



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PWU  
Title : Crystal Structure of Anthrax Lethal Factor complexed with (3-(N-hydroxycarbonyl)-2-isobutylpropanoyl-Trp-methylamide), a known small molecule inhibitor of matrix metalloproteases.  
Authors : Wong, T.Y.; Schwarzenbacher, R.; Liddington, R.C.  
Deposited on : 2003-07-02  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

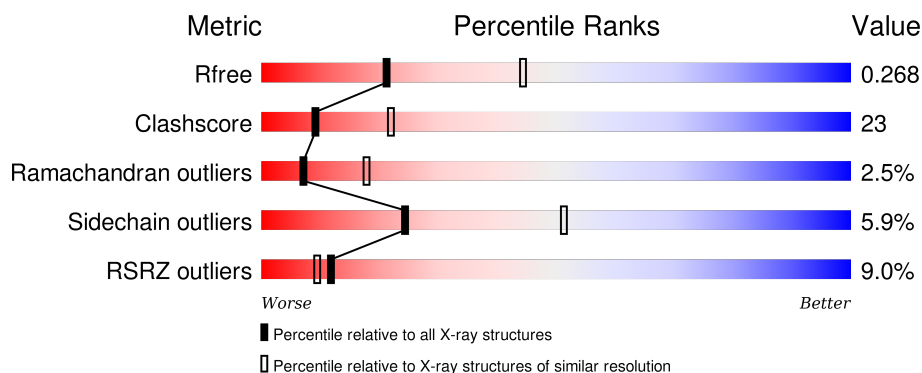
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	776	<div> <div>10%</div> <div>55%</div> <div>36%</div> <div>5%</div> <div>.</div> </div>
1	B	776	<div> <div>8%</div> <div>57%</div> <div>33%</div> <div>5%</div> <div>5%</div> </div>

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	GM6	A	1001	-	-	X	X
3	GM6	B	2001	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12238 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	747	Total	C	N	O	S	0	0	0
			6134	3897	1032	1197	8			
1	B	736	Total	C	N	O	S	0	0	0
			6046	3846	1014	1178	8			

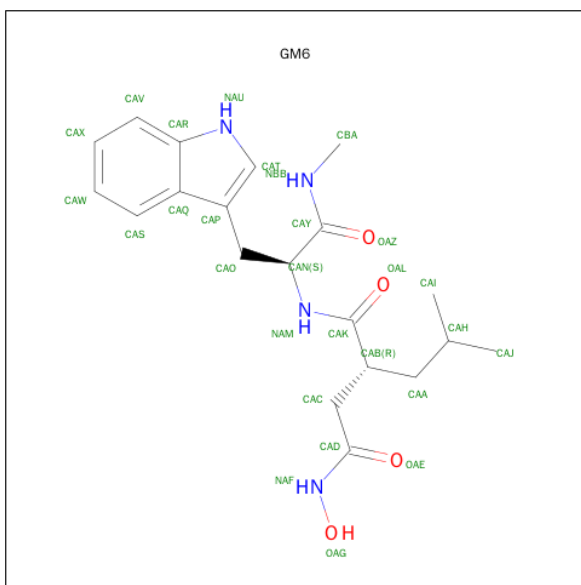
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	687	CYS	GLU	engineered	UNP P15917
B	687	CYS	GLU	engineered	UNP P15917

- 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 3-(N-HYDROXYCARBOXAMIDO)-2-ISOBUTYLPROPANOYL-TRP-MET HYLAMIDE (three-letter code: GM6) (formula: C<sub>20</sub>H<sub>28</sub>N<sub>4</sub>O<sub>4</sub>).

