Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 10:29 AM EDT

PDB ID	:	3D47
Title	:	Crystal structure of L-rhamnonate dehydratase from Salmonella typhimurium complexed with Mg and D-malate
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Sauder, J.M.; Burley, S.K.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-05-14
Resolution	:	1.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

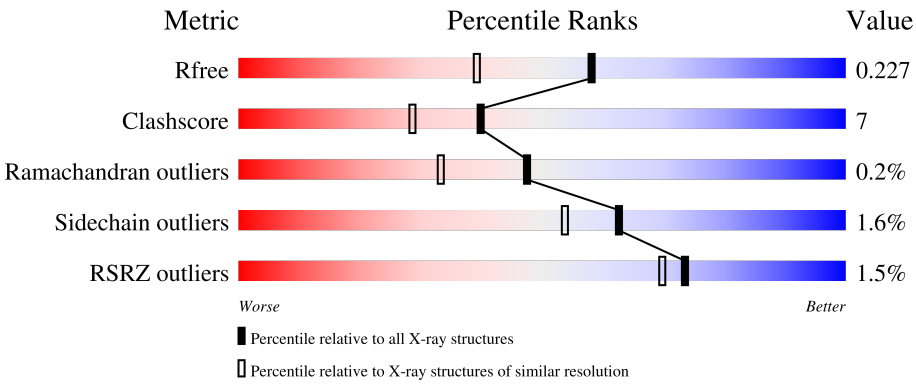
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	405	86% 14%
1	B	405	2% 85% 15%
1	C	405	2% 83% 17%
1	D	405	% 84% 15%
1	E	405	% 85% 15%

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Mol	Chain	Length	Quality of chain
1	F	405	% 83% 16%
1	G	405	% 84% 15%
1	H	405	3% 81% 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26892 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 Putative galactonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3137	1988	543	579	27	0	0	0
1	B	405	3137	1988	543	579	27	0	0	0
1	C	405	3137	1988	543	579	27	0	0	0
1	D	405	3137	1988	543	579	27	0	0	0
1	E	405	3137	1988	543	579	27	0	0	0
1	F	405	3137	1988	543	579	27	0	0	0
1	G	405	3137	1988	543	579	27	0	0	0
1	H	405	3137	1988	543	579	27	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

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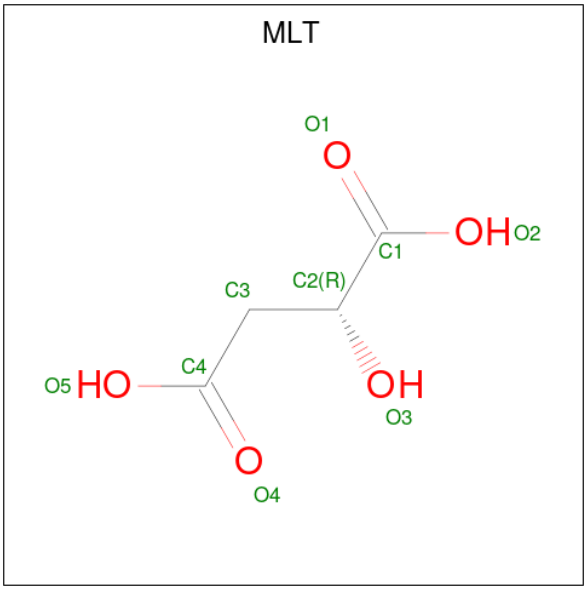
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 4 5	0	0
3	B	1	Total C O 9 4 5	0	0
3	C	1	Total C O 9 4 5	0	0
3	D	1	Total C O 9 4 5	0	0
3	E	1	Total C O 9 4 5	0	0
3	F	1	Total C O 9 4 5	0	0
3	G	1	Total C O 9 4 5	0	0
3	H	1	Total C O 9 4 5	0	0

- Molecule 4 is water.

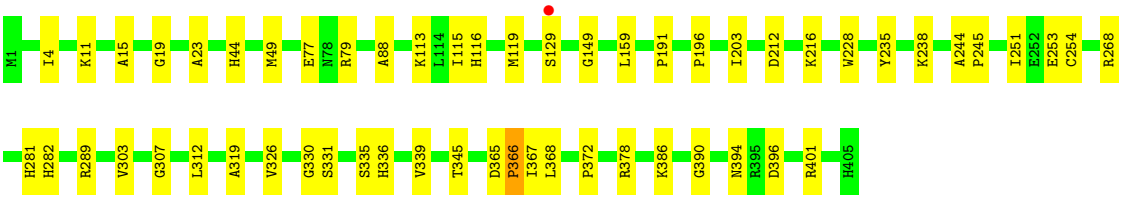
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	274	274	274	0	0
			Total	O		
4	B	202	202	202	0	0
			Total	O		
4	C	237	237	237	0	0
			Total	O		
4	D	165	165	165	0	0
			Total	O		
4	E	194	194	194	0	0
			Total	O		
4	F	225	225	225	0	0
			Total	O		
4	G	267	267	267	0	0
			Total	O		
4	H	152	152	152	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.

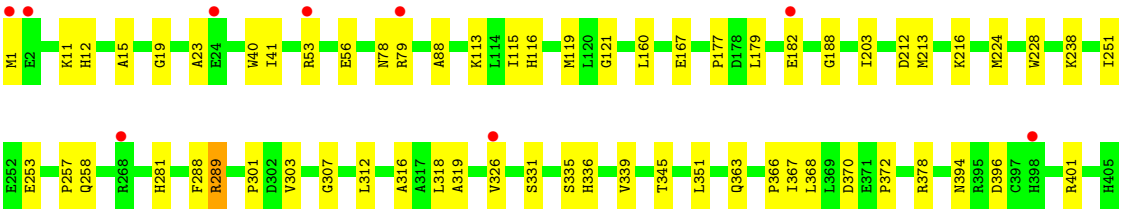
• Molecule 1: Putative galactonate dehydratase

Chain A:



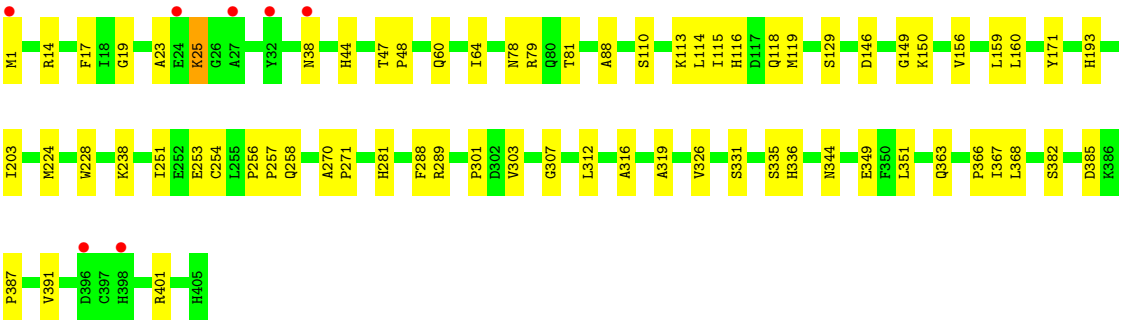
• Molecule 1: Putative galactonate dehydratase

