Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:09 AM GMT

PDB ID	:	1ZXV
Title	:	X-Ray Crystal Structure of the Anthrax Lethal Factor Bound to a Small Molecule Inhibitor, BI-MFM3, 3-{5-[5-(4-Chloro-phenyl)-furan-2-ylmethylene]-4-oxo-2-thioxo-thiazolidin-3-yl}-propionic acid.
Authors	:	Wong, T.Y.; Liddington, R.C.
Deposited on	:	2005-06-08
Resolution	:	2.67 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:

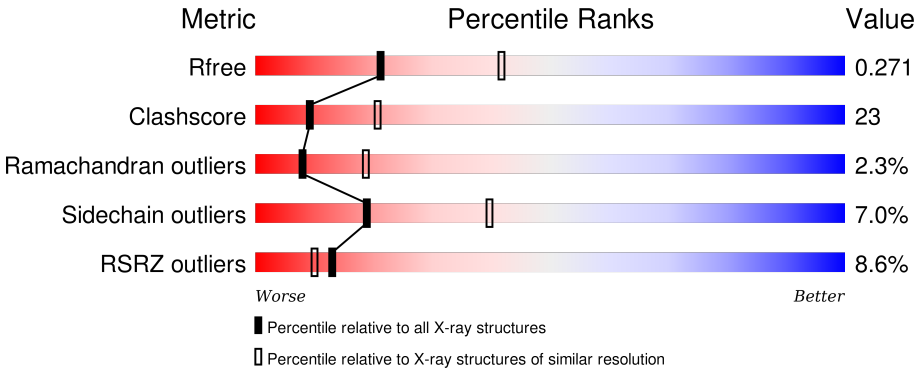
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.67 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}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	776	9% 50% 38% 5% 6%
1	B	776	7% 56% 35% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MFM	A	9002	-	-	-	X
3	MFM	B	9003	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12088 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.

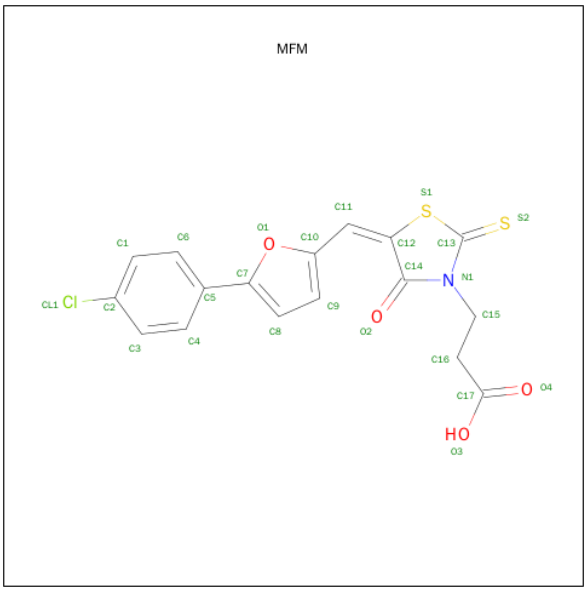
- Molecule 1 is a protein called lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5988	3809	1007	1165	7			
1	B	736	Total	C	N	O	S	0	0	0
			6048	3841	1019	1181	7			

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

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

- Molecule 3 is (E)-3-(5((5-(4-CHLOROPHENYL)FURAN-2-YL)METHYLENE)-4-OXO-2 -THIOXOTHIAZOLIDIN-3-YL)PROPANOIC ACID (three-letter code: MFM) (formula: $C_{17}H_{12}ClNO_4S_2$).



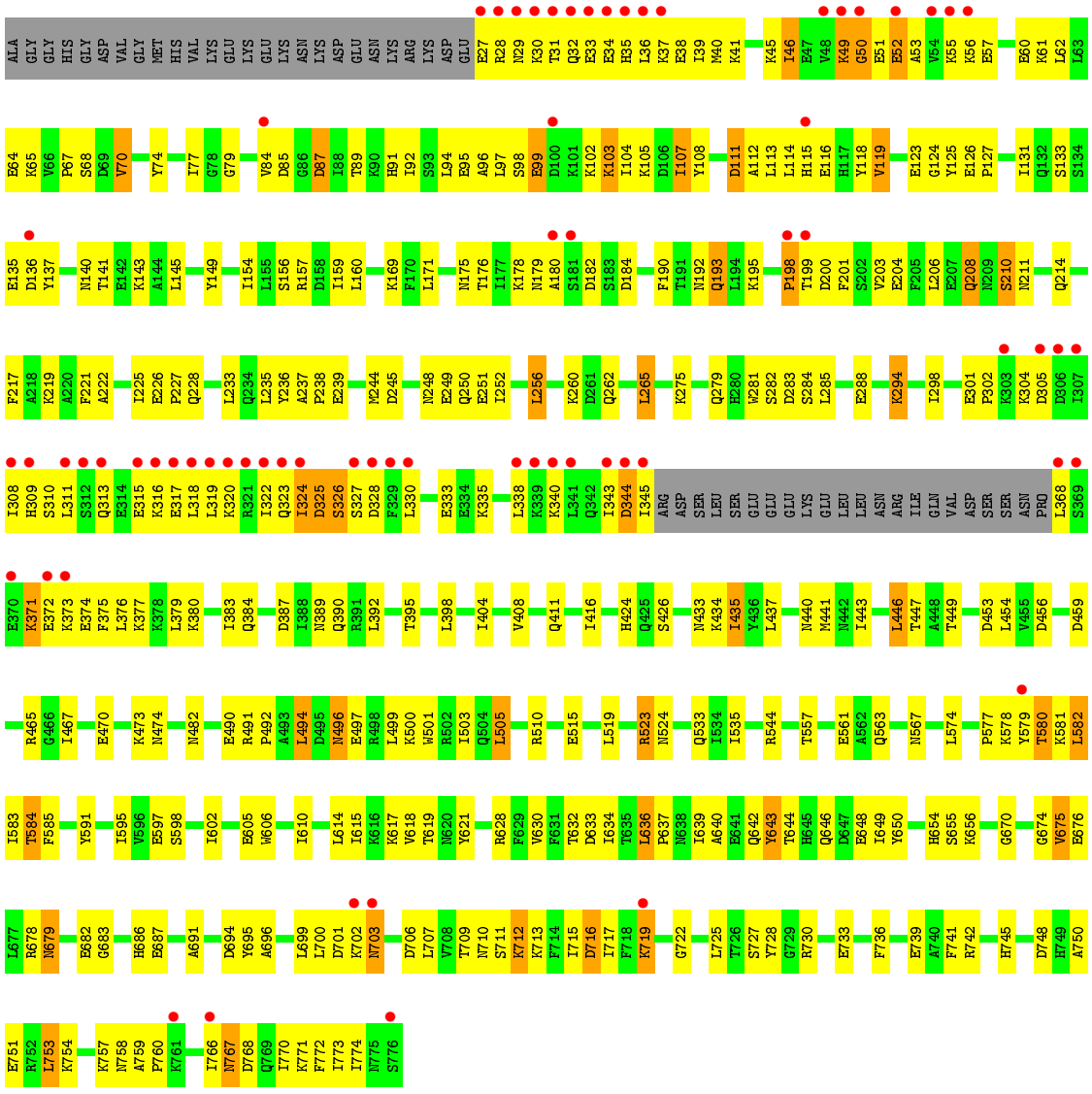
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			25	17	1	1	4	2		
3	B	1	Total	C	Cl	N	O	S	0	0
			25	17	1	1	4	2		

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.

