Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 04:27 AM EDT

PDB ID	:	1LT8
Title	:	Reduced Homo sapiens Betaine-Homocysteine S-Methyltransferase in Complex with S-(delta-carboxybutyl)-L-Homocysteine
Authors	:	Evans, J.C.; Huddler, D.P.; Jiracek, J.; Castro, C.; Millian, N.S.; Garrow, T.A.; Ludwig, M.L.
Deposited on	:	2002-05-20
Resolution	:	2.05 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 (i) symbol.

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

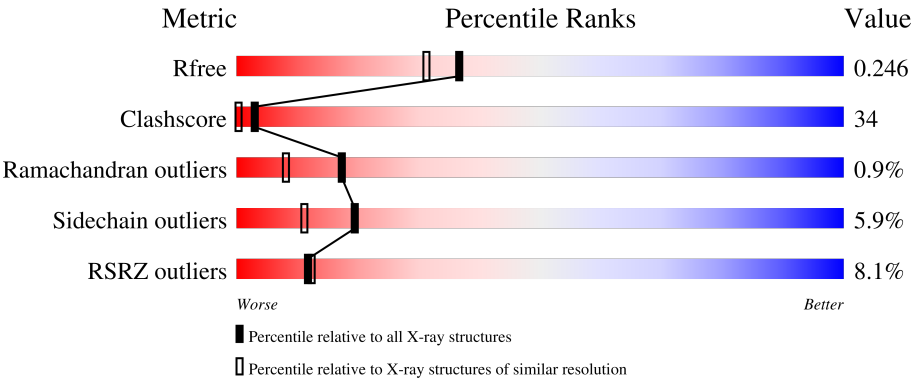
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	406	8% 48% 34% · 14%
1	B	406	6% 47% 33% · 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5826 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 BETAINE-HOMOCYSTEINE METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2700	1722	469	499	10			
1	B	340	Total	C	N	O	S	0	0	0
			2637	1686	458	483	10			

There are 14 discrepancies between the modelled and reference sequences:

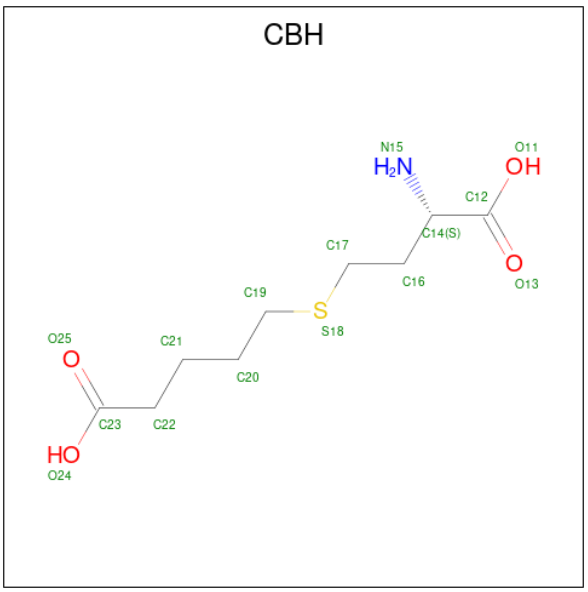
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	engineered mutation	UNP Q93088
A	104	ALA	CYS	engineered mutation	UNP Q93088
A	131	ALA	CYS	engineered mutation	UNP Q93088
A	186	ALA	CYS	engineered mutation	UNP Q93088
A	201	ALA	CYS	engineered mutation	UNP Q93088
A	239	GLN	ARG	SEE REMARK 999	UNP Q93088
A	256	ALA	CYS	engineered mutation	UNP Q93088
B	2	ALA	PRO	engineered mutation	UNP Q93088
B	104	ALA	CYS	engineered mutation	UNP Q93088
B	131	ALA	CYS	engineered mutation	UNP Q93088
B	186	ALA	CYS	engineered mutation	UNP Q93088
B	201	ALA	CYS	engineered mutation	UNP Q93088
B	239	GLN	ARG	SEE REMARK 999	UNP Q93088
B	256	ALA	CYS	engineered mutation	UNP Q93088

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

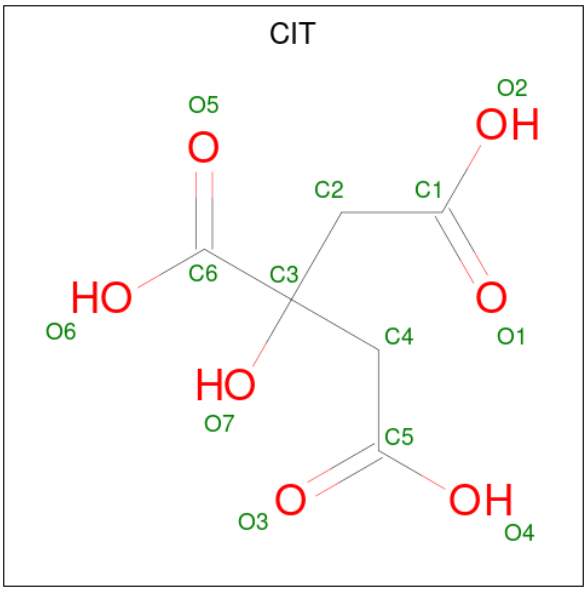
- Molecule 3 is S-(D-CARBOXYBUTYL)-L-HOMOCYSTEINE (three-letter code: CBH)

(formula: $C_9H_{17}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	9	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