Chain B:



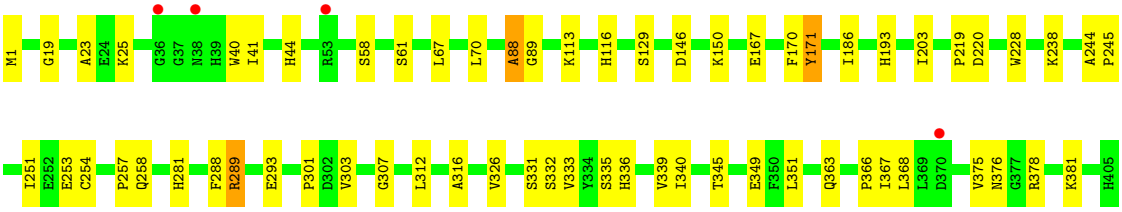
• Molecule 1: Putative galactonate dehydratase

Chain C:



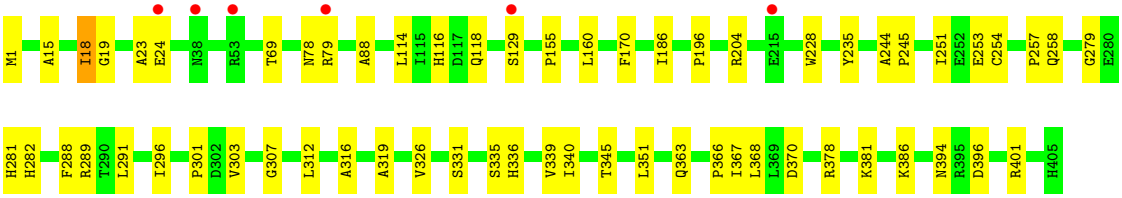
• Molecule 1: Putative galactonate dehydratase

Chain D:



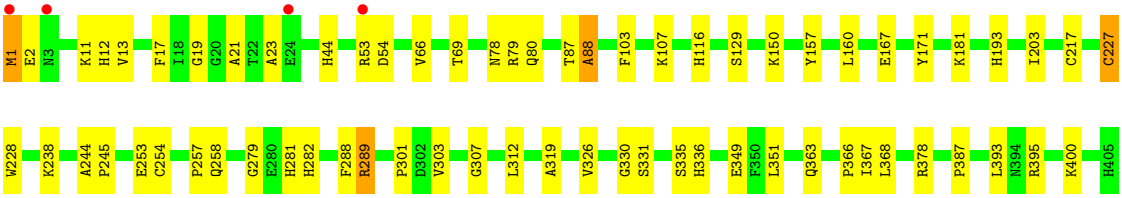
• Molecule 1: Putative galactonate dehydratase

Chain E:



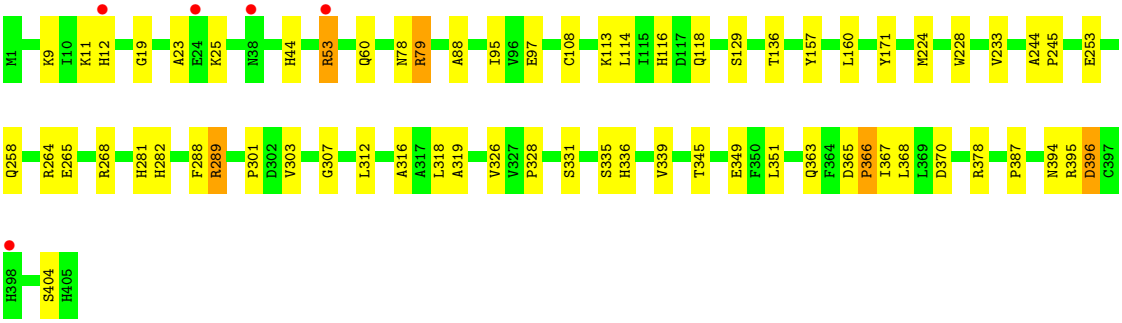
• Molecule 1: Putative galactonate dehydratase

Chain F:



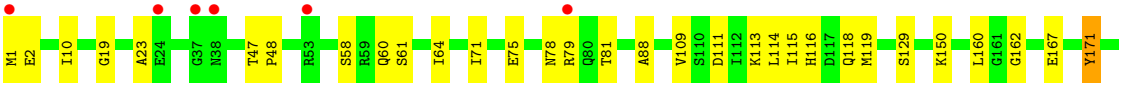
• Molecule 1: Putative galactonate dehydratase

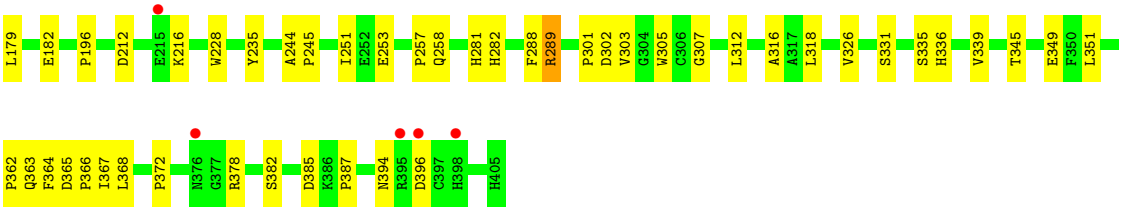
Chain G:



• Molecule 1: Putative galactonate dehydratase

Chain H:




L179
E182
P196
D212
E215
K216
W228
Y235
A244
P245
I251
E252
E253
P257
Q258
H281
H282
F288
R289
P301
D302
V303
G304
W305
C306
G307
L312
A316
A317
L318
V326
S331
S335
H336
V339
T345
E349
F350
L351
P362
Q363
F364
D365
P366
I367
L368
P372
N376
G377
R378
S382
D385
K386
P387
N394
R395
D396
C397
H398
H405

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.22Å 122.00Å 141.35Å 90.00° 108.24° 90.00°	Depositor
Resolution (Å)	24.88 – 1.80 38.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (24.88-1.80) 96.7 (38.95-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.232 0.198 , 0.227	Depositor DCC
R_{free} test set	14317 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26892	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLT, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.33	0/3218	0.64	0/4358
1	B	0.32	0/3218	0.62	0/4358
1	C	0.32	0/3218	0.63	0/4358
1	D	0.31	0/3218	0.61	1/4358 (0.0%)
1	E	0.31	0/3218	0.61	0/4358
1	F	0.34	1/3218 (0.0%)	0.63	0/4358
1	G	0.33	0/3218	0.62	0/4358
1	H	0.31	0/3218	0.61	1/4358 (0.0%)
All	All	0.32	1/25744 (0.0%)	0.62	2/34864 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	227	CYS	CB-SG	-6.37	1.71	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	171	TYR	N-CA-C	-5.29	96.72	111.00
1	H	171	TYR	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3137	0	3059	42	0
1	B	3137	0	3059	42	0
1	C	3137	0	3059	56	0
1	D	3137	0	3059	47	0
1	E	3137	0	3059	47	0
1	F	3137	0	3059	54	0
1	G	3137	0	3059	58	0
1	H	3137	0	3059	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	9	0	3	0	0
3	B	9	0	3	0	0
3	C	9	0	4	0	0
3	D	9	0	4	0	0
3	E	9	0	3	0	0
3	F	9	0	3	0	0
3	G	9	0	3	0	0
3	H	9	0	3	0	0
4	A	274	0	0	7	0
4	B	202	0	0	3	0
4	C	237	0	0	4	0
4	D	165	0	0	5	0
4	E	194	0	0	7	0
4	F	225	0	0	4	0
4	G	267	0	0	9	0
4	H	152	0	0	5	0
All	All	26892	0	24498	363	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 7.