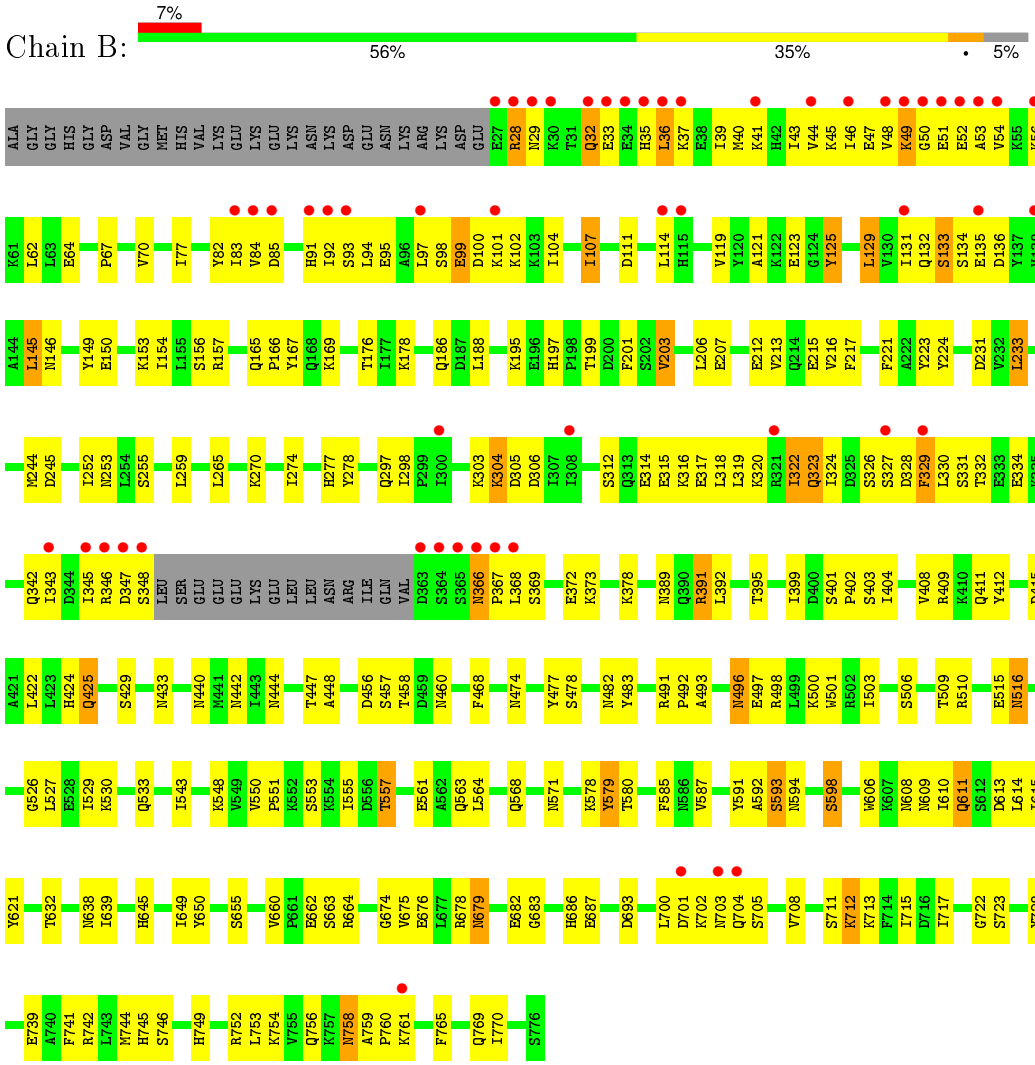
- Molecule 1: lethal factor

Chain A:



- Molecule 1: lethal factor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.96Å 136.65Å 97.90Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	49.00 – 2.67 45.90 – 2.67	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.00-2.67) 92.0 (45.90-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.272 0.231 , 0.271	Depositor DCC
R_{free} test set	3306 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.5	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 70887 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12088	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, MFM

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	0.38	0/6095	0.63	0/8208
1	B	0.40	0/6156	0.64	0/8291
All	All	0.39	0/12251	0.64	0/16499

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	5988	0	5977	307	0
1	B	6048	0	6026	241	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	11	5	0
3	B	25	0	11	4	0
All	All	12088	0	12025	553	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 23.