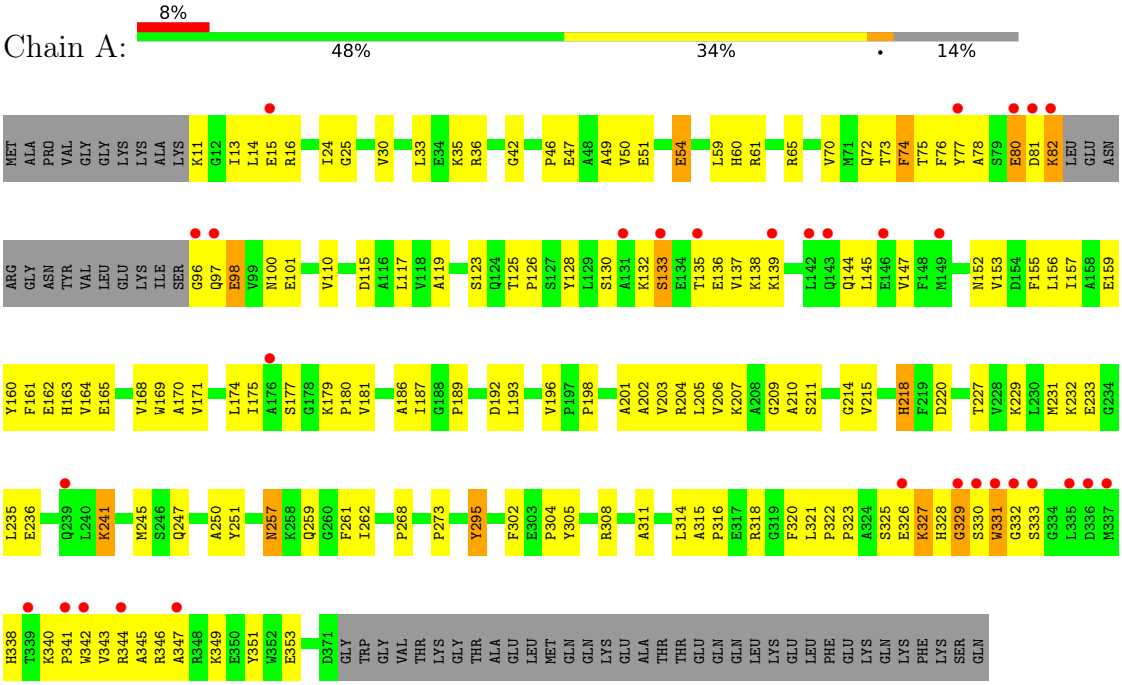
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	240	Total O 240 240	0	0
5	B	191	Total O 191 191	0	0

3 Residue-property plots (i)

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

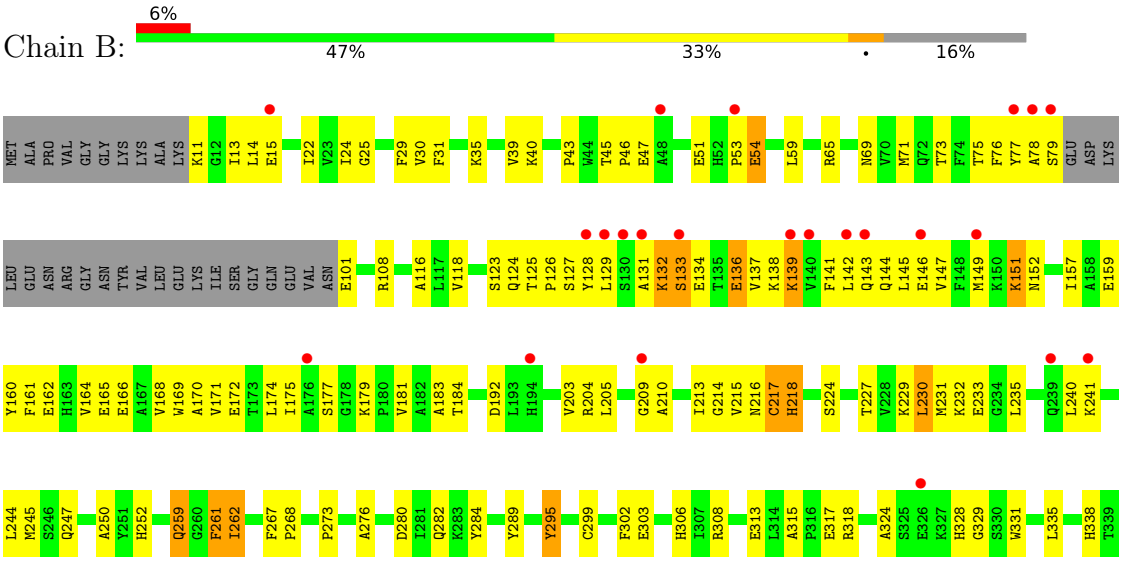
• Molecule 1: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE

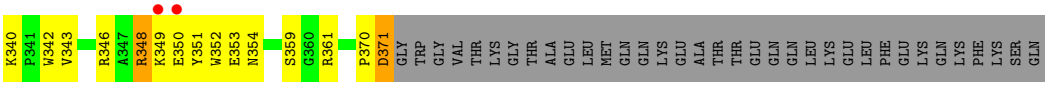
Chain A:



• Molecule 1: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE

Chain B:




K340
P341
W342
V343
R346
A347
R348
K349
E350
Y351
W352
E353
N354
S359
G360
R361
P370
D371
GLY
TRP
GLY
VAL
THR
LYS
GLY
THR
ALA
GLU
LEU
MET
GLN
GLN
LYS
GLU
ALA
THR
THR
GLU
GLN
GLN
LEU
LYS
GLU
LEU
PHE
GLU
LYS
GLN
LYS
PHE
LYS
SER
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.70Å 90.84Å 88.40Å 90.00° 122.28° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 9.99 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-2.05) 99.9 (9.99-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.255 0.218 , 0.246	Depositor DCC
R_{free} test set	2317 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 83.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5826	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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, 0.333 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: CIT, ZN, CBH