All (363) 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:G:303:VAL:HG23	4:G:942:HOH:O	1.59	1.01
1:C:303:VAL:HG22	1:C:312:LEU:HD22	1.44	1.00
1:A:129:SER:HB3	1:B:258:GLN:HE21	1.25	0.99
1:F:227:CYS:SG	1:F:254:CYS:HA	2.02	0.98
1:G:258:GLN:HE21	1:H:129:SER:HB3	1.27	0.98
1:C:129:SER:HB3	1:D:258:GLN:NE2	1.79	0.97
1:G:129:SER:HB3	1:H:258:GLN:HE21	1.24	0.97
1:G:258:GLN:NE2	1:H:129:SER:HB3	1.81	0.93
1:E:258:GLN:HE21	1:F:129:SER:HB3	1.32	0.92
1:C:367:ILE:HG23	1:C:368:LEU:HD13	1.53	0.91
1:E:258:GLN:NE2	1:F:129:SER:HB3	1.85	0.90
1:G:129:SER:HB3	1:H:258:GLN:NE2	1.85	0.89
1:A:129:SER:HB3	1:B:258:GLN:NE2	1.86	0.89
1:C:303:VAL:HG23	4:C:697:HOH:O	1.73	0.89
1:G:303:VAL:HG22	1:G:312:LEU:HD22	1.56	0.88
1:C:129:SER:HB3	1:D:258:GLN:HE21	1.37	0.87
1:H:351:LEU:HB3	1:H:363:GLN:HE22	1.39	0.87
1:E:18:ILE:HG23	1:E:69:THR:HB	1.57	0.86
1:E:367:ILE:HG23	1:E:368:LEU:HD13	1.57	0.85
1:G:367:ILE:HG23	1:G:368:LEU:HD13	1.57	0.84
1:E:129:SER:HB3	1:F:258:GLN:NE2	1.93	0.83
1:A:367:ILE:HG23	1:A:368:LEU:HD13	1.62	0.82
1:C:258:GLN:NE2	1:D:129:SER:HB3	1.94	0.82
1:B:367:ILE:HG23	1:B:368:LEU:HD13	1.62	0.81
1:G:351:LEU:HB3	1:G:363:GLN:HE22	1.46	0.79
1:H:367:ILE:HG23	1:H:368:LEU:HD13	1.67	0.76
1:C:316:ALA:HA	1:C:326:VAL:HG21	1.67	0.75
1:C:351:LEU:HB3	1:C:363:GLN:HE22	1.52	0.75
1:E:129:SER:HB3	1:F:258:GLN:HE21	1.53	0.73
1:H:303:VAL:HG22	1:H:312:LEU:HD22	1.69	0.73
1:G:253:GLU:OE2	1:G:281:HIS:HD2	1.72	0.72
1:H:331:SER:HB2	1:H:335:SER:HB2	1.72	0.72
1:F:253:GLU:OE2	1:F:281:HIS:HD2	1.72	0.71
1:D:253:GLU:OE2	1:D:281:HIS:HD2	1.74	0.70
1:D:1:MET:HE1	1:F:387:PRO:HD2	1.74	0.69
1:G:336:HIS:HD2	4:G:801:HOH:O	1.75	0.69
1:H:58:SER:O	1:H:61:SER:HB3	1.92	0.69
1:D:281:HIS:HE1	4:D:517:HOH:O	1.75	0.69
1:G:316:ALA:HA	1:G:326:VAL:HG21	1.76	0.68
1:C:1:MET:HE3	1:H:150:LYS:HE2	1.76	0.67
1:A:253:GLU:OE2	1:A:281:HIS:HD2	1.77	0.67
1:D:58:SER:O	1:D:61:SER:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:HIS:HD2	4:A:531:HOH:O	1.77	0.66
1:E:253:GLU:OE2	1:E:281:HIS:HD2	1.79	0.66
1:C:156:VAL:O	1:C:160:LEU:HD13	1.95	0.66
1:H:167:GLU:OE2	1:H:378:ARG:HD3	1.96	0.65
1:F:11:LYS:HE3	1:F:12:HIS:NE2	2.12	0.65
1:H:316:ALA:HA	1:H:326:VAL:HG21	1.77	0.65
1:B:177:PRO:HG2	1:B:213:MET:SD	2.37	0.65
1:D:146:ASP:O	1:D:150:LYS:HG2	1.96	0.64
1:A:44:HIS:HE1	4:A:533:HOH:O	1.79	0.64
1:D:336:HIS:HD2	4:D:592:HOH:O	1.80	0.64
1:A:116:HIS:HE1	1:A:307:GLY:O	1.81	0.64
1:G:331:SER:HB2	1:G:335:SER:HB2	1.80	0.64
1:H:339:VAL:HB	1:H:345:THR:HG21	1.80	0.64
1:B:116:HIS:HD2	4:G:976:HOH:O	1.79	0.63
1:B:253:GLU:OE2	1:B:281:HIS:HD2	1.81	0.63
1:B:351:LEU:HB3	1:B:363:GLN:HE22	1.64	0.63
1:G:268:ARG:HB3	1:G:268:ARG:NH1	2.13	0.63
1:G:394:ASN:OD1	1:G:396:ASP:HB2	1.99	0.62
1:E:303:VAL:HG22	1:E:312:LEU:HD22	1.82	0.62
1:G:11:LYS:HE3	1:G:12:HIS:NE2	2.15	0.61
1:C:253:GLU:OE2	1:C:281:HIS:HD2	1.83	0.61
1:C:319:ALA:CB	1:C:326:VAL:HG22	2.31	0.61
1:F:303:VAL:HG22	1:F:312:LEU:HD22	1.82	0.61
1:C:258:GLN:HE21	1:D:129:SER:HB3	1.64	0.60
1:C:19:GLY:O	1:C:23:ALA:HB3	2.01	0.60
1:D:1:MET:HE3	1:F:150:LYS:HE2	1.81	0.60
1:C:326:VAL:HG23	1:C:344:ASN:ND2	2.15	0.60
4:D:590:HOH:O	1:F:116:HIS:HD2	1.83	0.60
1:H:281:HIS:HE1	4:H:577:HOH:O	1.83	0.60
1:C:336:HIS:HD2	4:C:616:HOH:O	1.84	0.60
1:F:351:LEU:HB3	1:F:363:GLN:HE22	1.67	0.60
1:G:233:VAL:HG11	1:G:265:GLU:HG2	1.85	0.59
1:G:78:ASN:O	1:G:79:ARG:HB2	2.01	0.59
1:B:167:GLU:OE2	1:B:378:ARG:HD3	2.02	0.59
1:D:367:ILE:HG23	1:D:368:LEU:CD1	2.32	0.59
1:A:378:ARG:HG3	1:A:378:ARG:HH11	1.67	0.58
1:B:331:SER:HB2	1:B:335:SER:HB2	1.85	0.58
1:G:44:HIS:HE1	4:G:893:HOH:O	1.86	0.58
1:A:116:HIS:HD2	4:E:608:HOH:O	1.87	0.58
1:D:113:LYS:HE3	1:F:160:LEU:O	2.04	0.58
1:C:319:ALA:HB3	1:C:326:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ASP:OD2	1:C:150:LYS:HE2	2.03	0.58
1:F:257:PRO:HG2	1:F:258:GLN:NE2	2.19	0.57
1:H:253:GLU:OE2	1:H:281:HIS:HD2	1.86	0.57
1:B:303:VAL:HG22	1:B:312:LEU:HD22	1.86	0.57
1:D:19:GLY:O	1:D:23:ALA:HB3	2.05	0.57
1:H:351:LEU:HB3	1:H:363:GLN:NE2	2.17	0.57
1:C:257:PRO:HG2	1:C:258:GLN:NE2	2.20	0.57
1:A:281:HIS:HE1	4:A:560:HOH:O	1.88	0.57
1:F:44:HIS:HE1	4:F:684:HOH:O	1.88	0.57
1:C:319:ALA:HB3	1:C:326:VAL:CG2	2.35	0.56
1:D:331:SER:HB2	1:D:335:SER:HB2	1.87	0.56
1:D:367:ILE:HG23	1:D:368:LEU:HD13	1.87	0.56
1:A:339:VAL:HB	1:A:345:THR:HG21	1.87	0.56
1:E:316:ALA:HA	1:E:326:VAL:HG21	1.86	0.56
1:A:331:SER:HB2	1:A:335:SER:HB2	1.87	0.55
1:A:113:LYS:HE3	1:E:160:LEU:O	2.05	0.55
1:B:11:LYS:HE3	1:B:12:HIS:NE2	2.21	0.55
1:C:129:SER:CB	1:D:258:GLN:HE21	2.13	0.55
1:F:331:SER:HB2	1:F:335:SER:HB2	1.88	0.55
1:D:303:VAL:HG22	1:D:312:LEU:HD22	1.88	0.55
1:E:19:GLY:O	1:E:23:ALA:HB3	2.07	0.55
1:F:116:HIS:HE1	1:F:307:GLY:O	1.90	0.55
1:G:319:ALA:HB3	1:G:326:VAL:CG2	2.37	0.55
1:F:19:GLY:O	1:F:23:ALA:HB3	2.06	0.55
1:D:150:LYS:HE2	1:F:1:MET:HE3	1.89	0.54
1:D:171:TYR:CZ	1:D:349:GLU:HB2	2.42	0.54
1:F:79:ARG:HD2	1:F:79:ARG:N	2.23	0.54
1:H:378:ARG:HG3	1:H:378:ARG:HH11	1.71	0.54
1:B:288:PHE:CZ	1:B:301:PRO:HB3	2.43	0.54
1:B:319:ALA:CB	1:B:326:VAL:HG23	2.37	0.54
1:C:303:VAL:CG2	1:C:312:LEU:HD22	2.29	0.54
1:B:19:GLY:O	1:B:23:ALA:HB3	2.07	0.54
1:C:203:ILE:CD1	1:C:238:LYS:HE2	2.37	0.54
1:F:367:ILE:HG23	1:F:368:LEU:HD13	1.89	0.54
1:D:351:LEU:HB3	1:D:363:GLN:HE22	1.72	0.54
1:F:53:ARG:HG3	1:F:54:ASP:N	2.23	0.54
1:F:319:ALA:CB	1:F:326:VAL:HG23	2.38	0.54
1:B:113:LYS:HE3	1:G:160:LEU:O	2.07	0.53
1:B:116:HIS:HE1	1:B:307:GLY:O	1.91	0.53
1:E:257:PRO:HG2	1:E:258:GLN:NE2	2.23	0.53