All (553) 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:B:483:TYR:HB3	1:B:520:ILE:HD11	1.29	1.15
1:B:121:ALA:HB1	1:B:154:ILE:HD11	1.31	1.11
1:A:446:LEU:HD12	1:A:591:TYR:HB2	1.34	1.08
1:A:34:GLU:HA	1:A:37:LYS:HD3	1.36	1.04
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.42	1.01
1:A:435:ILE:H	1:A:435:ILE:HD12	1.29	0.98
1:B:712:LYS:HD2	1:B:712:LYS:H	1.29	0.96
1:A:434:LYS:HB3	1:A:434:LYS:NZ	1.80	0.96
1:A:581:LYS:HD3	1:A:628:ARG:HH21	1.28	0.96
1:A:104:ILE:HG22	1:A:105:LYS:H	1.33	0.93
1:A:712:LYS:H	1:A:712:LYS:HD3	1.30	0.93
1:B:104:ILE:HD13	1:B:114:LEU:CD2	1.97	0.93
1:A:434:LYS:HZ2	1:A:434:LYS:HB3	1.30	0.92
3:B:9003:MFM:H9	3:B:9003:MFM:O2	1.69	0.92
1:A:102:LYS:HA	1:A:114:LEU:HD12	1.53	0.91
1:A:298:ILE:O	1:A:298:ILE:HD12	1.70	0.91
1:A:32:GLN:HE22	1:A:68:SER:HB2	1.34	0.91
1:B:510:ARG:H	1:B:522:GLN:HE21	0.90	0.90
1:B:510:ARG:H	1:B:522:GLN:NE2	1.69	0.90
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.53	0.90
1:A:301:GLU:HG3	1:A:302:PRO:HD2	1.51	0.90
3:A:9002:MFM:O2	3:A:9002:MFM:H9	1.72	0.90
1:A:563:GLN:NE2	1:A:585:PHE:H	1.70	0.89
1:B:33:GLU:O	1:B:36:LEU:HB3	1.74	0.87
1:B:510:ARG:N	1:B:522:GLN:HE21	1.73	0.87
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.57	0.85
1:A:92:ILE:HD12	1:A:92:ILE:H	1.41	0.85
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.42	0.85
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.56	0.84
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.59	0.84
1:A:435:ILE:HD12	1:A:435:ILE:N	1.92	0.84
1:A:55:LYS:HD2	1:A:133:SER:HB2	1.59	0.84
1:B:483:TYR:HB3	1:B:520:ILE:CD1	2.08	0.84
1:A:70:VAL:HG12	1:A:252:ILE:HD11	1.59	0.82
1:A:649:ILE:HD12	1:A:649:ILE:H	1.45	0.82
1:B:107:ILE:HG21	1:B:145:LEU:HD13	1.59	0.82
1:B:104:ILE:HD13	1:B:114:LEU:HD21	1.61	0.82
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.62	0.81
1:A:563:GLN:HE21	1:A:585:PHE:H	1.25	0.81
1:A:30:LYS:O	1:A:34:GLU:HG3	1.81	0.81
1:B:104:ILE:HD13	1:B:114:LEU:HD23	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:HD23	1:B:345:ILE:HD12	1.64	0.80
1:B:564:LEU:O	1:B:568:GLN:HG3	1.81	0.79
1:A:728:TYR:OH	3:A:9002:MFM:H161	1.82	0.79
1:B:712:LYS:CD	1:B:712:LYS:H	1.94	0.78
1:A:31:THR:HA	1:A:34:GLU:HG3	1.65	0.78
1:A:33:GLU:O	1:A:37:LYS:HG3	1.83	0.78
1:B:483:TYR:CB	1:B:520:ILE:HD11	2.13	0.77
1:B:392:LEU:HD21	1:B:416:ILE:HD13	1.67	0.76
1:A:46:ILE:H	1:A:46:ILE:HD12	1.50	0.76
1:B:496:ASN:H	1:B:496:ASN:HD22	1.34	0.75
1:A:317:GLU:HA	1:A:320:LYS:CE	2.16	0.75
1:B:94:LEU:O	1:B:97:LEU:HG	1.87	0.75
1:B:97:LEU:HB2	1:B:102:LYS:HE3	1.66	0.75
1:B:717:ILE:HD12	1:B:761:LYS:HB3	1.68	0.75
1:B:408:VAL:HA	1:B:411:GLN:HG3	1.69	0.75
1:A:87:ASP:OD1	1:A:115:HIS:HB2	1.88	0.74
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.52	0.74
1:A:107:ILE:CD1	1:A:219:LYS:HG3	2.18	0.74
1:A:581:LYS:HD3	1:A:628:ARG:NH2	2.03	0.74
1:A:567:ASN:HD21	1:A:583:ILE:H	1.36	0.74
1:B:84:VAL:O	1:B:132:GLN:HA	1.88	0.74
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.69	0.73
1:B:712:LYS:HD2	1:B:712:LYS:N	2.04	0.73
1:B:496:ASN:N	1:B:496:ASN:HD22	1.86	0.73
1:A:210:SER:O	1:A:214:GLN:HG3	1.90	0.72
1:A:713:LYS:O	1:A:717:ILE:HG12	1.90	0.72
1:A:140:ASN:HB3	1:A:143:LYS:HZ3	1.55	0.72
1:A:577:PRO:O	1:A:580:THR:HG23	1.89	0.71
1:B:711:SER:O	1:B:715:ILE:HG13	1.90	0.71
1:B:578:LYS:O	1:B:579:TYR:HB2	1.90	0.71
1:A:325:ASP:HA	1:A:335:LYS:HE2	1.73	0.71
1:A:317:GLU:HA	1:A:320:LYS:HE2	1.71	0.71
1:B:759:ALA:N	1:B:760:PRO:HD3	2.06	0.70
1:B:322:ILE:HD13	1:B:323:GLN:N	2.06	0.70
1:B:136:ASP:HB2	1:B:143:LYS:HD2	1.73	0.70
1:A:739:GLU:CD	1:A:742:ARG:HH21	1.95	0.70
1:A:70:VAL:HG12	1:A:252:ILE:CD1	2.22	0.69
1:B:754:LYS:O	1:B:758:ASN:HB2	1.92	0.69
3:A:9002:MFM:O2	3:A:9002:MFM:C9	2.40	0.69
1:A:640:ALA:HB2	1:A:643:TYR:CZ	2.28	0.69
1:A:640:ALA:HB1	1:A:644:THR:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.20	0.68
3:B:9003:MFM:C9	3:B:9003:MFM:O2	2.40	0.68
1:B:28:ARG:CG	1:B:32:GLN:HB2	2.24	0.68
1:B:134:SER:HB3	1:B:136:ASP:OD1	1.93	0.68
1:B:332:THR:O	1:B:336:GLU:HG2	1.93	0.68
1:B:366:ASN:HB2	1:B:367:PRO:CD	2.24	0.68
1:A:411:GLN:NE2	1:A:411:GLN:HA	2.08	0.67
1:A:192:ASN:HA	1:A:195:LYS:HB2	1.76	0.67
1:B:45:LYS:HB2	1:B:82:TYR:CD2	2.29	0.67
1:B:186:GLN:HE21	1:B:195:LYS:HG2	1.60	0.66
1:A:324:ILE:HG22	1:A:335:LYS:HD3	1.78	0.66
1:A:703:ASN:ND2	1:A:703:ASN:H	1.92	0.66
1:B:496:ASN:H	1:B:496:ASN:ND2	1.92	0.66
1:A:99:GLU:OE2	1:A:102:LYS:HD2	1.96	0.66
1:A:87:ASP:OD2	1:A:115:HIS:HA	1.96	0.66
1:A:30:LYS:O	1:A:34:GLU:CG	2.43	0.66
1:A:682:GLU:OE1	1:A:742:ARG:NH1	2.25	0.66
1:A:766:ILE:O	1:A:770:ILE:HG12	1.96	0.66
1:B:693:ASP:OD2	1:B:708:VAL:HG12	1.94	0.66
1:A:389:ASN:OD1	1:A:482:ASN:HB2	1.96	0.65
1:A:27:GLU:O	1:A:29:ASN:N	2.27	0.65
1:B:331:SER:OG	1:B:334:GLU:HG3	1.96	0.65
1:B:474:ASN:O	1:B:593:SER:OG	2.13	0.65
1:A:535:ILE:HD13	1:A:544:ARG:HB2	1.79	0.65
1:A:674:GLY:O	1:A:676:GLU:N	2.30	0.65
1:A:94:LEU:HD22	1:A:97:LEU:HD11	1.78	0.65
1:B:104:ILE:CD1	1:B:114:LEU:HD23	2.27	0.65
1:A:136:ASP:HB3	1:A:140:ASN:ND2	2.12	0.64
1:A:649:ILE:HD12	1:A:649:ILE:N	2.13	0.64
1:B:571:ASN:ND2	1:B:580:THR:HB	2.13	0.64
1:A:32:GLN:HE22	1:A:68:SER:CB	2.10	0.64
1:A:317:GLU:HA	1:A:320:LYS:CG	2.28	0.63
1:A:203:VAL:HG21	1:A:465:ARG:NH2	2.14	0.63
1:A:317:GLU:HA	1:A:320:LYS:HG2	1.79	0.63
1:A:679:ASN:C	1:A:679:ASN:HD22	2.02	0.63
1:B:136:ASP:HB2	1:B:143:LYS:CD	2.29	0.63
1:B:440:ASN:HD21	1:B:500:LYS:NZ	1.97	0.63
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.33	0.63
1:B:28:ARG:HG3	1:B:32:GLN:HB2	1.81	0.62
1:B:342:GLN:O	1:B:346:ARG:HG3	1.97	0.62
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:LYS:O	1:B:717:ILE:HG12	1.99	0.62
1:A:103:LYS:HG2	1:A:112:ALA:O	1.98	0.62
1:B:733:GLU:CD	1:B:733:GLU:H	2.01	0.62
1:A:404:ILE:HD12	1:A:408:VAL:HG23	1.81	0.62
1:A:453:ASP:HB2	1:A:467:ILE:HG12	1.82	0.62
1:B:39:ILE:O	1:B:43:ILE:HG12	1.99	0.62
1:B:41:LYS:HG2	1:B:41:LYS:O	1.98	0.62
1:B:460:ASN:O	1:B:498:ARG:NH2	2.32	0.62
1:B:611:GLN:HE22	1:B:613:ASP:N	1.97	0.61
1:A:333:GLU:H	1:A:333:GLU:CD	2.01	0.61
1:A:34:GLU:HA	1:A:37:LYS:CD	2.23	0.61
1:B:51:GLU:OE2	1:B:53:ALA:HB2	2.00	0.61
1:A:171:LEU:HD21	1:A:206:LEU:HB2	1.81	0.61
1:A:712:LYS:HD3	1:A:712:LYS:N	2.08	0.61
1:B:40:MET:HA	1:B:44:VAL:HG23	1.81	0.61
1:B:169:LYS:HB2	1:B:533:GLN:NE2	2.15	0.61
1:A:281:TRP:CH2	1:A:285:LEU:HD11	2.36	0.61
1:B:683:GLY:O	1:B:687:GLU:HG2	2.01	0.61
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.31	0.61
1:B:608:ASN:C	1:B:609:ASN:HD22	2.04	0.61
1:A:434:LYS:CB	1:A:434:LYS:HZ2	2.10	0.61
1:B:312:SER:OG	1:B:315:GLU:HG3	2.00	0.61
1:A:107:ILE:HD13	1:A:219:LYS:HG3	1.82	0.60
1:B:679:ASN:HB2	1:B:682:GLU:HG3	1.83	0.60
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.82	0.60
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.34	0.60
1:B:36:LEU:HG	1:B:40:MET:HE2	1.83	0.60
1:B:516:ASN:H	1:B:516:ASN:ND2	2.00	0.60
1:B:611:GLN:HE22	1:B:613:ASP:CB	2.13	0.60
1:A:56:LYS:O	1:A:60:GLU:HG3	2.01	0.60
1:B:36:LEU:HG	1:B:40:MET:CE	2.32	0.60
1:A:157:ARG:HG3	1:A:214:GLN:HE22	1.66	0.60
1:B:571:ASN:HD21	1:B:580:THR:HB	1.68	0.59
1:B:366:ASN:HB2	1:B:367:PRO:HD3	1.85	0.59
1:A:38:GLU:O	1:A:41:LYS:HB3	2.01	0.59
1:B:303:LYS:HB2	1:B:306:ASP:OD2	2.02	0.59
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.01	0.59
1:B:530:LYS:HE3	1:B:548:LYS:HE2	1.84	0.59
1:A:426:SER:HA	1:A:510:ARG:HA	1.84	0.59
1:B:678:ARG:C	1:B:679:ASN:HD22	2.06	0.59
1:B:611:GLN:NE2	1:B:613:ASP:N	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:NE2	1:B:195:LYS:HG2	2.18	0.59
1:A:715:ILE:O	1:A:719:LYS:HE2	2.03	0.59
1:B:516:ASN:HD22	1:B:516:ASN:N	2.00	0.59
1:A:741:PHE:O	1:A:745:HIS:HD2	1.86	0.59
1:B:741:PHE:O	1:B:745:HIS:HD2	1.86	0.59
1:A:193:GLN:HE21	1:A:193:GLN:HA	1.66	0.59
1:B:49:LYS:HE2	1:B:85:ASP:OD1	2.02	0.58
1:B:304:LYS:HG2	1:B:305:ASP:H	1.68	0.58
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.38	0.58
1:B:169:LYS:HB2	1:B:533:GLN:HE21	1.67	0.58
1:A:304:LYS:HD2	1:A:344:ASP:OD2	2.03	0.58
1:B:339:LYS:O	1:B:343:ILE:HG12	2.03	0.58
1:A:107:ILE:HG21	1:A:145:LEU:HD11	1.86	0.58
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.33	0.57
1:B:28:ARG:HG2	1:B:32:GLN:HB2	1.86	0.57
1:A:31:THR:CA	1:A:34:GLU:HG3	2.34	0.57
1:B:318:LEU:O	1:B:322:ILE:HB	2.04	0.57
1:A:703:ASN:HD22	1:A:703:ASN:H	1.52	0.57