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	0.36	0/2768	0.60	0/3750
1	B	0.34	0/2705	0.61	0/3666
All	All	0.35	0/5473	0.60	0/7416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2700	0	2653	182	0
1	B	2637	0	2598	188	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	15	3	0
3	B	15	0	15	5	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0
5	A	240	0	0	90	0
5	B	191	0	0	78	0
All	All	5826	0	5291	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (368) 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:156:LEU:HD13	1:A:174:LEU:HD12	1.23	1.09
1:A:241:LYS:HA	1:A:241:LYS:HE2	1.46	0.97
1:A:24:ILE:HG13	5:A:840:HOH:O	1.63	0.97
1:B:151:LYS:HE2	1:B:151:LYS:HA	1.52	0.92
1:B:77:TYR:HB2	5:B:851:HOH:O	1.70	0.91
1:A:170:ALA:O	1:A:174:LEU:HD23	1.70	0.89
1:B:215:VAL:HG21	5:B:841:HOH:O	1.73	0.89
1:B:24:ILE:H	1:B:69:ASN:HD22	1.19	0.89
1:B:303:GLU:H	1:B:306:HIS:HD2	1.11	0.88
1:B:116:ALA:HB1	5:B:855:HOH:O	1.74	0.86
1:A:227:THR:HG23	5:A:900:HOH:O	1.75	0.86
1:A:33:LEU:HA	5:A:781:HOH:O	1.76	0.85
1:A:327:LYS:HE3	1:A:327:LYS:HA	1.59	0.85
1:A:80:GLU:OE2	1:A:80:GLU:HA	1.75	0.84
1:B:45:THR:HA	5:B:851:HOH:O	1.76	0.84
1:B:125:THR:HG23	1:B:128:TYR:H	1.43	0.82
1:B:73:THR:HB	5:B:826:HOH:O	1.79	0.82
1:A:156:LEU:HD13	1:A:174:LEU:CD1	2.08	0.82
1:A:70:VAL:HG11	5:A:941:HOH:O	1.78	0.81
1:B:151:LYS:HA	1:B:151:LYS:CE	2.10	0.81
1:A:330:SER:HB2	1:A:333:SER:OG	1.83	0.79
1:B:126:PRO:O	1:B:129:LEU:HB3	1.82	0.79
1:B:262:ILE:HD13	1:B:262:ILE:H	1.49	0.78
1:B:213:ILE:HG13	5:B:877:HOH:O	1.82	0.77
1:A:110:VAL:HG13	5:A:891:HOH:O	1.84	0.77
1:B:73:THR:HG22	1:B:75:THR:HG23	1.67	0.77
1:A:33:LEU:HD23	5:A:781:HOH:O	1.84	0.77
1:A:157:ILE:HD11	5:A:941:HOH:O	1.85	0.77
1:A:125:THR:HG23	1:A:128:TYR:H	1.50	0.77
1:A:82:LYS:HA	1:A:82:LYS:HE2	1.67	0.75
1:A:132:LYS:HB2	5:A:784:HOH:O	1.86	0.75
1:B:217:CYS:HB2	5:B:864:HOH:O	1.86	0.75
1:B:159:GLU:HA	5:B:829:HOH:O	1.87	0.75
1:B:370:PRO:O	1:B:371:ASP:HB2	1.87	0.74
1:B:229:LYS:O	1:B:233:GLU:HG3	1.88	0.73
1:B:227:THR:HB	5:B:841:HOH:O	1.89	0.72
1:B:125:THR:HG22	1:B:166:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLU:HB2	5:B:839:HOH:O	1.89	0.72
1:B:303:GLU:H	1:B:306:HIS:CD2	2.01	0.72
1:B:308:ARG:HG3	5:B:853:HOH:O	1.89	0.72
1:A:332:GLY:HA3	5:A:844:HOH:O	1.90	0.71
1:A:210:ALA:N	5:A:852:HOH:O	2.23	0.71
1:A:36:ARG:HD2	5:A:781:HOH:O	1.90	0.71
1:A:54:GLU:CD	1:A:54:GLU:H	1.94	0.71
1:A:82:LYS:HB2	5:A:932:HOH:O	1.90	0.70
1:B:137:VAL:HG11	1:B:169:TRP:CE3	2.27	0.70
1:B:340:LYS:HB3	5:B:825:HOH:O	1.92	0.70
1:A:80:GLU:CD	1:A:81:ASP:H	1.94	0.70
1:B:128:TYR:CD2	1:B:166:GLU:HB2	2.26	0.70
1:B:24:ILE:H	1:B:69:ASN:ND2	1.89	0.70
1:B:123:SER:HA	1:B:159:GLU:O	1.90	0.70
1:A:132:LYS:HE2	5:A:784:HOH:O	1.92	0.69
1:B:168:VAL:O	1:B:172:GLU:HG3	1.91	0.69
1:A:218:HIS:HD2	5:A:707:HOH:O	1.76	0.69
1:B:299:CYS:SG	5:B:864:HOH:O	2.50	0.69
1:A:206:VAL:HA	5:A:852:HOH:O	1.91	0.69
1:A:163:HIS:HB3	5:A:930:HOH:O	1.93	0.68
1:A:130:SER:HB2	5:A:784:HOH:O	1.92	0.68
1:B:203:VAL:HG22	5:B:830:HOH:O	1.93	0.68
1:A:100:ASN:HD21	1:A:144:GLN:HE21	1.42	0.68
1:A:61:ARG:HG2	5:A:891:HOH:O	1.94	0.67
1:A:257:ASN:HD21	1:A:259:GLN:HB2	1.59	0.67
1:B:164:VAL:O	1:B:168:VAL:HG23	1.95	0.67
1:A:73:THR:HG23	5:A:893:HOH:O	1.95	0.67
1:B:25:GLY:HA2	5:B:880:HOH:O	1.94	0.66
1:A:165:GLU:HB2	5:A:930:HOH:O	1.96	0.66