1:B:336:HIS:HD2	4:B:533:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:HG2	4:C:585:HOH:O	2.08	0.53
1:G:114:LEU:O	1:G:118:GLN:HG3	2.08	0.53
1:H:75:GLU:HG3	1:H:81:THR:HG22	1.90	0.53
1:B:281:HIS:HE1	4:B:517:HOH:O	1.91	0.53
1:E:336:HIS:HD2	4:E:509:HOH:O	1.92	0.53
1:E:331:SER:HB2	1:E:335:SER:HB2	1.90	0.52
1:F:319:ALA:HB3	1:F:326:VAL:HG23	1.92	0.52
1:A:4:ILE:HG21	1:E:155:PRO:HD3	1.92	0.52
1:A:386:LYS:HB3	1:E:1:MET:HE3	1.91	0.52
1:C:251:ILE:HG12	1:C:254:CYS:SG	2.50	0.52
1:B:1:MET:HE1	1:G:387:PRO:HD2	1.93	0.51
1:D:251:ILE:HG12	1:D:254:CYS:SG	2.50	0.51
1:D:332:SER:OG	1:D:333:VAL:N	2.44	0.51
1:E:339:VAL:HB	1:E:345:THR:HG21	1.93	0.51
1:H:336:HIS:HD2	4:H:521:HOH:O	1.92	0.51
1:F:336:HIS:HD2	4:F:548:HOH:O	1.93	0.51
1:D:339:VAL:HB	1:D:345:THR:HG21	1.93	0.51
1:H:335:SER:O	1:H:339:VAL:HG22	2.11	0.51
1:H:47:THR:HB	1:H:48:PRO:HD2	1.92	0.51
1:B:319:ALA:HB3	1:B:326:VAL:HG23	1.93	0.51
1:F:244:ALA:N	1:F:245:PRO:HD2	2.26	0.50
1:B:257:PRO:HG2	1:B:258:GLN:NE2	2.27	0.50
1:E:281:HIS:HE1	4:E:579:HOH:O	1.93	0.50
1:D:1:MET:CE	1:F:150:LYS:HE2	2.42	0.50
1:E:116:HIS:HE1	1:E:307:GLY:O	1.95	0.50
1:H:212:ASP:OD1	1:H:216:LYS:NZ	2.45	0.50
1:H:19:GLY:O	1:H:23:ALA:HB3	2.12	0.49
1:B:160:LEU:O	1:G:113:LYS:HE3	2.12	0.49
1:C:17:PHE:HE1	1:C:23:ALA:HB2	1.77	0.49
1:F:103:PHE:O	1:F:107:LYS:NZ	2.45	0.49
1:C:288:PHE:CZ	1:C:301:PRO:HB3	2.47	0.49
1:F:393:LEU:HD23	1:F:395:ARG:HH11	1.77	0.49
1:G:129:SER:CB	1:H:258:GLN:HE21	2.10	0.49
1:A:49:MET:CE	1:B:121:GLY:HA3	2.42	0.49
1:G:339:VAL:HB	1:G:345:THR:HG21	1.94	0.49
1:H:257:PRO:HG2	1:H:258:GLN:NE2	2.28	0.49
1:E:204:ARG:HG3	4:E:590:HOH:O	2.12	0.49
1:G:288:PHE:CZ	1:G:301:PRO:HB3	2.48	0.49
1:H:71:ILE:HD12	1:H:71:ILE:N	2.27	0.49
1:H:367:ILE:HG23	1:H:368:LEU:CD1	2.40	0.49
1:C:368:LEU:HG	1:C:391:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:PRO:HG2	1:F:258:GLN:HE22	1.78	0.49
1:G:19:GLY:O	1:G:23:ALA:HB3	2.13	0.49
1:H:111:ASP:O	1:H:115:ILE:HG13	2.13	0.49
1:C:78:ASN:O	1:C:79:ARG:HB2	2.12	0.48
1:C:146:ASP:O	1:C:150:LYS:HG3	2.12	0.48
1:G:395:ARG:HG2	1:G:395:ARG:HH11	1.78	0.48
1:B:339:VAL:HB	1:B:345:THR:HG21	1.95	0.48
1:C:81:THR:O	1:C:150:LYS:HD2	2.13	0.48
1:F:281:HIS:HE1	4:F:579:HOH:O	1.95	0.48
1:G:264:ARG:O	1:G:268:ARG:HG3	2.13	0.48
1:F:167:GLU:OE2	1:F:378:ARG:HD3	2.13	0.48
1:D:70:LEU:HB2	1:D:88:ALA:HB3	1.96	0.48
1:A:191:PRO:HB3	4:A:688:HOH:O	2.13	0.48
1:A:203:ILE:CD1	1:A:238:LYS:HE2	2.44	0.48
1:D:316:ALA:HA	1:D:326:VAL:HG21	1.95	0.48
1:B:177:PRO:HB3	1:B:188:GLY:HA3	1.96	0.48
1:B:203:ILE:HD13	1:B:238:LYS:HB3	1.95	0.47
1:E:288:PHE:CZ	1:E:301:PRO:HB3	2.48	0.47
1:E:378:ARG:HH11	1:E:378:ARG:HG3	1.79	0.47
1:H:362:PRO:HB2	1:H:365:ASP:HB2	1.96	0.47
1:C:25:LYS:HD3	1:C:25:LYS:C	2.34	0.47
1:D:257:PRO:HG2	1:D:258:GLN:NE2	2.29	0.47
1:G:9:LYS:HE3	4:G:925:HOH:O	2.13	0.47
1:B:179:LEU:O	1:B:182:GLU:HB2	2.15	0.47
1:F:21:ALA:HB2	1:F:66:VAL:HG13	1.95	0.47
1:G:268:ARG:HB3	1:G:268:ARG:HH11	1.78	0.47
1:H:116:HIS:HE1	1:H:307:GLY:O	1.98	0.47
1:C:160:LEU:O	1:H:113:LYS:HE3	2.15	0.47
1:D:25:LYS:HE2	4:D:599:HOH:O	2.14	0.47
1:F:288:PHE:CZ	1:F:301:PRO:HB3	2.50	0.47
1:C:281:HIS:HE1	4:C:512:HOH:O	1.97	0.47
1:F:279:GLY:HA2	1:F:282:HIS:HD2	1.79	0.47
1:C:110:SER:O	1:H:162:GLY:HA3	2.14	0.47
1:C:113:LYS:HE3	1:H:160:LEU:O	2.14	0.47
1:E:291:LEU:HG	1:E:296:ILE:HD11	1.97	0.47
1:D:244:ALA:N	1:D:245:PRO:CD	2.78	0.47
1:D:288:PHE:CZ	1:D:301:PRO:HB3	2.50	0.47
1:B:378:ARG:HG3	1:B:378:ARG:HH11	1.80	0.47
1:E:251:ILE:HG12	1:E:254:CYS:SG	2.55	0.47
1:A:303:VAL:HG22	1:A:312:LEU:HD22	1.96	0.46
1:C:14:ARG:HB3	1:C:401:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:HIS:HE1	1:C:307:GLY:O	1.98	0.46
1:F:203:ILE:HD13	1:F:238:LYS:HB3	1.97	0.46
1:C:387:PRO:O	1:H:1:MET:HE1	2.16	0.46
1:F:253:GLU:OE2	1:F:281:HIS:CD2	2.61	0.46
1:D:289:ARG:C	1:D:289:ARG:HD3	2.36	0.46
1:F:171:TYR:CZ	1:F:349:GLU:HB2	2.50	0.46
1:F:279:GLY:HA2	1:F:282:HIS:CD2	2.50	0.46
1:C:115:ILE:O	1:C:119:MET:HG3	2.15	0.46
1:F:78:ASN:O	1:F:79:ARG:HB2	2.15	0.46
1:C:331:SER:HB2	1:C:335:SER:HB2	1.98	0.46
1:E:19:GLY:HA2	1:E:24:GLU:O	2.16	0.46
1:E:244:ALA:HB3	1:E:245:PRO:HD3	1.98	0.46
1:E:319:ALA:HB3	1:E:326:VAL:HG23	1.96	0.46
1:F:378:ARG:HG3	1:F:378:ARG:HH11	1.81	0.46
1:G:367:ILE:HG23	1:G:368:LEU:CD1	2.39	0.46
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.80	0.46
1:D:167:GLU:OE2	1:D:378:ARG:HD3	2.15	0.46
1:E:351:LEU:HB3	1:E:363:GLN:HE22	1.81	0.46
1:B:115:ILE:O	1:B:119:MET:HG3	2.16	0.46
1:E:282:HIS:CD2	4:E:505:HOH:O	2.68	0.46
1:E:335:SER:O	1:E:339:VAL:HG22	2.16	0.45
1:E:394:ASN:OD1	1:E:396:ASP:HB2	2.16	0.45
1:F:17:PHE:HA	1:F:69:THR:O	2.16	0.45
1:G:378:ARG:HG3	1:G:378:ARG:HH11	1.81	0.45
1:A:378:ARG:HG3	1:A:378:ARG:NH1	2.30	0.45
1:A:11:LYS:HB2	1:A:77:GLU:HG2	1.98	0.45
1:D:150:LYS:HE2	1:F:1:MET:CE	2.46	0.45
1:H:378:ARG:HG3	1:H:378:ARG:NH1	2.31	0.45
1:E:244:ALA:N	1:E:245:PRO:CD	2.80	0.45
1:H:78:ASN:O	1:H:79:ARG:HB2	2.17	0.45
1:B:78:ASN:O	1:B:79:ARG:HB2	2.17	0.45
1:B:372:PRO:HG2	4:B:593:HOH:O	2.15	0.45
1:D:375:VAL:O	1:D:376:ASN:HB3	2.17	0.45
1:G:116:HIS:HE1	1:G:307:GLY:O	1.99	0.45
1:A:282:HIS:HD2	4:A:532:HOH:O	2.00	0.45
1:G:303:VAL:CG2	1:G:312:LEU:HD22	2.39	0.45
1:A:196:PRO:HA	1:A:235:TYR:CD1	2.52	0.44
1:B:15:ALA:O	1:B:401:ARG:HD2	2.16	0.44
1:C:14:ARG:HB3	1:C:401:ARG:HH12	1.82	0.44
1:F:258:GLN:H	1:F:258:GLN:CD	2.20	0.44
1:H:364:PHE:O	1:H:367:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLY:O	1:E:1:MET:HE1	2.17	0.44
1:D:203:ILE:HD13	1:D:238:LYS:HB3	1.99	0.44
1:E:196:PRO:HA	1:E:235:TYR:CD1	2.52	0.44