1:A:557:THR:O	1:A:561:GLU:HG3	2.04	0.57
1:A:84:VAL:HG11	1:A:91:HIS:HD2	1.68	0.57
1:B:48:VAL:HG12	1:B:85:ASP:N	2.20	0.57
1:A:584:THR:HG23	1:A:630:VAL:HG22	1.87	0.57
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.40	0.57
1:B:45:LYS:HB2	1:B:82:TYR:HD2	1.70	0.57
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.86	0.57
1:B:167:TYR:CZ	1:B:203:VAL:HG21	2.40	0.56
1:A:649:ILE:H	1:A:649:ILE:CD1	2.18	0.56
1:A:711:SER:O	1:A:715:ILE:HG13	2.05	0.56
1:A:250:GLN:HG3	1:A:251:GLU:H	1.70	0.56
1:B:674:GLY:O	1:B:676:GLU:N	2.39	0.56
1:A:113:LEU:HD12	1:A:116:GLU:OE2	2.04	0.56
1:B:57:GLU:O	1:B:60:GLU:HB3	2.05	0.56
1:A:32:GLN:NE2	1:A:68:SER:HB2	2.12	0.56
1:B:206:LEU:HD23	1:B:213:VAL:HG21	1.88	0.56
1:B:237:ALA:N	1:B:238:PRO:HD3	2.21	0.56
1:B:611:GLN:HE22	1:B:613:ASP:CA	2.19	0.56
1:A:577:PRO:HD2	1:A:580:THR:HG21	1.87	0.56
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.06	0.56
1:B:645:HIS:CD2	1:B:663:SER:HB3	2.41	0.55
1:B:769:GLN:NE2	1:B:769:GLN:HA	2.21	0.55
1:A:140:ASN:CB	1:A:143:LYS:HZ3	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LYS:O	1:A:374:GLU:HB3	2.07	0.55
1:A:107:ILE:HG22	1:A:108:TYR:CD1	2.42	0.55
1:A:496:ASN:HD22	1:A:497:GLU:N	2.04	0.55
1:B:415:ASP:O	1:B:419:ILE:HG13	2.06	0.55
1:B:47:GLU:O	1:B:84:VAL:HG23	2.06	0.55
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.07	0.55
1:B:402:PRO:O	1:B:649:ILE:HD12	2.07	0.55
1:A:95:GLU:C	1:A:97:LEU:H	2.10	0.54
1:B:516:ASN:ND2	1:B:516:ASN:N	2.56	0.54
1:B:440:ASN:HD21	1:B:500:LYS:HZ2	1.53	0.54
1:A:496:ASN:C	1:A:496:ASN:HD22	2.10	0.54
1:B:401:SER:OG	1:B:638:ASN:ND2	2.33	0.54
1:B:104:ILE:HG21	1:B:114:LEU:HD21	1.88	0.54
1:B:749:HIS:HA	1:B:752:ARG:HD3	1.87	0.54
1:A:768:ASP:O	1:A:771:LYS:HG3	2.08	0.54
1:B:129:LEU:HD22	1:B:131:ILE:HD11	1.89	0.54
1:A:679:ASN:ND2	1:A:682:GLU:H	2.06	0.54
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.42	0.54
1:B:54:VAL:O	1:B:58:ALA:HB2	2.07	0.54
1:A:27:GLU:O	1:A:27:GLU:HG3	2.08	0.54
1:B:51:GLU:HG3	1:B:53:ALA:HB3	1.89	0.54
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.37	0.54
1:B:403:SER:OG	1:B:638:ASN:ND2	2.37	0.53
1:B:129:LEU:HD22	1:B:131:ILE:CD1	2.38	0.53
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.39	0.53
1:A:379:LEU:O	1:A:383:ILE:HG12	2.08	0.53
1:B:679:ASN:N	1:B:679:ASN:HD22	2.04	0.53
1:A:683:GLY:O	1:A:687:GLU:HG2	2.09	0.53
1:A:748:ASP:OD1	1:A:750:ALA:HB3	2.08	0.53
1:B:223:TYR:HB3	1:B:233:LEU:HG	1.91	0.53
1:B:119:VAL:HG23	1:B:131:ILE:HD13	1.91	0.53
1:A:318:LEU:O	1:A:322:ILE:HG22	2.08	0.53
1:A:104:ILE:HG22	1:A:105:LYS:N	2.14	0.53
1:A:159:ILE:N	1:A:159:ILE:HD12	2.23	0.53
1:B:48:VAL:HG13	1:B:84:VAL:HA	1.90	0.53
1:A:327:SER:OG	1:A:335:LYS:HE3	2.08	0.53
1:A:753:LEU:HD12	1:A:757:LYS:HD2	1.90	0.53
1:A:89:THR:CG2	1:A:114:LEU:HB3	2.38	0.53
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.38	0.53
1:B:553:SER:O	1:B:557:THR:HG23	2.08	0.53
1:B:67:PRO:HB2	1:B:70:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD13	1:B:338:LEU:HD12	1.91	0.53
1:B:125:TYR:CD2	1:B:125:TYR:N	2.77	0.53
1:A:567:ASN:HD21	1:A:583:ILE:N	2.06	0.52
1:B:662:GLU:H	1:B:662:GLU:CD	2.10	0.52
1:A:32:GLN:O	1:A:36:LEU:HB2	2.09	0.52
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.91	0.52
1:B:563:GLN:NE2	1:B:585:PHE:H	2.08	0.52
1:A:99:GLU:O	1:A:102:LYS:HB2	2.10	0.52
1:A:310:SER:O	1:A:311:LEU:HD23	2.10	0.52
1:A:31:THR:O	1:A:35:HIS:N	2.38	0.52
1:A:640:ALA:C	1:A:642:GLN:N	2.63	0.52
1:B:129:LEU:HD13	1:B:131:ILE:HD11	1.92	0.52
1:B:252:ILE:O	1:B:255:SER:HB2	2.09	0.52
1:B:46:ILE:HG13	1:B:56:LYS:HG3	1.90	0.52
1:A:700:LEU:O	1:A:702:LYS:N	2.43	0.52
1:A:298:ILE:CD1	1:A:298:ILE:O	2.53	0.52
1:A:107:ILE:HG13	1:A:145:LEU:CD1	2.40	0.52
1:A:193:GLN:HE21	1:A:193:GLN:CA	2.22	0.52
1:B:123:GLU:HG3	1:B:157:ARG:NE	2.25	0.52
1:A:79:GLY:CA	1:A:127:PRO:HG2	2.40	0.52
1:A:67:PRO:O	1:A:70:VAL:HG13	2.10	0.51
1:A:392:LEU:HD21	1:A:416:ILE:HD13	1.92	0.51
1:B:741:PHE:O	1:B:745:HIS:CD2	2.63	0.51
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.45	0.51
1:B:759:ALA:N	1:B:760:PRO:CD	2.73	0.51
1:A:739:GLU:OE2	1:A:742:ARG:NH2	2.40	0.51
1:B:37:LYS:O	1:B:37:LYS:HG2	2.11	0.51
1:A:169:LYS:HD2	1:A:533:GLN:OE1	2.10	0.51
1:B:611:GLN:NE2	1:B:613:ASP:HB2	2.23	0.51
1:B:578:LYS:O	1:B:579:TYR:CB	2.58	0.51
1:A:748:ASP:HB3	1:A:751:GLU:HG3	1.93	0.51
1:A:380:LYS:O	1:A:384:GLN:HG2	2.11	0.51
1:B:95:GLU:OE1	1:B:95:GLU:HA	2.10	0.51
1:B:739:GLU:HA	1:B:739:GLU:OE1	2.10	0.51
1:A:27:GLU:HB2	1:A:29:ASN:ND2	2.25	0.51
1:B:609:ASN:N	1:B:609:ASN:HD22	2.09	0.51
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.91	0.51
1:B:212:GLU:O	1:B:216:VAL:HG23	2.10	0.51
3:A:9002:MFM:H9	3:A:9002:MFM:C14	2.41	0.51
1:A:175:ASN:HA	1:A:178:LYS:HG2	1.93	0.51
1:B:324:ILE:HD12	1:B:339:LYS:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:N	1:A:118:TYR:CD1	2.79	0.51
1:B:491:ARG:HB3	1:B:492:PRO:HD2	1.92	0.51
1:A:79:GLY:HA2	1:A:127:PRO:HG2	1.93	0.51
1:B:682:GLU:HB3	1:B:742:ARG:HD3	1.92	0.51
1:A:169:LYS:NZ	1:A:251:GLU:OE2	2.44	0.51
1:A:49:LYS:HG3	1:A:85:ASP:OD1	2.10	0.50
1:A:281:TRP:CZ3	1:A:285:LEU:HD11	2.46	0.50
1:A:92:ILE:H	1:A:92:ILE:CD1	2.15	0.50
1:A:368:LEU:HB3	1:A:373:LYS:HE3	1.93	0.50
1:A:767:ASN:O	1:A:771:LYS:HG2	2.12	0.50
1:A:315:GLU:HB3	1:A:375:PHE:CE1	2.47	0.50
1:A:244:MET:CE	1:A:248:ASN:HD21	2.24	0.50
1:A:748:ASP:HB3	1:A:751:GLU:CG	2.40	0.50
3:B:9003:MFM:C14	3:B:9003:MFM:H9	2.40	0.50
1:A:340:LYS:HG2	1:A:344:ASP:OD2	2.11	0.50
1:A:441:MET:SD	1:A:446:LEU:HD21	2.52	0.50
1:A:434:LYS:HZ3	1:A:434:LYS:HB3	1.71	0.50
1:A:318:LEU:HB3	1:A:372:GLU:OE2	2.12	0.50
1:A:50:GLY:C	1:A:52:GLU:H	2.15	0.50
1:A:435:ILE:CD1	1:A:435:ILE:N	2.59	0.50
1:A:36:LEU:O	1:A:40:MET:HG2	2.11	0.50
1:A:176:THR:O	1:A:180:ALA:HB2	2.12	0.50
1:A:637:PRO:HD3	1:A:654:HIS:HB2	1.94	0.49
1:B:686:HIS:CE1	1:B:728:TYR:HE2	2.30	0.49
1:A:373:LYS:O	1:A:377:LYS:HG3	2.13	0.49
1:A:578:LYS:HD3	1:A:579:TYR:CE2	2.46	0.49
1:B:97:LEU:HD22	1:B:101:LYS:HD3	1.94	0.49
1:A:325:ASP:HA	1:A:335:LYS:CE	2.42	0.49
1:A:340:LYS:HG2	1:A:340:LYS:O	2.11	0.49
1:A:125:TYR:CD1	1:A:126:GLU:HG3	2.47	0.49
1:A:490:GLU:OE2	1:A:500:LYS:HE3	2.12	0.49
1:A:687:GLU:OE2	3:A:9002:MFM:S1	2.71	0.49
1:B:701:ASP:OD2	1:B:704:GLN:HB3	2.12	0.49
1:A:675:VAL:O	1:A:675:VAL:HG22	2.12	0.49
1:A:35:HIS:O	1:A:39:ILE:HG13	2.12	0.49
1:B:611:GLN:NE2	1:B:614:LEU:H	2.11	0.49
1:A:74:TYR:HD2	1:A:77:ILE:HD11	1.77	0.49
1:A:135:GLU:OE1	1:A:135:GLU:N	2.46	0.49
1:B:121:ALA:CB	1:B:154:ILE:HD11	2.21	0.49
1:A:703:ASN:N	1:A:703:ASN:ND2	2.61	0.49
1:A:606:TRP:CH2	1:A:615:ILE:HG23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLN:O	1:A:324:ILE:C	2.51	0.49
1:A:34:GLU:O	1:A:37:LYS:HB2	2.12	0.48
1:B:610:ILE:CG2	1:B:614:LEU:HD23	2.43	0.48
1:B:477:TYR:H	1:B:593:SER:HB3	1.78	0.48
1:A:567:ASN:ND2	1:A:583:ILE:H	2.06	0.48
1:A:97:LEU:O	1:A:98:SER:C	2.51	0.48
1:A:119:VAL:CG1	1:A:131:ILE:HG12	2.43	0.48
1:B:156:SER:HB2	1:B:217:PHE:CD2	2.49	0.48
1:B:48:VAL:CG1	1:B:84:VAL:HA	2.44	0.48
1:B:35:HIS:C	1:B:37:LYS:H	2.17	0.48
1:A:456:ASP:HB3	1:A:459:ASP:O	2.14	0.48
1:A:699:LEU:HB3	1:A:772:PHE:HE1	1.78	0.48
1:A:615:ILE:O	1:A:619:THR:HG23	2.13	0.48
1:A:754:LYS:O	1:A:758:ASN:HB2	2.14	0.48
1:A:326:SER:HB3	1:A:368:LEU:HD21	1.96	0.48
1:B:769:GLN:HA	1:B:769:GLN:HE21	1.77	0.48
1:B:478:SER:HB3	1:B:527:LEU:HB2	1.95	0.48
1:A:61:LYS:O	1:A:64:GLU:HG2	2.14	0.48
1:B:49:LYS:O	1:B:51:GLU:N	2.47	0.48
1:B:756:GLN:O	1:B:760:PRO:HG3	2.14	0.48
1:A:404:ILE:HD12	1:A:408:VAL:CG2	2.43	0.48
1:B:765:PHE:O	1:B:769:GLN:HG2	2.14	0.48
1:B:346:ARG:C	1:B:348:SER:H	2.16	0.47
1:A:156:SER:HB3	1:A:217:PHE:CD2	2.49	0.47
1:A:433:ASN:O	1:A:435:ILE:HG13	2.14	0.47
1:B:48:VAL:HG12	1:B:85:ASP:H	1.79	0.47
1:A:107:ILE:HG12	1:A:149:TYR:CG	2.49	0.47
1:B:686:HIS:CD2	1:B:686:HIS:C	2.87	0.47
1:B:165:GLN:HA	1:B:166:PRO:C	2.35	0.47
1:B:368:LEU:O	1:B:373:LYS:HE3	2.14	0.47
1:A:441:MET:SD	1:A:446:LEU:CD2	3.03	0.47
1:A:710:ASN:O	1:A:715:ILE:HD11	2.14	0.47
1:A:318:LEU:HB3	1:A:372:GLU:CD	2.35	0.47
1:B:252:ILE:HG23	1:B:253:ASN:N	2.30	0.47
1:B:107:ILE:HG12	1:B:149:TYR:CG	2.49	0.47
1:A:27:GLU:C	1:A:29:ASN:N	2.68	0.47
1:A:640:ALA:HA	1:A:643:TYR:CG	2.49	0.47
1:A:424:HIS:O	1:A:510:ARG:HD2	2.15	0.47
1:A:727:SER:O	1:A:730:ARG:HB3	2.14	0.47
1:A:275:LYS:NZ	1:A:279:GLN:HE22	2.13	0.47