1:B:69:ASN:HD21	1:B:318:ARG:HH12	1.43	0.66
1:B:128:TYR:HA	1:B:131:ALA:O	1.95	0.66
1:A:168:VAL:HA	5:A:909:HOH:O	1.95	0.66
1:A:257:ASN:ND2	1:A:259:GLN:H	1.93	0.66
1:A:137:VAL:HG11	1:A:169:TRP:CE3	2.31	0.66
1:A:257:ASN:C	1:A:257:ASN:HD22	1.97	0.66
1:A:314:LEU:O	1:A:318:ARG:HG3	1.95	0.66
1:A:49:ALA:HB2	5:A:914:HOH:O	1.95	0.65
1:A:333:SER:HA	1:A:347:ALA:HB1	1.78	0.65
1:B:137:VAL:HG13	1:B:138:LYS:N	2.10	0.65
1:B:184:THR:OG1	5:B:829:HOH:O	2.15	0.65
1:A:137:VAL:HG11	1:A:169:TRP:HE3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TRP:HE3	1:A:331:TRP:H	1.46	0.64
1:A:60:HIS:HB3	1:A:110:VAL:HG11	1.80	0.64
1:B:170:ALA:O	1:B:174:LEU:HG	1.98	0.64
1:A:42:GLY:HA2	5:B:776:HOH:O	1.98	0.64
1:A:179:LYS:HD2	5:A:850:HOH:O	1.98	0.64
1:B:171:VAL:HG21	5:B:860:HOH:O	1.97	0.63
1:B:216:ASN:ND2	5:B:864:HOH:O	2.30	0.63
1:B:230:LEU:HD13	5:B:889:HOH:O	1.99	0.63
1:B:152:ASN:HD22	1:B:179:LYS:NZ	1.97	0.63
1:B:259:GLN:O	1:B:262:ILE:HD11	1.99	0.63
1:B:145:LEU:O	1:B:149:MET:HB2	1.98	0.63
1:A:196:VAL:HG11	5:A:934:HOH:O	1.99	0.62
1:A:162:GLU:O	1:A:192:ASP:HB2	1.99	0.62
1:B:315:ALA:HB1	5:B:842:HOH:O	1.99	0.62
1:B:46:PRO:HD3	5:B:851:HOH:O	1.99	0.61
1:A:210:ALA:HB2	5:A:912:HOH:O	1.98	0.61
1:A:169:TRP:HB3	5:A:939:HOH:O	2.00	0.61
1:B:71:MET:HG2	5:B:855:HOH:O	1.99	0.61
1:A:137:VAL:HG12	5:A:783:HOH:O	1.99	0.61
1:A:11:LYS:HE2	5:A:876:HOH:O	2.00	0.60
1:A:119:ALA:HA	5:A:866:HOH:O	2.01	0.60
1:A:331:TRP:HB3	1:A:349:LYS:HD2	1.82	0.60
1:B:152:ASN:HD22	1:B:179:LYS:HZ1	1.48	0.60
1:A:153:VAL:HB	5:A:866:HOH:O	2.01	0.60
1:B:331:TRP:HB3	1:B:349:LYS:HA	1.83	0.60
1:A:147:VAL:HG23	5:A:851:HOH:O	2.01	0.60
1:A:304:PRO:HD2	5:B:890:HOH:O	2.01	0.60
1:A:25:GLY:N	5:A:896:HOH:O	2.35	0.60
1:A:164:VAL:HG11	5:A:934:HOH:O	2.02	0.59
1:B:76:PHE:HB3	5:B:821:HOH:O	2.02	0.59
1:B:138:LYS:HB3	5:B:886:HOH:O	2.01	0.59
1:B:149:MET:CE	1:B:177:SER:HB2	2.33	0.59
1:A:138:LYS:HG2	5:A:939:HOH:O	2.01	0.59
1:A:320:PHE:HD1	5:A:857:HOH:O	1.84	0.59
1:B:352:TRP:HB2	5:B:813:HOH:O	2.03	0.58
1:A:180:PRO:HB3	5:A:864:HOH:O	2.02	0.58
1:B:138:LYS:HE2	1:B:169:TRP:HB3	1.84	0.58
1:B:210:ALA:HB2	5:B:860:HOH:O	2.03	0.58
1:B:241:LYS:NZ	1:B:241:LYS:HB3	2.19	0.58
1:B:210:ALA:HA	5:B:763:HOH:O	2.03	0.58
1:A:341:PRO:HG3	1:A:344:ARG:HH22	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:N	5:A:780:HOH:O	2.30	0.57
1:A:73:THR:O	1:A:75:THR:N	2.36	0.57
1:A:232:LYS:O	1:A:236:GLU:HG3	2.05	0.57
1:A:189:PRO:HA	5:A:900:HOH:O	2.05	0.56
1:A:349:LYS:HG3	5:A:872:HOH:O	2.05	0.56
1:A:82:LYS:HE2	1:A:82:LYS:CA	2.35	0.56
1:B:181:VAL:HB	5:B:763:HOH:O	2.04	0.56
1:A:325:SER:O	1:A:329:GLY:N	2.39	0.56
1:A:341:PRO:HG3	1:A:344:ARG:NH2	2.21	0.56
1:A:119:ALA:HB1	5:A:923:HOH:O	2.05	0.56
1:A:315:ALA:HB3	1:A:316:PRO:HD3	1.87	0.56
1:A:50:VAL:HG11	5:A:865:HOH:O	2.05	0.56
1:B:245:MET:HG3	1:B:295:TYR:CD1	2.41	0.56
1:A:47:GLU:HB2	5:A:901:HOH:O	2.04	0.56
1:A:211:SER:HB2	5:A:864:HOH:O	2.04	0.55
1:B:152:ASN:ND2	1:B:179:LYS:NZ	2.53	0.55
1:B:79:SER:CB	1:B:144:GLN:HG2	2.37	0.55
1:B:338:HIS:ND1	5:B:776:HOH:O	2.33	0.55
1:B:343:VAL:N	5:B:825:HOH:O	2.28	0.55
1:A:137:VAL:HG13	1:A:138:LYS:N	2.21	0.55
1:B:137:VAL:HG11	1:B:169:TRP:HE3	1.71	0.55
1:A:36:ARG:HB2	5:A:781:HOH:O	2.05	0.55
1:A:11:LYS:HB3	5:A:876:HOH:O	2.06	0.55
1:A:203:VAL:O	1:A:206:VAL:HG22	2.07	0.55