1:G:25:LYS:HE3	1:G:60:GLN:OE1	2.17	0.44
1:D:253:GLU:OE2	1:D:281:HIS:CD2	2.64	0.44
1:E:251:ILE:HG23	1:E:251:ILE:O	2.17	0.44
1:H:289:ARG:HA	1:H:318:LEU:HD21	2.00	0.44
1:H:382:SER:HA	1:H:385:ASP:OD2	2.18	0.44
1:G:395:ARG:HG2	1:G:395:ARG:NH1	2.32	0.44
1:H:171:TYR:CZ	1:H:349:GLU:HB2	2.52	0.44
1:G:19:GLY:C	1:G:23:ALA:HB3	2.39	0.44
1:E:258:GLN:CD	1:E:258:GLN:H	2.21	0.43
1:E:282:HIS:HD2	4:E:505:HOH:O	2.00	0.43
1:F:330:GLY:O	1:F:331:SER:HB2	2.18	0.43
1:H:302:ASP:HB3	1:H:305:TRP:HB2	2.00	0.43
1:H:251:ILE:HG23	1:H:251:ILE:O	2.18	0.43
1:A:19:GLY:O	1:A:23:ALA:HB3	2.18	0.43
1:A:372:PRO:HG2	4:A:657:HOH:O	2.17	0.43
1:B:316:ALA:HA	1:B:326:VAL:HG21	2.00	0.43
1:C:203:ILE:HD13	1:C:238:LYS:HE2	2.00	0.43
1:D:340:ILE:HD11	1:D:381:LYS:HB3	1.99	0.43
1:G:95:ILE:HB	1:G:136:THR:HG21	2.00	0.43
1:G:171:TYR:CZ	1:G:349:GLU:HB2	2.54	0.43
1:H:179:LEU:O	1:H:182:GLU:HG2	2.19	0.43
1:A:365:ASP:HA	1:A:366:PRO:HA	1.82	0.43
1:A:394:ASN:OD1	1:A:396:ASP:HB2	2.18	0.43
1:C:171:TYR:CZ	1:C:349:GLU:HB2	2.54	0.43
1:E:114:LEU:O	1:E:118:GLN:HG3	2.18	0.43
1:G:319:ALA:CB	1:G:326:VAL:HG22	2.49	0.43
1:C:47:THR:HB	1:C:48:PRO:HD2	2.01	0.43
1:G:53:ARG:NH2	4:G:971:HOH:O	2.51	0.43
1:G:328:PRO:HG3	1:G:339:VAL:CG1	2.49	0.43
1:G:365:ASP:HA	1:G:366:PRO:HA	1.85	0.43
1:G:258:GLN:HE21	1:H:129:SER:CB	2.14	0.43
1:H:394:ASN:OD1	1:H:396:ASP:HB2	2.18	0.43
1:A:319:ALA:HB3	1:A:326:VAL:HG23	2.00	0.43
1:C:1:MET:HE1	1:H:387:PRO:HD2	2.01	0.43
1:D:378:ARG:HG3	1:D:378:ARG:HH11	1.83	0.43
1:A:282:HIS:CD2	4:A:532:HOH:O	2.71	0.42
1:F:203:ILE:CD1	1:F:238:LYS:HE2	2.49	0.42
1:G:244:ALA:N	1:G:245:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:GLN:HA	1:H:64:ILE:HG22	2.01	0.42
1:H:115:ILE:O	1:H:119:MET:HG3	2.19	0.42
1:B:394:ASN:OD1	1:B:396:ASP:HB2	2.19	0.42
1:C:146:ASP:CG	1:C:150:LYS:HE2	2.40	0.42
1:D:116:HIS:HE1	1:D:307:GLY:O	2.02	0.42
1:G:9:LYS:HD3	1:G:108:CYS:HA	2.01	0.42
1:E:24:GLU:HB3	4:E:664:HOH:O	2.19	0.42
1:E:257:PRO:HG2	1:E:258:GLN:HE22	1.84	0.42
1:F:400:LYS:HE2	4:F:727:HOH:O	2.19	0.42
1:G:97:GLU:OE1	1:G:404:SER:HA	2.18	0.42
1:H:288:PHE:CZ	1:H:301:PRO:HB3	2.55	0.42
1:A:268:ARG:HB3	1:A:268:ARG:CZ	2.49	0.42
1:E:170:PHE:O	1:E:186:ILE:HG12	2.19	0.42
1:F:181:LYS:HE3	1:F:217:CYS:O	2.19	0.42
1:G:282:HIS:HD2	4:G:735:HOH:O	2.01	0.42
1:B:212:ASP:OD1	1:B:216:LYS:NZ	2.52	0.42
1:C:44:HIS:HD2	1:C:193:HIS:O	2.02	0.42
1:G:44:HIS:O	1:G:44:HIS:CD2	2.72	0.42
1:D:40:TRP:CG	1:D:41:ILE:N	2.87	0.42
1:E:15:ALA:O	1:E:401:ARG:HD2	2.20	0.42
1:E:370:ASP:OD2	1:E:386:LYS:NZ	2.53	0.42
1:A:244:ALA:N	1:A:245:PRO:CD	2.83	0.42
1:C:60:GLN:HA	1:C:64:ILE:HG22	2.02	0.42
1:C:257:PRO:HG2	1:C:258:GLN:HE22	1.82	0.42
1:C:382:SER:HA	1:C:385:ASP:OD2	2.20	0.42
1:G:281:HIS:HE1	4:G:777:HOH:O	2.02	0.42
1:A:330:GLY:O	1:A:331:SER:HB2	2.20	0.42
1:H:244:ALA:N	1:H:245:PRO:CD	2.83	0.42
1:B:251:ILE:O	1:B:251:ILE:HG23	2.20	0.42
1:D:67:LEU:O	1:D:89:GLY:HA3	2.19	0.42
1:E:78:ASN:O	1:E:79:ARG:HB2	2.19	0.42
1:E:258:GLN:HE21	1:F:129:SER:CB	2.18	0.42
1:G:328:PRO:HG3	1:G:339:VAL:HG11	2.01	0.42
1:E:340:ILE:HD11	1:E:381:LYS:HB3	2.02	0.42
1:A:212:ASP:OD1	1:A:216:LYS:HE3	2.20	0.41
1:A:251:ILE:HG12	1:A:254:CYS:SG	2.59	0.41
1:A:49:MET:HE3	1:B:121:GLY:HA3	2.02	0.41
1:F:319:ALA:CB	1:F:326:VAL:CG2	2.98	0.41
1:G:335:SER:O	1:G:339:VAL:HG22	2.20	0.41
1:G:336:HIS:CE1	4:G:823:HOH:O	2.73	0.41
1:H:196:PRO:HA	1:H:235:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ALA:CB	1:A:326:VAL:HG23	2.50	0.41
1:D:44:HIS:HE1	4:D:653:HOH:O	2.02	0.41
1:D:289:ARG:O	1:D:293:GLU:HG3	2.19	0.41
1:G:253:GLU:OE2	1:G:281:HIS:CD2	2.63	0.41
1:A:115:ILE:O	1:A:119:MET:HG3	2.20	0.41
1:E:279:GLY:HA2	1:E:282:HIS:CD2	2.54	0.41
1:A:149:GLY:HA2	1:A:159:LEU:HD11	2.01	0.41
1:B:253:GLU:OE2	1:B:281:HIS:CD2	2.69	0.41
1:C:351:LEU:HB3	1:C:363:GLN:NE2	2.29	0.41
1:B:53:ARG:NH2	1:B:56:GLU:OE1	2.54	0.41
1:D:44:HIS:CD2	1:D:193:HIS:O	2.72	0.41
1:F:87:THR:O	1:F:88:ALA:HB2	2.19	0.41
1:H:281:HIS:CE1	4:H:577:HOH:O	2.65	0.41
1:C:149:GLY:HA2	1:C:159:LEU:HD11	2.02	0.41
1:H:282:HIS:CD2	4:H:518:HOH:O	2.73	0.41
1:A:15:ALA:O	1:A:401:ARG:HD2	2.21	0.41
1:C:270:ALA:HA	1:C:271:PRO:HD3	1.96	0.41
1:D:219:PRO:HG2	1:D:220:ASP:OD1	2.21	0.41
1:G:258:GLN:H	1:G:258:GLN:CD	2.24	0.41
1:H:372:PRO:HG2	4:H:641:HOH:O	2.20	0.41
1:A:268:ARG:CB	1:A:268:ARG:NH1	2.84	0.41
1:D:170:PHE:O	1:D:186:ILE:HG12	2.20	0.40
1:H:10:ILE:HD13	1:H:109:VAL:HG12	2.03	0.40
1:G:319:ALA:CB	1:G:326:VAL:CG2	2.99	0.40
1:H:114:LEU:O	1:H:118:GLN:HG3	2.21	0.40
1:F:289:ARG:HD3	1:F:289:ARG:C	2.41	0.40
1:B:289:ARG:HA	1:B:318:LEU:HD21	2.04	0.40
1:C:114:LEU:O	1:C:118:GLN:HG3	2.21	0.40
1:C:253:GLU:OE2	1:C:281:HIS:CD2	2.70	0.40
1:F:13:VAL:O	1:F:13:VAL:HG13	2.21	0.40
1:G:289:ARG:HA	1:G:318:LEU:HD21	2.02	0.40
1:B:40:TRP:CG	1:B:41:ILE:N	2.90	0.40
1:B:367:ILE:HG23	1:B:368:LEU:CD1	2.44	0.40
1:F:44:HIS:HD2	1:F:193:HIS:O	2.05	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	403/405 (100%)	391 (97%)	11 (3%)	1 (0%)	47	33
1	B	403/405 (100%)	384 (95%)	18 (4%)	1 (0%)	47	33
1	C	403/405 (100%)	389 (96%)	13 (3%)	1 (0%)	47	33
1	D	403/405 (100%)	383 (95%)	19 (5%)	1 (0%)	47	33
1	E	403/405 (100%)	385 (96%)	17 (4%)	1 (0%)	47	33
1	F	403/405 (100%)	386 (96%)	16 (4%)	1 (0%)	47	33
1	G	403/405 (100%)	390 (97%)	12 (3%)	1 (0%)	47	33
1	H	403/405 (100%)	383 (95%)	19 (5%)	1 (0%)	47	33
All	All	3224/3240 (100%)	3091 (96%)	125 (4%)	8 (0%)	47	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	88	ALA
1	A	88	ALA
1	B	88	ALA
1	C	88	ALA
1	G	88	ALA
1	H	88	ALA
1	D	88	ALA
1	E	88	ALA