1:A:316:LYS:O	1:A:319:LEU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LYS:CD	1:A:712:LYS:H	2.13	0.47
1:B:655:SER:OG	3:B:9003:MFM:H152	2.14	0.47
1:B:35:HIS:C	1:B:37:LYS:N	2.68	0.47
1:A:474:ASN:HB3	1:A:597:GLU:HG3	1.97	0.47
1:A:221:PHE:O	1:A:225:ILE:HG12	2.14	0.47
1:B:277:HIS:CD2	1:B:429:SER:HB2	2.49	0.47
1:A:640:ALA:HA	1:A:643:TYR:CD2	2.50	0.47
1:B:28:ARG:O	1:B:32:GLN:HB2	2.15	0.47
1:B:244:MET:HA	1:B:244:MET:HE3	1.97	0.47
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.96	0.47
1:A:103:LYS:HD3	1:A:111:ASP:HB3	1.97	0.46
1:A:178:LYS:HG3	1:A:179:ASN:N	2.30	0.46
1:A:249:GLU:OE2	1:A:249:GLU:HA	2.15	0.46
1:B:36:LEU:O	1:B:40:MET:HE2	2.14	0.46
1:A:317:GLU:CA	1:A:320:LYS:HE2	2.44	0.46
1:A:159:ILE:HG22	1:A:160:LEU:N	2.30	0.46
1:B:378:LYS:HE2	1:B:650:TYR:CE2	2.51	0.46
1:A:29:ASN:O	1:A:32:GLN:HB3	2.16	0.46
1:B:404:ILE:HD11	1:B:409:ARG:HA	1.97	0.46
1:A:74:TYR:CZ	1:A:154:ILE:HD13	2.50	0.46
1:B:468:PHE:HE1	1:B:543:ILE:HG23	1.81	0.46
1:A:99:GLU:HG2	1:A:102:LYS:NZ	2.31	0.46
1:B:632:THR:CG2	1:B:639:ILE:HD11	2.37	0.46
1:B:107:ILE:O	1:B:107:ILE:HD13	2.16	0.46
1:A:311:LEU:HB3	1:A:315:GLU:HB2	1.98	0.46
1:A:440:ASN:HD21	1:A:500:LYS:NZ	2.13	0.46
1:A:65:LYS:HE2	1:A:227:PRO:HG3	1.98	0.45
1:A:204:GLU:O	1:A:208:GLN:HG2	2.15	0.45
1:A:294:LYS:O	1:A:298:ILE:HG13	2.16	0.45
1:A:178:LYS:HB3	1:A:190:PHE:HE1	1.81	0.45
1:A:610:ILE:CG2	1:A:614:LEU:HD23	2.46	0.45
1:B:51:GLU:C	1:B:53:ALA:H	2.19	0.45
1:A:318:LEU:HB3	1:A:372:GLU:OE1	2.16	0.45
1:A:441:MET:O	1:A:499:LEU:HB2	2.17	0.45
1:A:699:LEU:HB3	1:A:772:PHE:CE1	2.52	0.45
1:B:149:TYR:OH	1:B:215:GLU:OE1	2.32	0.45
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.63	0.45
1:B:369:SER:OG	1:B:372:GLU:HG3	2.16	0.45
1:B:233:LEU:CD2	1:B:237:ALA:HB3	2.47	0.45
1:A:315:GLU:OE1	1:A:375:PHE:HE1	1.99	0.45
1:A:730:ARG:HG3	1:A:730:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LYS:O	1:B:320:LYS:HG3	2.17	0.45
1:A:324:ILE:O	1:A:335:LYS:HE2	2.16	0.45
1:A:440:ASN:ND2	1:A:500:LYS:HG2	2.31	0.45
1:A:282:SER:O	1:A:284:SER:N	2.50	0.45
1:A:309:HIS:ND1	1:A:309:HIS:O	2.50	0.45
1:A:656:LYS:HB2	1:A:674:GLY:HA2	1.99	0.44
1:A:318:LEU:HD13	1:A:372:GLU:OE2	2.17	0.44
1:B:85:ASP:HB3	1:B:133:SER:OG	2.17	0.44
1:A:515:GLU:HB2	1:B:207:GLU:OE1	2.17	0.44
1:A:29:ASN:O	1:A:32:GLN:N	2.48	0.44
1:A:149:TYR:HA	1:A:222:ALA:HB2	2.00	0.44
1:A:74:TYR:CD2	1:A:77:ILE:HD11	2.53	0.44
1:B:493:ALA:HB1	1:B:497:GLU:HB2	1.97	0.44
1:A:598:SER:O	1:A:602:ILE:HG13	2.17	0.44
1:A:107:ILE:HG12	1:A:149:TYR:HB2	1.99	0.44
1:A:748:ASP:O	1:A:751:GLU:HB2	2.17	0.44
1:B:47:GLU:OE1	1:B:91:HIS:HE1	2.00	0.44
1:A:315:GLU:HB3	1:A:375:PHE:CZ	2.52	0.44
1:A:330:LEU:HD11	1:A:376:LEU:HD13	2.00	0.44
1:A:387:ASP:HB3	1:A:390:GLN:HB3	1.99	0.44
1:B:197:HIS:HD2	1:B:199:THR:O	2.00	0.44
1:A:437:LEU:HD11	1:A:519:LEU:HD12	2.00	0.44
1:A:107:ILE:HG13	1:A:145:LEU:HD11	1.98	0.44
1:A:716:ASP:HA	1:A:719:LYS:HB2	1.99	0.44
1:A:198:PRO:HG2	1:A:199:THR:H	1.83	0.44
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.81	0.44
1:A:395:THR:O	1:A:398:LEU:HG	2.18	0.44
1:A:343:ILE:O	1:A:343:ILE:HG22	2.17	0.44
1:A:618:VAL:O	1:A:621:TYR:HB3	2.18	0.44
1:A:178:LYS:NZ	1:A:199:THR:O	2.48	0.44
1:B:723:SER:HB2	1:B:730:ARG:CZ	2.47	0.43
1:A:759:ALA:N	1:A:760:PRO:CD	2.81	0.43
1:B:660:VAL:O	1:B:664:ARG:N	2.51	0.43
1:A:324:ILE:O	1:A:326:SER:N	2.51	0.43
1:B:587:VAL:CG1	1:B:592:ALA:HA	2.49	0.43
1:B:611:GLN:NE2	1:B:613:ASP:H	2.15	0.43
1:A:265:LEU:HA	1:A:265:LEU:HD12	1.82	0.43
1:A:36:LEU:O	1:A:40:MET:CG	2.65	0.43
1:A:123:GLU:HG2	1:A:124:GLY:H	1.82	0.43
1:B:77:ILE:O	1:B:77:ILE:HG23	2.18	0.43
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLN:CA	1:A:411:GLN:NE2	2.76	0.43
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.89	0.43
1:B:516:ASN:H	1:B:516:ASN:HD22	1.61	0.43
1:B:529:ILE:HD12	1:B:529:ILE:N	2.33	0.43
1:B:206:LEU:CD2	1:B:213:VAL:HG21	2.47	0.43
1:A:496:ASN:C	1:A:496:ASN:ND2	2.71	0.43
1:B:662:GLU:OE2	1:B:662:GLU:N	2.29	0.43
1:B:391:ARG:NH1	1:B:399:ILE:O	2.50	0.43
1:B:153:LYS:O	1:B:157:ARG:HB3	2.19	0.43
1:A:696:ALA:HB2	1:A:773:ILE:HD11	2.01	0.43
1:B:424:HIS:CA	1:B:510:ARG:HD2	2.40	0.43
1:A:637:PRO:CD	1:A:654:HIS:HB2	2.48	0.43
1:B:297:GLN:O	1:B:298:ILE:HD13	2.19	0.43
1:B:136:ASP:O	1:B:140:ASN:N	2.52	0.43
1:A:371:LYS:HA	1:A:371:LYS:HD3	1.83	0.43
1:B:744:MET:O	1:B:752:ARG:HG2	2.19	0.43
1:A:617:LYS:HB3	1:A:695:TYR:HE2	1.83	0.43
1:A:235:LEU:HD23	1:A:236:TYR:CE2	2.54	0.43
1:A:107:ILE:HG12	1:A:149:TYR:CB	2.49	0.43
1:A:311:LEU:HA	1:A:315:GLU:OE2	2.18	0.42
1:B:48:VAL:HB	1:B:85:ASP:OD2	2.20	0.42
1:B:304:LYS:HD3	1:B:304:LYS:H	1.83	0.42
1:B:746:SER:O	1:B:752:ARG:HD2	2.19	0.42
1:A:632:THR:OG1	1:A:633:ASP:N	2.52	0.42
1:B:594:ASN:O	1:B:598:SER:HB3	2.20	0.42
1:A:686:HIS:HB2	1:A:742:ARG:HD3	2.00	0.42
1:A:741:PHE:O	1:A:745:HIS:CD2	2.71	0.42
1:A:368:LEU:CB	1:A:373:LYS:HE3	2.50	0.42
1:B:188:LEU:HD11	1:B:223:TYR:CE2	2.54	0.42
1:B:506:SER:HB3	1:B:509:THR:OG1	2.20	0.42
1:A:494:LEU:HD12	1:A:494:LEU:HA	1.89	0.42
1:A:694:ASP:C	1:A:694:ASP:OD1	2.58	0.42
1:A:770:ILE:O	1:A:774:ILE:HG13	2.20	0.42
1:A:392:LEU:HD13	1:A:482:ASN:HA	2.01	0.42
1:A:178:LYS:HB2	1:A:178:LYS:HE3	1.86	0.42
1:A:491:ARG:HB3	1:A:492:PRO:HD2	2.00	0.42
1:B:84:VAL:HG22	1:B:85:ASP:N	2.35	0.42
1:B:60:GLU:O	1:B:64:GLU:HB2	2.19	0.42
1:B:557:THR:O	1:B:561:GLU:HG3	2.19	0.42
1:A:245:ASP:O	1:A:249:GLU:HG2	2.19	0.42
1:A:330:LEU:HD13	1:A:338:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:VAL:O	1:B:621:TYR:HB3	2.20	0.42
1:A:294:LYS:HA	1:A:294:LYS:HD3	1.87	0.42
1:B:550:VAL:HB	1:B:551:PRO:HD2	2.01	0.42
1:A:104:ILE:CG2	1:A:105:LYS:H	2.11	0.41
1:A:244:MET:HE2	1:A:248:ASN:HD21	1.84	0.41
1:A:404:ILE:CD1	1:A:408:VAL:HG23	2.49	0.41
1:A:226:GLU:HA	1:A:227:PRO:HD2	1.84	0.41
1:B:59:ALA:O	1:B:62:LEU:HB3	2.20	0.41
1:A:36:LEU:HD23	1:A:36:LEU:O	2.20	0.41
1:A:85:ASP:OD2	1:A:133:SER:OG	2.38	0.41
1:B:442:ASN:ND2	1:B:496:ASN:HB2	2.35	0.41
1:B:48:VAL:HG23	1:B:52:GLU:HG2	2.01	0.41
1:A:437:LEU:HD12	1:A:505:LEU:HD21	2.01	0.41
1:B:224:TYR:CZ	1:B:245:ASP:HA	2.55	0.41
1:B:270:LYS:O	1:B:274:ILE:HG12	2.19	0.41
1:A:523:ARG:O	1:A:524:ASN:HB2	2.20	0.41
1:A:715:ILE:HG22	1:A:719:LYS:HE3	2.02	0.41
1:A:199:THR:OG1	1:A:200:ASP:N	2.52	0.41
1:A:322:ILE:HG23	1:A:322:ILE:O	2.20	0.41
1:B:123:GLU:CD	1:B:157:ARG:HD2	2.41	0.41
1:B:47:GLU:OE1	1:B:91:HIS:CE1	2.74	0.41
1:B:591:TYR:CD2	1:B:594:ASN:HB3	2.55	0.41
1:A:634:ILE:HD11	1:A:639:ILE:HD13	2.02	0.41
1:B:563:GLN:HE21	1:B:585:PHE:HB2	1.86	0.41
1:B:526:GLY:CA	1:B:555:ILE:HD12	2.51	0.41
1:A:176:THR:CG2	1:A:239:GLU:HG3	2.41	0.41
1:B:99:GLU:O	1:B:102:LYS:HB2	2.20	0.41
1:B:45:LYS:HB2	1:B:82:TYR:CE2	2.56	0.41
1:A:275:LYS:HZ2	1:A:279:GLN:HE22	1.69	0.41
1:A:33:GLU:O	1:A:37:LYS:CG	2.63	0.41
1:B:686:HIS:CE1	1:B:728:TYR:CE2	3.09	0.41
1:B:77:ILE:HD13	1:B:259:LEU:HD21	2.03	0.41
1:A:725:LEU:HD12	1:A:736:PHE:CE1	2.56	0.41
1:B:150:GLU:O	1:B:154:ILE:HG12	2.21	0.41
1:B:733:GLU:N	1:B:733:GLU:CD	2.71	0.41
1:B:236:TYR:C	1:B:238:PRO:HD3	2.41	0.41
1:B:46:ILE:HD13	1:B:83:ILE:HB	2.03	0.41
1:A:437:LEU:CD1	1:A:519:LEU:HD12	2.51	0.41
1:B:77:ILE:CG2	1:B:77:ILE:O	2.67	0.41
1:A:595:ILE:CD1	1:A:670:GLY:HA3	2.50	0.41
1:B:456:ASP:OD1	1:B:458:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:LEU:HD12	1:A:636:LEU:HA	1.79	0.41
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.49	0.41
1:B:278:TYR:CE2	1:B:425:GLN:HB3	2.57	0.41
1:A:140:ASN:HB3	1:A:143:LYS:NZ	2.31	0.40
1:A:340:LYS:O	1:A:344:ASP:HB2	2.21	0.40
1:A:123:GLU:HG2	1:A:124:GLY:N	2.36	0.40
1:A:62:LEU:HD22	1:A:137:TYR:CD1	2.56	0.40
1:A:691:ALA:O	1:A:694:ASP:HB3	2.21	0.40
1:A:237:ALA:N	1:A:238:PRO:HD3	2.35	0.40
1:A:567:ASN:ND2	1:A:582:LEU:H	2.18	0.40
1:A:739:GLU:HA	1:A:739:GLU:OE1	2.20	0.40
1:A:330:LEU:CD1	1:A:376:LEU:HD13	2.52	0.40
1:A:182:ASP:OD1	1:A:184:ASP:HB2	2.21	0.40
1:B:613:ASP:O	1:B:617:LYS:HG2	2.21	0.40
1:B:395:THR:HG22	1:B:638:ASN:ND2	2.36	0.40
1:A:154:ILE:HG22	1:A:159:ILE:HD13	2.03	0.40
1:A:648:GLU:HG3	1:A:650:TYR:OH	2.20	0.40
1:B:98:SER:O	1:B:102:LYS:HD3	2.21	0.40
1:B:614:LEU:HD13	1:B:770:ILE:HG23	2.03	0.40
1:B:327:SER:HB2	1:B:329:PHE: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	724/776 (93%)	645 (89%)	62 (9%)	17 (2%)	8	19
1	B	732/776 (94%)	660 (90%)	56 (8%)	16 (2%)	8	20
All	All	1456/1552 (94%)	1305 (90%)	118 (8%)	33 (2%)	8	19