1:A:157:ILE:HG13	5:A:923:HOH:O	2.05	0.55
1:B:137:VAL:HG13	1:B:138:LYS:H	1.72	0.54
1:A:80:GLU:OE2	1:A:80:GLU:CA	2.52	0.54
1:B:371:ASP:HA	5:B:820:HOH:O	2.07	0.54
1:B:127:SER:HA	1:B:132:LYS:HE2	1.89	0.54
1:B:240:LEU:HD12	5:B:830:HOH:O	2.08	0.54
1:B:261:PHE:HD1	5:B:847:HOH:O	1.91	0.54
1:B:276:ALA:O	1:B:306:HIS:HE1	1.90	0.54
1:B:147:VAL:HG12	5:B:844:HOH:O	2.07	0.54
1:B:338:HIS:HD2	1:B:340:LYS:H	1.56	0.54
1:A:125:THR:HG21	1:A:137:VAL:HG23	1.90	0.54
1:B:342:TRP:N	5:B:825:HOH:O	2.41	0.54
5:A:917:HOH:O	1:B:40:LYS:HE3	2.09	0.53
1:A:175:ILE:HG21	1:A:209:GLY:HA3	1.90	0.53
1:A:345:ALA:HB2	5:A:764:HOH:O	2.09	0.53
1:B:124:GLN:HA	1:B:161:PHE:CE1	2.44	0.53
1:B:128:TYR:CE2	1:B:166:GLU:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG21	5:A:863:HOH:O	2.08	0.53
1:A:187:ILE:HD12	5:A:908:HOH:O	2.08	0.52
1:A:353:GLU:HB2	5:A:793:HOH:O	2.07	0.52
1:A:262:ILE:HG21	5:B:823:HOH:O	2.08	0.52
1:A:338:HIS:CD2	1:A:343:VAL:HG11	2.44	0.52
1:B:159:GLU:HG3	5:B:829:HOH:O	2.10	0.52
1:B:183:ALA:O	1:B:213:ILE:HA	2.09	0.52
1:A:97:GLN:O	1:A:101:GLU:HG3	2.09	0.52
1:A:321:LEU:HD11	1:A:331:TRP:HH2	1.75	0.52
1:B:157:ILE:HG22	1:B:159:GLU:HB2	1.91	0.52
1:A:76:PHE:HB3	5:A:884:HOH:O	2.09	0.52
1:A:132:LYS:HG2	1:A:136:GLU:HG2	1.93	0.51
1:A:231:MET:SD	5:A:853:HOH:O	2.59	0.51
1:B:218:HIS:HD2	5:B:717:HOH:O	1.94	0.51
1:B:143:GLN:O	1:B:147:VAL:HG23	2.11	0.51
1:B:172:GLU:HB2	5:B:852:HOH:O	2.09	0.51
1:A:100:ASN:ND2	1:A:144:GLN:HE21	2.07	0.51
1:A:201:ALA:HA	5:A:934:HOH:O	2.10	0.51
1:B:78:ALA:HB3	5:B:862:HOH:O	2.10	0.51
1:B:172:GLU:HG2	5:B:881:HOH:O	2.11	0.51
1:B:160:TYR:CE2	3:B:602:CBH:H102	2.46	0.51
1:A:160:TYR:HB2	5:A:858:HOH:O	2.11	0.51
1:B:214:GLY:HA3	1:B:245:MET:O	2.11	0.50
1:A:171:VAL:HG22	5:A:912:HOH:O	2.11	0.50
1:A:204:ARG:HD3	5:A:934:HOH:O	2.11	0.50
1:B:79:SER:HB2	1:B:144:GLN:HG2	1.93	0.50
1:A:47:GLU:HG3	1:A:51:GLU:OE2	2.10	0.50
1:A:203:VAL:HG23	5:A:883:HOH:O	2.11	0.50
1:B:124:GLN:NE2	1:B:162:GLU:H	2.08	0.50
1:B:308:ARG:HD2	5:B:707:HOH:O	2.10	0.50
1:A:136:GLU:O	1:A:139:LYS:HB2	2.11	0.50
1:B:73:THR:O	1:B:75:THR:N	2.44	0.50
1:B:134:GLU:OE1	1:B:138:LYS:HE3	2.10	0.49
1:B:139:LYS:O	1:B:143:GLN:HG3	2.12	0.49
1:B:349:LYS:HA	5:B:813:HOH:O	2.11	0.49
1:A:250:ALA:HB2	1:A:302:PHE:CD1	2.47	0.49
1:A:46:PRO:HG3	1:A:78:ALA:HB2	1.95	0.49
1:A:72:GLN:HE22	1:A:247:GLN:HE22	1.58	0.49
1:A:198:PRO:HG3	5:A:900:HOH:O	2.12	0.49
1:B:11:LYS:HE2	5:B:866:HOH:O	2.12	0.49
1:B:224:SER:HA	5:B:841:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ASN:N	5:B:824:HOH:O	2.42	0.49
1:B:134:GLU:HG2	1:B:138:LYS:HD2	1.95	0.49
1:B:141:PHE:HB3	5:B:833:HOH:O	2.12	0.49
1:B:328:HIS:CG	1:B:329:GLY:H	2.31	0.49
1:B:151:LYS:HD2	5:B:836:HOH:O	2.11	0.49
1:B:159:GLU:HG3	1:B:216:ASN:ND2	2.27	0.48
1:B:131:ALA:HB3	5:B:786:HOH:O	2.11	0.48
1:A:123:SER:HA	1:A:159:GLU:O	2.13	0.48
1:A:137:VAL:HG13	1:A:138:LYS:H	1.78	0.48
1:A:181:VAL:HG11	5:A:863:HOH:O	2.12	0.48
1:B:276:ALA:HB1	1:B:280:ASP:HB2	1.95	0.48
1:B:152:ASN:ND2	1:B:179:LYS:HZ1	2.08	0.48
1:B:235:LEU:HD12	5:B:830:HOH:O	2.13	0.48
1:A:177:SER:HB2	5:A:892:HOH:O	2.12	0.48
1:A:202:ALA:O	1:A:206:VAL:HG13	2.14	0.48
1:B:349:LYS:HE3	5:B:882:HOH:O	2.13	0.48
3:B:602:CBH:O13	3:B:602:CBH:H172	2.14	0.48
1:A:126:PRO:HD2	5:A:843:HOH:O	2.14	0.48
1:A:51:GLU:HG3	5:A:901:HOH:O	2.13	0.48