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	333/333 (100%)	330 (99%)	3 (1%)	78	75
1	B	333/333 (100%)	328 (98%)	5 (2%)	65	56
1	C	333/333 (100%)	326 (98%)	7 (2%)	53	42
1	D	333/333 (100%)	330 (99%)	3 (1%)	78	75
1	E	333/333 (100%)	329 (99%)	4 (1%)	71	65
1	F	333/333 (100%)	326 (98%)	7 (2%)	53	42
1	G	333/333 (100%)	324 (97%)	9 (3%)	44	31
1	H	333/333 (100%)	329 (99%)	4 (1%)	71	65
All	All	2664/2664 (100%)	2622 (98%)	42 (2%)	62	54

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	TRP
1	A	289	ARG
1	A	366	PRO
1	B	224	MET
1	B	228	TRP
1	B	289	ARG
1	B	366	PRO
1	B	370	ASP
1	C	25	LYS
1	C	38	ASN
1	C	224	MET
1	C	228	TRP
1	C	256	PRO
1	C	289	ARG
1	C	366	PRO
1	D	228	TRP
1	D	289	ARG
1	D	366	PRO
1	E	18	ILE
1	E	228	TRP
1	E	289	ARG
1	E	366	PRO
1	F	1	MET
1	F	2	GLU
1	F	80	GLN
1	F	157	TYR
1	F	228	TRP