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	675	VAL
1	B	32	GLN
1	B	50	GLY
1	B	366	ASN
1	B	702	LYS
1	A	53	ALA
1	A	87	ASP
1	A	198	PRO
1	A	473	LYS
1	A	722	GLY
1	B	29	ASN
1	B	92	ILE
1	B	140	ASN
1	B	675	VAL
1	B	700	LEU
1	B	722	GLY
1	A	52	GLU
1	A	283	ASP
1	B	133	SER
1	B	329	PHE
1	A	51	GLU
1	A	324	ILE
1	A	326	SER
1	B	326	SER
1	A	28	ARG
1	A	96	ALA
1	A	678	ARG
1	B	93	SER
1	B	579	TYR
1	B	758	ASN
1	A	733	GLU
1	A	50	GLY

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	667/710 (94%)	616 (92%)	51 (8%)	16 35
1	B	675/710 (95%)	632 (94%)	43 (6%)	22 44
All	All	1342/1420 (94%)	1248 (93%)	94 (7%)	19 40

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	46	ILE
1	A	57	GLU
1	A	70	VAL
1	A	99	GLU
1	A	103	LYS
1	A	107	ILE
1	A	111	ASP
1	A	119	VAL
1	A	193	GLN
1	A	208	GLN
1	A	210	SER
1	A	211	ASN
1	A	233	LEU
1	A	256	LEU
1	A	262	GLN
1	A	265	LEU
1	A	288	GLU
1	A	294	LYS
1	A	305	ASP
1	A	313	GLN
1	A	325	ASP
1	A	328	ASP
1	A	344	ASP
1	A	371	LYS
1	A	435	ILE
1	A	446	LEU
1	A	447	THR
1	A	449	THR
1	A	470	GLU
1	A	494	LEU
1	A	496	ASN
1	A	505	LEU
1	A	523	ARG
1	A	574	LEU