1:A:241:LYS:HA	1:A:241:LYS:CE	2.29	0.48
1:B:108:ARG:HA	1:B:118:VAL:HG21	1.95	0.48
1:B:348:ARG:NH2	5:B:879:HOH:O	2.46	0.47
1:B:340:LYS:HD2	1:B:342:TRP:CZ2	2.49	0.47
1:A:308:ARG:NH1	5:A:890:HOH:O	2.40	0.47
1:B:160:TYR:OH	3:B:602:CBH:H222	2.14	0.47
1:B:346:ARG:HG2	1:B:351:TYR:CZ	2.49	0.47
1:B:370:PRO:O	1:B:371:ASP:CB	2.59	0.47
1:B:349:LYS:NZ	1:B:349:LYS:HB3	2.29	0.47
1:A:72:GLN:NE2	1:A:247:GLN:HE22	2.13	0.47
1:A:179:LYS:HB2	5:A:850:HOH:O	2.15	0.47
1:B:137:VAL:CG1	1:B:138:LYS:N	2.76	0.47
1:B:54:GLU:HB3	5:B:781:HOH:O	2.14	0.47
1:A:257:ASN:ND2	1:A:257:ASN:C	2.68	0.47
1:A:326:GLU:HB3	5:A:885:HOH:O	2.15	0.47
1:B:133:SER:N	5:B:839:HOH:O	2.48	0.47
1:A:65:ARG:O	1:A:323:PRO:HG2	2.14	0.47
1:B:205:LEU:HB3	5:B:860:HOH:O	2.14	0.47
1:B:149:MET:HE2	5:B:784:HOH:O	2.15	0.47
1:B:159:GLU:CA	5:B:829:HOH:O	2.57	0.47
1:B:331:TRP:HE3	5:B:813:HOH:O	1.97	0.47
1:B:13:ILE:HG23	1:B:14:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:HD21	1:A:144:GLN:NE2	2.12	0.46
1:B:229:LYS:HB3	5:B:889:HOH:O	2.14	0.46
1:B:349:LYS:HG2	1:B:353:GLU:OE1	2.15	0.46
1:B:76:PHE:CE1	3:B:602:CBH:H191	2.50	0.46
1:A:311:ALA:HB2	5:A:840:HOH:O	2.14	0.46
1:B:101:GLU:N	5:B:812:HOH:O	2.49	0.46
1:B:69:ASN:HD21	1:B:318:ARG:NH1	2.10	0.46
1:A:165:GLU:OE1	1:A:165:GLU:N	2.46	0.46
1:B:127:SER:HB3	1:B:132:LYS:HE3	1.97	0.46
1:B:267:PHE:HZ	3:B:602:CBH:O24	1.98	0.46
1:A:98:GLU:HB3	5:A:849:HOH:O	2.15	0.46
5:A:913:HOH:O	1:B:54:GLU:HB2	2.16	0.46
1:B:45:THR:OG1	1:B:47:GLU:OE2	2.33	0.46
1:B:338:HIS:CD2	1:B:340:LYS:H	2.33	0.46
1:A:308:ARG:CZ	1:A:328:HIS:HB2	2.46	0.46
1:B:47:GLU:HB2	1:B:51:GLU:OE2	2.15	0.45
1:B:77:TYR:HE2	5:B:845:HOH:O	1.99	0.45
1:A:186:ALA:N	5:A:868:HOH:O	2.48	0.45
1:B:29:PHE:CD2	1:B:59:LEU:HD23	2.51	0.45
1:B:250:ALA:HB2	1:B:302:PHE:CD1	2.51	0.45
1:A:135:THR:C	5:A:780:HOH:O	2.55	0.45
1:A:229:LYS:O	1:A:233:GLU:HG3	2.16	0.45
1:A:311:ALA:HB1	1:A:322:PRO:HD3	1.98	0.45
1:A:152:ASN:HA	5:A:897:HOH:O	2.14	0.45
1:A:257:ASN:HD22	1:A:259:GLN:H	1.63	0.45
1:B:262:ILE:HD13	5:B:847:HOH:O	2.16	0.45
1:B:53:PRO:HB3	5:B:857:HOH:O	2.17	0.45
1:A:46:PRO:HD3	1:A:76:PHE:O	2.16	0.45
1:B:125:THR:CG2	1:B:127:SER:HB2	2.46	0.45
1:A:145:LEU:HD13	1:A:174:LEU:HD13	1.99	0.45
1:B:134:GLU:O	1:B:137:VAL:HG12	2.16	0.45
1:A:77:TYR:HE1	5:A:928:HOH:O	1.99	0.45
1:B:75:THR:O	1:B:77:TYR:O	2.35	0.45
1:B:162:GLU:O	1:B:192:ASP:HB2	2.17	0.45
1:B:282:GLN:O	1:B:313:GLU:HG2	2.16	0.44
1:B:353:GLU:HG2	5:B:824:HOH:O	2.17	0.44
1:A:155:PHE:HB2	1:A:180:PRO:O	2.17	0.44
1:A:305:TYR:CE2	1:B:35:LYS:HD2	2.53	0.44
1:B:146:GLU:HA	1:B:149:MET:HB2	1.99	0.44
1:A:16:ARG:NH2	1:A:115:ASP:OD2	2.39	0.44
1:B:216:ASN:HA	1:B:247:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:HIS:HE1	1:B:280:ASP:OD2	2.00	0.44
1:A:15:GLU:C	5:A:876:HOH:O	2.55	0.44
1:B:139:LYS:HA	1:B:139:LYS:HZ2	1.83	0.44
1:B:139:LYS:HA	1:B:139:LYS:NZ	2.31	0.44
1:B:76:PHE:O	1:B:77:TYR:HB2	2.18	0.44
1:B:126:PRO:C	1:B:129:LEU:HB3	2.38	0.44
1:B:151:LYS:HE3	5:B:818:HOH:O	2.17	0.44
1:A:201:ALA:O	1:A:205:LEU:HG	2.18	0.44
1:A:133:SER:HB2	5:A:771:HOH:O	2.17	0.44
1:A:331:TRP:CE3	1:A:331:TRP:N	2.86	0.44
1:B:227:THR:O	1:B:231:MET:HG3	2.18	0.44
1:B:348:ARG:HD3	5:B:879:HOH:O	2.18	0.44
1:A:80:GLU:O	1:A:81:ASP:HB3	2.18	0.44
1:A:308:ARG:HD2	5:A:719:HOH:O	2.17	0.44
1:A:136:GLU:HB2	5:A:771:HOH:O	2.16	0.43