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Mol	Chain	Res	Type
1	F	289	ARG
1	F	366	PRO
1	G	53	ARG
1	G	79	ARG
1	G	157	TYR
1	G	224	MET
1	G	228	TRP
1	G	289	ARG
1	G	366	PRO
1	G	370	ASP
1	G	396	ASP
1	H	2	GLU
1	H	228	TRP
1	H	289	ARG
1	H	366	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	116	HIS
1	A	281	HIS
1	A	282	HIS
1	A	336	HIS
1	B	44	HIS
1	B	116	HIS
1	B	169	GLN
1	B	193	HIS
1	B	258	GLN
1	B	269	ASN
1	B	281	HIS
1	B	282	HIS
1	B	336	HIS
1	C	44	HIS
1	C	116	HIS
1	C	258	GLN
1	C	281	HIS
1	C	282	HIS
1	C	336	HIS
1	D	44	HIS
1	D	116	HIS
1	D	258	GLN

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Mol	Chain	Res	Type
1	D	281	HIS
1	D	282	HIS
1	D	336	HIS
1	E	44	HIS
1	E	116	HIS
1	E	234	ASN
1	E	258	GLN
1	E	281	HIS
1	E	282	HIS
1	E	336	HIS
1	F	44	HIS
1	F	116	HIS
1	F	258	GLN
1	F	281	HIS
1	F	282	HIS
1	F	336	HIS
1	G	44	HIS
1	G	234	ASN
1	G	258	GLN
1	G	269	ASN
1	G	281	HIS
1	G	282	HIS
1	G	336	HIS
1	H	44	HIS
1	H	116	HIS
1	H	258	GLN
1	H	281	HIS
1	H	282	HIS
1	H	336	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MLT	D	502	2	8,8,8	1.01	1 (12%)	10,10,10	1.47	1 (10%)
3	MLT	G	502	2	8,8,8	1.01	1 (12%)	10,10,10	1.38	1 (10%)
3	MLT	H	502	2	8,8,8	0.96	1 (12%)	10,10,10	1.46	1 (10%)
3	MLT	A	502	2	8,8,8	0.99	1 (12%)	10,10,10	1.43	1 (10%)
3	MLT	B	502	2	8,8,8	0.97	1 (12%)	10,10,10	1.46	1 (10%)
3	MLT	F	502	2	8,8,8	0.98	1 (12%)	10,10,10	1.44	1 (10%)
3	MLT	E	502	2	8,8,8	1.02	1 (12%)	10,10,10	1.43	1 (10%)
3	MLT	C	502	2	8,8,8	0.93	1 (12%)	10,10,10	1.46	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLT	D	502	2	-	2/8/8/8	-
3	MLT	G	502	2	-	0/8/8/8	-
3	MLT	H	502	2	-	1/8/8/8	-
3	MLT	A	502	2	-	1/8/8/8	-
3	MLT	B	502	2	-	0/8/8/8	-
3	MLT	F	502	2	-	0/8/8/8	-
3	MLT	E	502	2	-	2/8/8/8	-
3	MLT	C	502	2	-	0/8/8/8	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	MLT	O2-C1	-2.47	1.22	1.30
3	E	502	MLT	O2-C1	-2.40	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	502	MLT	O2-C1	-2.38	1.22	1.30
3	D	502	MLT	O2-C1	-2.37	1.22	1.30
3	F	502	MLT	O2-C1	-2.36	1.22	1.30
3	B	502	MLT	O2-C1	-2.35	1.22	1.30
3	C	502	MLT	O2-C1	-2.26	1.23	1.30
3	H	502	MLT	O2-C1	-2.19	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	MLT	O2-C1-C2	3.29	119.95	112.72
3	D	502	MLT	O2-C1-C2	3.29	119.95	112.72
3	B	502	MLT	O2-C1-C2	3.24	119.83	112.72
3	H	502	MLT	O2-C1-C2	3.23	119.83	112.72
3	F	502	MLT	O2-C1-C2	3.23	119.82	112.72
3	E	502	MLT	O2-C1-C2	3.21	119.77	112.72
3	A	502	MLT	O2-C1-C2	3.17	119.68	112.72
3	G	502	MLT	O2-C1-C2	3.03	119.37	112.72

