLU:O	1:B:212:ALA:N	2.54	0.41
1:A:36:SER:HB3	1:A:96:VAL:HG11	2.03	0.41
1:B:179:PRO:N	1:B:180:PRO:HD2	2.32	0.41
1:B:210:GLU:C	1:B:212:ALA:N	2.69	0.41
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.74	0.41
1:B:122:THR:HG22	1:B:122:THR:O	2.20	0.41
1:B:7:ILE:HG13	1:B:115:TRP:CE2	2.56	0.41
1:A:8:ARG:HA	1:A:9:PRO:HD3	1.80	0.41
1:B:50:ILE:HG23	1:B:50:ILE:HD12	1.73	0.41
1:B:183:THR:O	1:B:185:TYR:N	2.54	0.41
1:B:162:ILE:HG22	1:B:166:LEU:HD11	2.04	0.40
1:B:50:ILE:O	1:B:53:ASP:N	2.54	0.40
1:B:31:PRO:O	1:B:35:ARG:NH1	2.50	0.40
1:B:32:PRO:C	1:B:35:ARG:NH1	2.73	0.40
1:A:142:ILE:HD11	1:A:191:THR:CG2	2.51	0.40
1:A:109:ASN:C	1:A:109:ASN:OD1	2.60	0.40
1:B:20:VAL:O	1:B:20:VAL:HG23	2.21	0.40
1:B:209:LEU:HD13	1:B:213:ARG:NH2	2.36	0.40
1:A:85:LEU:HD22	1:A:86:ILE:N	2.36	0.40
1:B:65:TYR:HD2	1:B:65:TYR:O	2.03	0.40
1:A:22:ALA:O	1:A:26:ARG:HG3	2.21	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:B:15:ARG:NH2	1:B:211:ILE:CG1[3_665]	1.79	0.41
1:A:15:ARG:NH2	1:A:211:ILE:CD1[2_665]	2.10	0.10

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	194/225 (86%)	138 (71%)	46 (24%)	10 (5%)	2	3
1	B	194/225 (86%)	143 (74%)	38 (20%)	13 (7%)	1	1
All	All	388/450 (86%)	281 (72%)	84 (22%)	23 (6%)	2	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ALA
1	B	214	ASN
1	B	215	PRO
1	A	49	TYR
1	B	3	ALA
1	B	51	ALA
1	B	111	ALA
1	B	120	GLN
1	B	155	PRO
1	A	175	THR
1	A	214	ASN
1	A	193	SER
1	B	108	GLU
1	B	141	GLY
1	B	196	ALA
1	A	91	PRO
1	A	141	GLY
1	A	170	ASP
1	A	199	ALA
1	A	155	PRO
1	B	6	LEU
1	B	11	VAL
1	B	162	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	152/169 (90%)	120 (79%)	32 (21%)	1 2
1	B	152/169 (90%)	120 (79%)	32 (21%)	1 2
All	All	304/338 (90%)	240 (79%)	64 (21%)	1 2

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	15	ARG
1	A	19	SER
1	A	23	ASP
1	A	24	PHE
1	A	29	LYS
1	A	32	PRO
1	A	33	HIS
1	A	35	ARG
1	A	43	ASP
1	A	44	SER
1	A	85	LEU
1	A	96	VAL
1	A	107	ILE
1	A	108	GLU
1	A	109	ASN
1	A	121	ASP
1	A	122	THR
1	A	131	ARG
1	A	143	THR
1	A	150	TYR
1	A	151	LEU
1	A	154	PRO
1	A	155	PRO
1	A	171	VAL
1	A	185	TYR
1	A	186	SER

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Mol	Chain	Res	Type
1	A	189	PHE
1	A	197	CYS
1	A	201	CYS
1	A	210	GLU
1	A	213	ARG
1	B	7	ILE
1	B	15	ARG
1	B	21	ASN
1	B	33	HIS
1	B	35	ARG
1	B	40	ILE
1	B	44	SER
1	B	65	TYR
1	B	69	LEU
1	B	86	ILE
1	B	87	MET
1	B	92	ASN
1	B	96	VAL
1	B	97	ARG
1	B	101	ASP
1	B	125	LEU
1	B	130	SER
1	B	132	THR
1	B	139	THR
1	B	142	ILE
1	B	144	LEU
1	B	147	PRO
1	B	150	TYR
1	B	157	GLU
1	B	170	ASP
1	B	173	LEU
1	B	184	ASN
1	B	193	SER
1	B	209	LEU
1	B	213	ARG
1	B	215	PRO
1	B	216	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	106	HIS
1	A	120	GLN
1	A	127	HIS
1	B	21	ASN
1	B	92	ASN
1	B	106	HIS
1	B	120	GLN
1	B	172	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 6 ligands modelled in this entry, 5 are 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	$\#\|Z\| > 2$
2	BME	A	226	3	3,3,3	0.37	0	2,2,2	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	A	226	3	-	0/1/1/1	0/0/0/0

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, 95^{th} 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	200/225 (88%)	0.76	15 (7%) 17 12	14, 34, 48, 64	0
1	B	200/225 (88%)	0.76	17 (8%) 13 9	20, 34, 50, 57	0
All	All	400/450 (88%)	0.76	32 (8%) 15 10	14, 34, 49, 64	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	THR	4.3
1	A	175	THR	4.1
1	A	174	ALA	3.9
1	B	215	PRO	3.7
1	B	175	THR	3.6
1	A	3	ALA	3.5
1	B	138	SER	3.3
1	B	15	ARG	3.1
1	B	7	ILE	3.1
1	B	141	GLY	3.1
1	A	15	ARG	3.0
1	A	216	ILE	2.9
1	A	67	ARG	2.9
1	A	215	PRO	2.9
1	B	214	ASN	2.8
1	B	142	ILE	2.8
1	B	176	TYR	2.7
1	A	213	ARG	2.7
1	B	69	LEU	2.7
1	A	25	ALA	2.6
1	A	183	THR	2.6
1	B	3	ALA	2.5
1	A	8	ARG	2.4
1	B	139	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	101	ASP	2.3
1	A	214	ASN	2.2
1	B	174	ALA	2.2
1	A	211	ILE	2.2
1	A	180	PRO	2.2
1	B	171	VAL	2.2
1	B	140	ALA	2.2
1	A	2	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 95^{th} 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(Å^2)	Q<0.9
2	BME	A	226	4/4	0.79	0.15	-1.61	33,35,40,50	0
3	ZN	A	903	1/1	0.91	0.05	-2.27	52,52,52,52	0
3	ZN	A	901	1/1	0.76	0.18	-	57,57,57,57	0
3	ZN	B	904	1/1	0.96	0.15	-	16,16,16,16	1
3	ZN	A	902	1/1	0.96	0.23	-	39,39,39,39	1
3	ZN	B	905	1/1	0.92	0.12	-	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.