1:B:78:ALA:HB2	5:B:814:HOH:O	2.18	0.43
1:B:137:VAL:CG1	1:B:138:LYS:H	2.31	0.43
1:A:214:GLY:N	5:A:853:HOH:O	2.50	0.43
1:A:262:ILE:HD11	3:A:601:CBH:H221	1.99	0.43
1:B:124:GLN:HG2	5:B:845:HOH:O	2.18	0.43
1:A:235:LEU:HD23	5:A:883:HOH:O	2.18	0.43
1:B:289:TYR:CE2	1:B:317:GLU:HG2	2.52	0.43
1:A:181:VAL:O	1:A:210:ALA:HA	2.18	0.43
1:A:332:GLY:O	1:A:347:ALA:HA	2.18	0.43
1:B:273:PRO:HG3	1:B:361:ARG:NH2	2.32	0.43
1:A:30:VAL:HG22	3:A:601:CBH:O13	2.17	0.43
1:A:163:HIS:CE1	1:A:193:LEU:HD12	2.53	0.43
1:A:50:VAL:HG21	5:A:865:HOH:O	2.19	0.43
1:A:245:MET:HG3	1:A:295:TYR:CD2	2.53	0.43
1:A:340:LYS:HA	1:A:341:PRO:HD3	1.92	0.43
1:B:124:GLN:NE2	5:B:778:HOH:O	2.51	0.43
1:B:138:LYS:O	1:B:142:LEU:HB2	2.19	0.43
1:A:35:LYS:HE2	5:A:775:HOH:O	2.18	0.43
1:A:174:LEU:HB2	5:A:863:HOH:O	2.18	0.43
1:A:202:ALA:HB3	5:A:883:HOH:O	2.19	0.43
1:A:273:PRO:HA	1:B:273:PRO:HA	2.00	0.43
1:B:73:THR:CG2	1:B:75:THR:HG23	2.45	0.42
1:A:73:THR:N	5:A:893:HOH:O	2.53	0.42
1:A:160:TYR:OH	3:A:601:CBH:H222	2.20	0.42
1:A:203:VAL:CG1	1:A:207:LYS:HE3	2.48	0.42
1:B:262:ILE:HD13	1:B:262:ILE:N	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HA	1:A:82:LYS:CE	2.43	0.42
1:A:96:GLY:N	5:A:849:HOH:O	2.53	0.42
1:B:22:ILE:HD11	1:B:289:TYR:CE2	2.55	0.42
1:B:31:PHE:O	1:B:35:LYS:HG2	2.19	0.42
1:A:76:PHE:O	1:A:77:TYR:HB2	2.20	0.42
1:B:331:TRP:HB3	1:B:349:LYS:CA	2.49	0.42
1:A:165:GLU:CD	1:A:204:ARG:HH12	2.23	0.42
1:A:33:LEU:HD12	1:A:74:PHE:CZ	2.54	0.42
1:A:161:PHE:HZ	5:A:848:HOH:O	2.02	0.42
1:B:15:GLU:OE1	1:B:15:GLU:N	2.50	0.42
1:B:261:PHE:N	5:B:847:HOH:O	2.53	0.42
1:A:13:ILE:HG23	1:A:14:LEU:N	2.35	0.41
1:A:214:GLY:HA3	1:A:245:MET:O	2.19	0.41
1:B:39:VAL:HG12	1:B:40:LYS:N	2.35	0.41
1:B:232:LYS:HD2	1:B:244:LEU:CD1	2.50	0.41
1:A:54:GLU:CD	1:A:54:GLU:N	2.68	0.41
1:A:175:ILE:HG23	5:A:863:HOH:O	2.21	0.41
1:A:80:GLU:CD	1:A:81:ASP:N	2.68	0.41
1:A:342:TRP:HA	1:A:342:TRP:CE3	2.54	0.41
1:A:164:VAL:HG23	1:A:192:ASP:OD1	2.21	0.41
1:B:232:LYS:HD2	1:B:244:LEU:HD11	2.02	0.41
1:B:30:VAL:HG11	5:B:821:HOH:O	2.19	0.41
1:A:220:ASP:HB3	1:A:251:TYR:O	2.21	0.41
1:A:346:ARG:HG2	1:A:351:TYR:CZ	2.56	0.41
1:B:349:LYS:CG	1:B:353:GLU:OE1	2.68	0.41
1:B:350:GLU:C	5:B:824:HOH:O	2.59	0.41
1:A:164:VAL:HG21	5:A:934:HOH:O	2.20	0.41
1:A:273:PRO:HB2	1:B:359:SER:HA	2.03	0.41
1:B:77:TYR:HA	5:B:858:HOH:O	2.21	0.41
1:B:141:PHE:CE1	1:B:170:ALA:HB2	2.56	0.41
1:B:151:LYS:HB2	5:B:844:HOH:O	2.20	0.41
1:A:202:ALA:HB2	1:A:231:MET:HB3	2.03	0.40
1:B:160:TYR:OH	1:B:218:HIS:HE1	2.04	0.40
1:B:175:ILE:HG21	1:B:209:GLY:HA3	2.03	0.40
1:B:40:LYS:O	1:B:43:PRO:HD2	2.21	0.40
1:B:65:ARG:HG2	1:B:324:ALA:HB2	2.02	0.40
1:B:132:LYS:O	1:B:133:SER:O	2.38	0.40
1:A:11:LYS:N	5:A:921:HOH:O	2.54	0.40
1:A:98:GLU:O	1:A:98:GLU:HG3	2.21	0.40
1:A:165:GLU:HA	5:A:910:HOH:O	2.21	0.40
1:B:262:ILE:HA	1:B:267:PHE:CG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ARG:NE	5:B:853:HOH:O	2.51	0.40
1:B:53:PRO:HD3	5:B:857:HOH:O	2.21	0.40
1:B:346:ARG:HG2	1:B:351:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	344/406 (85%)	323 (94%)	17 (5%)	4 (1%)	13 5
1	B	336/406 (83%)	313 (93%)	21 (6%)	2 (1%)	25 15
All	All	680/812 (84%)	636 (94%)	38 (6%)	6 (1%)	17 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	SER
1	A	133	SER
1	A	329	GLY
1	B	132	LYS
1	A	331	TRP
1	A	74	PHE