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	502	MLT	C1-C2-C3-C4
3	A	502	MLT	C1-C2-C3-C4
3	D	502	MLT	C1-C2-C3-C4
3	H	502	MLT	C1-C2-C3-C4
3	E	502	MLT	O3-C2-C3-C4
3	D	502	MLT	O3-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	405/405 (100%)	-0.45	1 (0%)	95	93	9, 16, 30, 45	0
1	B	405/405 (100%)	-0.20	9 (2%)	62	57	10, 20, 32, 45	0
1	C	405/405 (100%)	-0.29	7 (1%)	70	66	10, 19, 32, 44	0
1	D	405/405 (100%)	-0.12	4 (0%)	82	80	14, 22, 33, 44	0
1	E	405/405 (100%)	-0.07	6 (1%)	73	70	12, 21, 32, 42	0
1	F	405/405 (100%)	-0.24	4 (0%)	82	80	9, 19, 32, 45	0
1	G	405/405 (100%)	-0.30	5 (1%)	79	76	9, 19, 32, 44	0
1	H	405/405 (100%)	-0.03	11 (2%)	54	49	14, 23, 34, 44	0
All	All	3240/3240 (100%)	-0.21	47 (1%)	73	70	9, 20, 32, 45	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	38	ASN	4.4
1	H	37	GLY	4.0
1	H	1	MET	3.9
1	C	24	GLU	3.5
1	E	53	ARG	3.5
1	H	53	ARG	3.3
1	D	38	ASN	3.2
1	E	38	ASN	3.2
1	C	1	MET	3.1
1	C	32	TYR	3.1
1	B	24	GLU	3.1
1	G	12	HIS	3.0
1	B	2	GLU	3.0
1	H	24	GLU	2.9
1	F	1	MET	2.9
1	F	24	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	38	ASN	2.8
1	B	53	ARG	2.8
1	B	1	MET	2.6
1	F	53	ARG	2.5
1	H	79	ARG	2.5
1	H	395	ARG	2.5
1	E	24	GLU	2.5
1	C	27	ALA	2.5
1	H	396	ASP	2.5
1	D	370	ASP	2.5
1	G	53	ARG	2.5
1	E	79	ARG	2.4
1	G	38	ASN	2.4
1	D	53	ARG	2.4
1	B	79	ARG	2.4
1	B	182	GLU	2.4
1	G	24	GLU	2.4
1	H	215	GLU	2.4
1	E	215	GLU	2.3
1	C	398	HIS	2.2
1	H	398	HIS	2.2
1	B	398	HIS	2.1
1	E	129	SER	2.1
1	A	129	SER	2.1
1	G	398	HIS	2.1
1	F	3	ASN	2.1
1	H	376	ASN	2.1
1	C	396	ASP	2.0
1	B	268	ARG	2.0
1	B	326	VAL	2.0
1	D	36	GLY	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, 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(Å^2)	Q<0.9
3	MLT	E	502	9/9	0.88	0.10	26,27,29,30	0
2	MG	D	501	1/1	0.91	0.08	18,18,18,18	0
3	MLT	H	502	9/9	0.91	0.08	26,27,29,29	0
2	MG	F	501	1/1	0.92	0.07	14,14,14,14	0
3	MLT	F	502	9/9	0.92	0.10	18,21,26,28	0
3	MLT	G	502	9/9	0.92	0.09	16,21,28,30	0
2	MG	H	501	1/1	0.92	0.05	22,22,22,22	0
2	MG	C	501	1/1	0.94	0.07	15,15,15,15	0
2	MG	E	501	1/1	0.94	0.05	20,20,20,20	0
3	MLT	C	502	9/9	0.94	0.10	16,19,25,26	0
3	MLT	D	502	9/9	0.94	0.08	26,28,32,33	0
3	MLT	B	502	9/9	0.95	0.10	21,24,28,28	0
3	MLT	A	502	9/9	0.97	0.07	12,16,22,23	0
2	MG	G	501	1/1	0.97	0.04	15,15,15,15	0
2	MG	B	501	1/1	0.98	0.04	17,17,17,17	0
2	MG	A	501	1/1	1.00	0.04	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.