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Mol	Chain	Res	Type
1	A	580	THR
1	A	582	LEU
1	A	584	THR
1	A	605	GLU
1	A	636	LEU
1	A	643	TYR
1	A	655	SER
1	A	679	ASN
1	A	701	ASP
1	A	703	ASN
1	A	706	ASP
1	A	712	LYS
1	A	716	ASP
1	A	719	LYS
1	A	753	LEU
1	A	767	ASN
1	B	28	ARG
1	B	36	LEU
1	B	49	LYS
1	B	99	GLU
1	B	100	ASP
1	B	107	ILE
1	B	111	ASP
1	B	125	TYR
1	B	129	LEU
1	B	135	GLU
1	B	145	LEU
1	B	146	ASN
1	B	203	VAL
1	B	231	ASP
1	B	233	LEU
1	B	265	LEU
1	B	304	LYS
1	B	314	GLU
1	B	317	GLU
1	B	322	ILE
1	B	323	GLN
1	B	328	ASP
1	B	347	ASP
1	B	391	ARG
1	B	422	LEU
1	B	425	GLN

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Mol	Chain	Res	Type
1	B	433	ASN
1	B	447	THR
1	B	457	SER
1	B	496	ASN
1	B	515	GLU
1	B	516	ASN
1	B	520	ILE
1	B	523	ARG
1	B	557	THR
1	B	593	SER
1	B	598	SER
1	B	611	GLN
1	B	679	ASN
1	B	703	ASN
1	B	705	SER
1	B	712	LYS
1	B	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	32	GLN
1	A	132	GLN
1	A	140	ASN
1	A	164	ASN
1	A	179	ASN
1	A	193	GLN
1	A	209	ASN
1	A	214	GLN
1	A	248	ASN
1	A	262	GLN
1	A	276	GLN
1	A	277	HIS
1	A	279	GLN
1	A	313	GLN
1	A	411	GLN
1	A	425	GLN
1	A	440	ASN
1	A	496	ASN
1	A	524	ASN
1	A	563	GLN