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	275/323 (85%)	261 (95%)	14 (5%)	24 15
1	B	268/323 (83%)	250 (93%)	18 (7%)	16 9
All	All	543/646 (84%)	511 (94%)	32 (6%)	19 11

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	59	LEU
1	A	80	GLU
1	A	82	LYS
1	A	98	GLU
1	A	117	LEU
1	A	215	VAL
1	A	218	HIS
1	A	241	LYS
1	A	257	ASN
1	A	261	PHE
1	A	268	PRO
1	A	295	TYR
1	A	327	LYS
1	B	54	GLU
1	B	136	GLU
1	B	139	LYS
1	B	151	LYS
1	B	165	GLU
1	B	204	ARG
1	B	217	CYS
1	B	218	HIS
1	B	230	LEU
1	B	259	GLN
1	B	261	PHE
1	B	262	ILE
1	B	268	PRO
1	B	284	TYR
1	B	295	TYR
1	B	335	LEU
1	B	348	ARG
1	B	371	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	100	ASN
1	A	143	GLN
1	A	163	HIS
1	A	218	HIS
1	A	257	ASN
1	A	290	ASN
1	B	69	ASN
1	B	124	GLN
1	B	152	ASN
1	B	194	HIS
1	B	216	ASN
1	B	218	HIS
1	B	252	HIS
1	B	259	GLN
1	B	282	GLN
1	B	306	HIS
1	B	338	HIS
1	B	354	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	CIT	A	701	-	3,12,12	2.19	1 (33%)	3,17,17	0.78	0
4	CIT	B	702	-	3,12,12	2.29	1 (33%)	3,17,17	0.83	0
3	CBH	B	602	2	7,14,14	0.36	0	5,16,16	0.89	0
3	CBH	A	601	2	7,14,14	0.34	0	5,16,16	0.84	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
4	CIT	A	701	-	-	1/6/16/16	-
4	CIT	B	702	-	-	1/6/16/16	-
3	CBH	B	602	2	-	0/8/14/14	-
3	CBH	A	601	2	-	0/8/14/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	CIT	O7-C3	-3.96	1.36	1.43
4	A	701	CIT	O7-C3	-3.76	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	CIT	C1-C2-C3-C6
4	B	702	CIT	C1-C2-C3-C6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	CBH	5	0
3	A	601	CBH	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	348/406 (85%)	0.28	31 (8%)	9	10	16, 42, 74, 88	0
1	B	340/406 (83%)	0.25	25 (7%)	14	16	17, 44, 67, 83	0
All	All	688/812 (84%)	0.26	56 (8%)	12	12	16, 43, 71, 88	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	SER	13.2
1	A	329	GLY	9.7
1	B	129	LEU	7.3
1	A	331	TRP	6.1
1	A	342	TRP	5.6
1	B	128	TYR	5.5
1	A	80	GLU	5.3
1	B	77	TYR	4.9
1	B	130	SER	4.9
1	A	133	SER	4.9
1	A	335	LEU	4.3
1	B	78	ALA	4.2
1	A	81	ASP	4.2
1	A	82	LYS	3.9
1	B	349	LYS	3.8
1	B	131	ALA	3.5
1	B	79	SER	3.5
1	A	337	MET	3.4
1	B	239	GLN	3.4
1	B	149	MET	3.3
1	A	176	ALA	3.2
1	A	332	GLY	3.1
1	B	350	GLU	3.1
1	B	53	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	131	ALA	3.0
1	A	341	PRO	3.0
1	A	146	GLU	3.0
1	A	96	GLY	2.8
1	A	143	GLN	2.7
1	A	336	ASP	2.7
1	A	339	THR	2.6
1	B	326	GLU	2.6
1	A	142	LEU	2.6
1	B	176	ALA	2.6
1	B	15	GLU	2.5
1	B	194	HIS	2.5
1	A	15	GLU	2.5
1	B	140	VAL	2.5
1	B	133	SER	2.5
1	B	146	GLU	2.5
1	A	149	MET	2.4
1	B	241	LYS	2.4
1	A	239	GLN	2.4
1	A	344	ARG	2.4
1	B	143	GLN	2.3
1	B	139	LYS	2.3
1	A	139	LYS	2.3
1	A	97	GLN	2.2
1	A	347	ALA	2.2
1	A	135	THR	2.2
1	B	48	ALA	2.2
1	B	209	GLY	2.2
1	A	333	SER	2.1
1	A	326	GLU	2.1
1	B	142	LEU	2.1
1	A	77	TYR	2.0

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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
3	CBH	B	602	15/15	0.80	0.19	35,37,48,49	15
3	CBH	A	601	15/15	0.90	0.14	32,35,36,38	0
4	CIT	A	701	13/13	0.90	0.14	22,29,35,35	13
2	ZN	B	502	1/1	0.91	0.09	30,30,30,30	1
4	CIT	B	702	13/13	0.91	0.14	31,36,38,40	13
2	ZN	A	501	1/1	0.94	0.06	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.