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Mol	Chain	Res	Type
1	A	567	ASN
1	A	571	ASN
1	A	608	ASN
1	A	679	ASN
1	A	703	ASN
1	A	710	ASN
1	A	745	HIS
1	A	767	ASN
1	B	42	HIS
1	B	91	HIS
1	B	164	ASN
1	B	186	GLN
1	B	193	GLN
1	B	197	HIS
1	B	214	GLN
1	B	242	ASN
1	B	250	GLN
1	B	277	HIS
1	B	297	GLN
1	B	323	GLN
1	B	393	GLN
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	474	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	589	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	638	ASN
1	B	654	HIS
1	B	679	ASN
1	B	703	ASN

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Mol	Chain	Res	Type
1	B	710	ASN
1	B	745	HIS
1	B	756	GLN
1	B	767	ASN
1	B	769	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	MFM	A	9002	2	20,27,27	2.19	5 (25%)	27,38,38	2.42	10 (37%)
3	MFM	B	9003	2	20,27,27	2.10	5 (25%)	27,38,38	2.54	10 (37%)

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	MFM	A	9002	2	-	0/5/29/29	0/2/3/3
3	MFM	B	9003	2	-	0/5/29/29	0/2/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9002	MFM	C5-C7	-5.62	1.39	1.46
3	B	9003	MFM	C5-C7	-5.58	1.39	1.46
3	A	9002	MFM	C14-C12	-4.21	1.39	1.48
3	B	9003	MFM	C14-C12	-3.94	1.40	1.48
3	B	9003	MFM	C14-N1	-3.22	1.32	1.39
3	A	9002	MFM	C14-N1	-3.11	1.33	1.39
3	B	9003	MFM	C11-C12	2.86	1.38	1.34
3	A	9002	MFM	C11-C12	3.68	1.39	1.34
3	A	9002	MFM	C13-S2	3.68	1.75	1.66
3	B	9003	MFM	C13-S2	3.76	1.75	1.66

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	9003	MFM	C11-C12-S1	-5.34	123.37	129.31
3	A	9002	MFM	C11-C12-S1	-5.14	123.59	129.31
3	B	9003	MFM	C14-C12-S1	-4.96	105.66	110.72
3	A	9002	MFM	C14-C12-S1	-4.89	105.73	110.72
3	B	9003	MFM	C16-C15-N1	-3.39	108.80	112.25
3	A	9002	MFM	C16-C15-N1	-3.34	108.86	112.25
3	B	9003	MFM	O2-C14-C12	-3.21	122.67	126.50
3	A	9002	MFM	O2-C14-C12	-2.67	123.32	126.50
3	A	9002	MFM	C4-C5-C7	-2.44	118.09	120.45
3	A	9002	MFM	O2-C14-N1	-2.32	119.50	124.50
3	B	9003	MFM	C4-C5-C7	-2.15	118.38	120.45
3	B	9003	MFM	O2-C14-N1	-2.08	120.02	124.50
3	A	9002	MFM	C8-C9-C10	2.08	108.14	106.30
3	B	9003	MFM	C8-C9-C10	2.16	108.20	106.30
3	B	9003	MFM	S1-C13-S2	2.16	127.60	123.28
3	A	9002	MFM	S1-C13-S2	2.24	127.75	123.28
3	B	9003	MFM	C12-C14-N1	3.81	116.01	109.99
3	A	9002	MFM	C12-C14-N1	3.83	116.04	109.99
3	A	9002	MFM	C11-C12-C14	5.93	126.35	120.40
3	B	9003	MFM	C11-C12-C14	6.84	127.27	120.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9002	MFM	5	0
3	B	9003	MFM	4	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	728/776 (93%)	0.43	68 (9%) 11 8	20, 48, 96, 103	0
1	B	736/776 (94%)	0.35	58 (7%) 15 13	18, 45, 94, 103	0
All	All	1464/1552 (94%)	0.39	126 (8%) 13 10	18, 46, 96, 103	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	VAL	7.5
1	B	363	ASP	7.3
1	A	27	GLU	6.9
1	A	321	ARG	6.7
1	B	48	VAL	6.2
1	B	29	ASN	6.2
1	B	28	ARG	5.9
1	A	322	ILE	5.9
1	A	318	LEU	5.7
1	A	345	ILE	5.4
1	B	365	SER	5.3
1	B	33	GLU	5.2
1	A	319	LEU	5.0
1	B	27	GLU	5.0
1	A	29	ASN	5.0
1	A	28	ARG	5.0
1	A	307	ILE	4.9
1	A	308	ILE	4.9
1	A	341	LEU	4.9
1	B	115	HIS	4.8
1	A	316	LYS	4.7
1	B	37	LYS	4.7
1	A	368	LEU	4.7
1	A	372	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	366	ASN	4.6
1	A	338	LEU	4.6
1	A	320	LYS	4.6
1	B	34	GLU	4.5
1	A	54	VAL	4.5
1	B	84	VAL	4.5
1	B	46	ILE	4.5
1	B	364	SER	4.4
1	A	344	ASP	4.4
1	B	135	GLU	4.3
1	B	367	PRO	4.3
1	B	321	ARG	4.3
1	A	49	LYS	4.2
1	A	31	THR	4.2
1	B	50	GLY	4.2
1	B	52	GLU	4.2
1	B	51	GLU	4.2
1	B	97	LEU	4.1
1	A	30	LYS	4.0
1	A	324	ILE	4.0
1	A	313	GLN	3.9
1	A	703	ASN	3.7
1	B	114	LEU	3.7
1	B	49	LYS	3.6
1	A	48	VAL	3.6
1	A	309	HIS	3.6
1	B	703	ASN	3.5
1	A	306	ASP	3.5
1	A	32	GLN	3.5
1	A	56	LYS	3.5
1	B	35	HIS	3.4
1	A	52	GLU	3.4
1	B	32	GLN	3.4
1	B	60	GLU	3.4
1	B	329	PHE	3.3
1	A	329	PHE	3.3
1	B	138	VAL	3.3
1	A	311	LEU	3.3
1	A	36	LEU	3.3
1	A	303	LYS	3.2
1	B	346	ARG	3.2
1	A	34	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	369	SER	3.1
1	B	53	ALA	3.1
1	B	345	ILE	3.1
1	B	56	LYS	3.0
1	B	91	HIS	3.1
1	A	330	LEU	2.9
1	A	84	VAL	2.8
1	B	348	SER	2.8
1	A	33	GLU	2.8
1	A	317	GLU	2.8
1	B	30	LYS	2.7
1	B	101	LYS	2.7
1	B	92	ILE	2.7
1	B	368	LEU	2.7
1	B	343	ILE	2.7
1	A	136	ASP	2.7
1	B	85	ASP	2.7
1	A	35	HIS	2.6
1	A	327	SER	2.6
1	A	702	LYS	2.6
1	B	701	ASP	2.6
1	A	199	THR	2.5
1	A	37	LYS	2.5
1	A	55	LYS	2.5
1	B	93	SER	2.4
1	A	373	LYS	2.4
1	A	315	GLU	2.4
1	B	83	ILE	2.4
1	B	131	ILE	2.4
1	A	198	PRO	2.4
1	B	704	GLN	2.4
1	A	115	HIS	2.4
1	A	370	GLU	2.4
1	A	776	SER	2.3
1	B	308	ILE	2.3
1	A	50	GLY	2.3
1	A	343	ILE	2.3
1	A	305	ASP	2.3
1	B	327	SER	2.3
1	A	328	ASP	2.2
1	A	579	TYR	2.2
1	B	41	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	719	LYS	2.2
1	A	181	SER	2.2
1	B	139	GLU	2.2
1	B	36	LEU	2.1
1	A	340	LYS	2.1
1	A	761	LYS	2.1
1	B	44	VAL	2.1
1	A	339	LYS	2.1
1	A	180	ALA	2.1
1	A	766	ILE	2.1
1	A	100	ASP	2.1
1	B	730	ARG	2.1
1	A	312	SER	2.1
1	B	337	PHE	2.1
1	B	761	LYS	2.1
1	B	300	ILE	2.0
1	B	347	ASP	2.0
1	A	323	GLN	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 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
3	MFM	B	9003	25/25	0.54	0.41	6.99	90,90,90,90	0
3	MFM	A	9002	25/25	0.69	0.30	3.61	90,90,90,90	0
2	ZN	A	9001	1/1	0.99	0.17	-0.47	49,49,49,49	0
2	ZN	B	9002	1/1	0.99	0.13	-2.01	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.