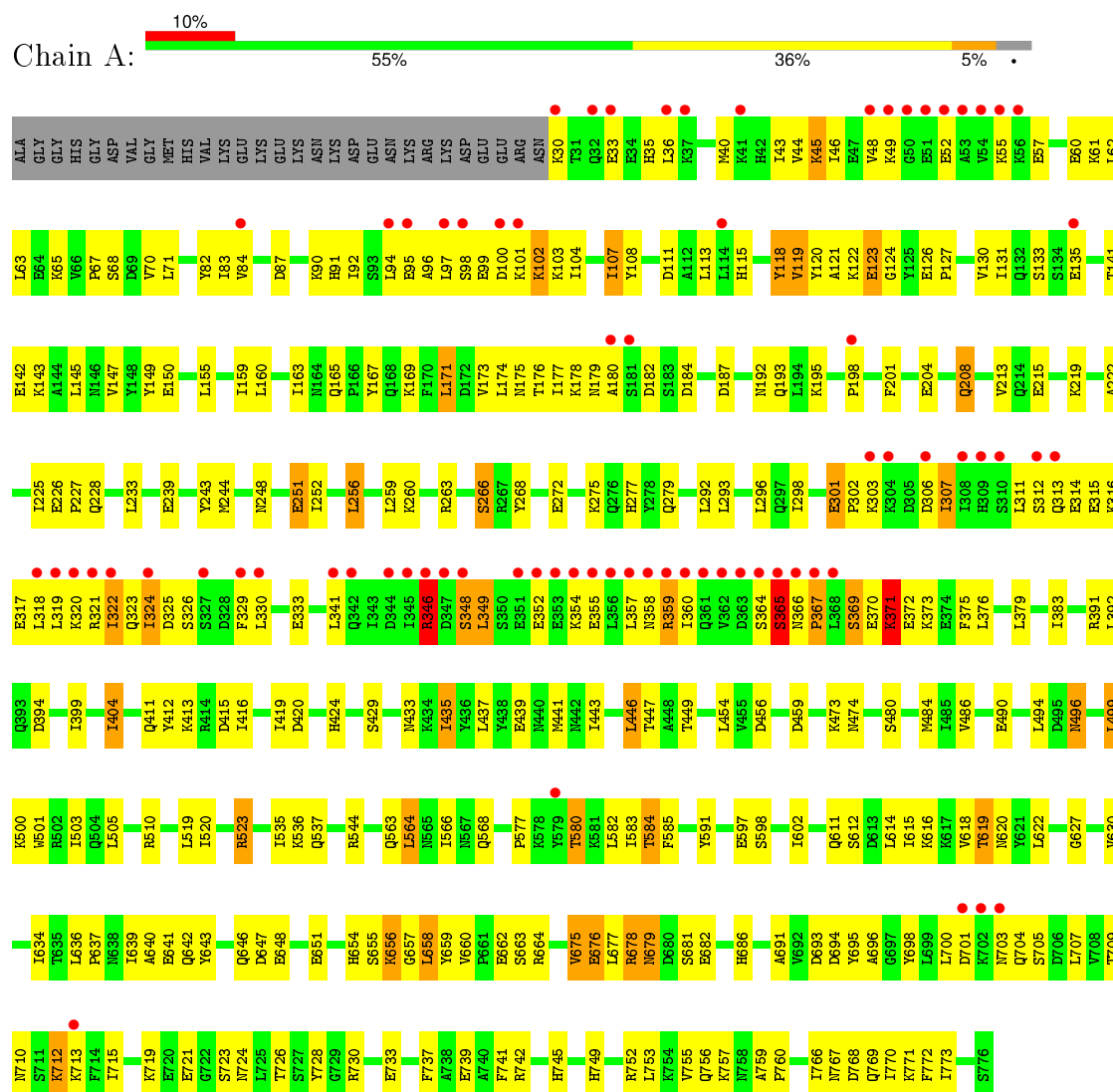


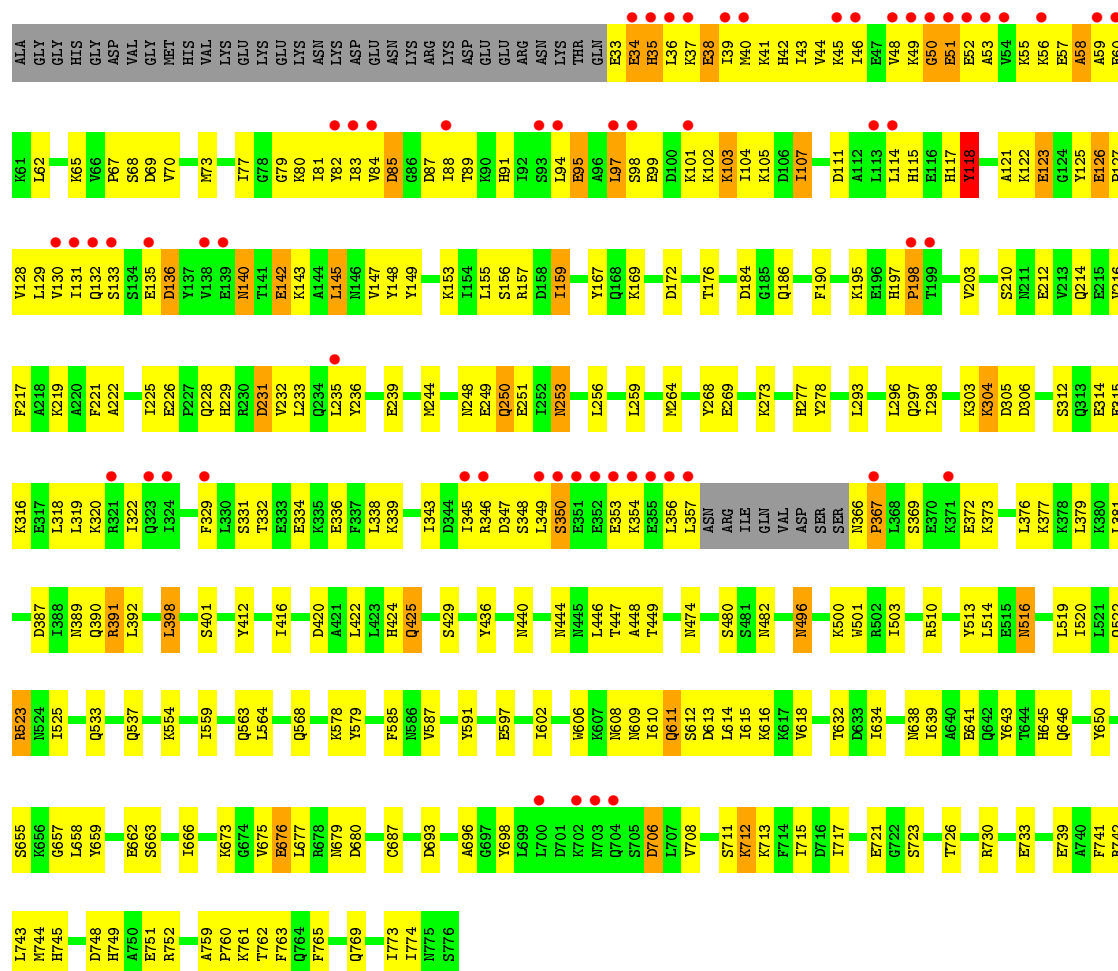
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 28	C 20	N 4	O 4	0	0
3	B	1	Total 28	C 20	N 4	O 4	0	0

### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.70 Å 137.40 Å 98.30 Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	33.10 – 2.70 46.05 – 2.71	Depositor EDS
% Data completeness (in resolution range)	93.7 (33.10-2.70) 93.7 (46.05-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.69 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.270 0.234 , 0.268	Depositor DCC
$R_{free}$ test set	3280 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.8	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 68460 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12238	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, GM6

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	0/6243	0.63	1/8411 (0.0%)
1	B	0.41	0/6154	0.65	3/8290 (0.0%)
All	All	0.39	0/12397	0.64	4/16701 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	B	118	TYR	CB-CG-CD1	7.54	125.52	121.00
1	B	97	LEU	CB-CA-C	-5.88	99.02	110.20
1	A	365	SER	N-CA-C	5.26	125.20	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	6134	0	6123	283	0
1	B	6046	0	6033	283	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	28	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	28	5	0
All	All	12238	0	12212	563	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 (563) 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:104:ILE:CD1	1:B:114:LEU:HD23	1.48	1.39
1:B:104:ILE:HD11	1:B:114:LEU:CD2	1.54	1.36
1:A:48:VAL:CG2	1:A:52:GLU:HG2	1.63	1.29
1:A:99:GLU:HA	1:A:102:LYS:HD2	1.11	1.10
1:B:366:ASN:HB3	1:B:367:PRO:HD3	1.26	1.09
1:A:324:ILE:HD12	1:A:324:ILE:H	0.93	1.04
1:A:48:VAL:HG23	1:A:52:GLU:HG2	1.35	1.04
1:A:324:ILE:H	1:A:324:ILE:CD1	1.69	1.02
1:A:99:GLU:HA	1:A:102:LYS:CD	1.92	1.00
1:A:324:ILE:HD12	1:A:324:ILE:N	1.76	1.00
1:B:48:VAL:HG23	1:B:84:VAL:HA	1.47	0.95
1:B:48:VAL:CG2	1:B:84:VAL:HA	1.97	0.94
1:B:97:LEU:CD1	1:B:102:LYS:HG3	1.97	0.94
1:B:712:LYS:HD2	1:B:712:LYS:H	1.34	0.93
1:A:563:GLN:HE21	1:A:585:PHE:H	1.08	0.93
1:B:51:GLU:OE2	1:B:53:ALA:HB2	1.70	0.91
1:A:99:GLU:CA	1:A:102:LYS:HD2	2.00	0.90
1:A:435:ILE:H	1:A:435:ILE:HD12	1.33	0.89
1:A:30:LYS:HD3	1:A:33:GLU:HG3	1.52	0.88
1:B:510:ARG:H	1:B:522:GLN:HE21	0.91	0.88
1:A:354:LYS:HB3	1:A:358:ASN:HD21	1.38	0.87
1:B:98:SER:OG	1:B:101:LYS:HG2	1.73	0.87
1:A:704:GLN:HG2	1:A:705:SER:H	1.40	0.87
1:A:615:ILE:O	1:A:619:THR:HG23	1.75	0.86
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.56	0.86
1:A:48:VAL:CG2	1:A:52:GLU:CG	2.53	0.85
1:A:369:SER:O	1:A:373:LYS:HG2	1.76	0.85
1:A:712:LYS:HD2	1:A:713:LYS:H	1.42	0.85
1:A:355:GLU:O	1:A:359:ARG:HB2	1.77	0.84
1:B:611:GLN:HE21	1:B:774:ILE:HD13	1.41	0.84
1:B:97:LEU:HD13	1:B:102:LYS:HG3	1.55	0.84
1:B:366:ASN:HB3	1:B:367:PRO:CD	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:GLU:HA	1:B:676:GLU:OE1	1.76	0.83
1:B:103:LYS:HE2	1:B:111:ASP:OD1	1.79	0.83
1:A:354:LYS:HB3	1:A:358:ASN:ND2	1.93	0.83
1:A:721:GLU:HA	1:A:724:ASN:HD22	1.41	0.83
1:A:715:ILE:HG22	1:A:719:LYS:HE2	1.61	0.82
1:B:510:ARG:H	1:B:522:GLN:NE2	1.76	0.82
1:B:366:ASN:CB	1:B:367:PRO:HD3	2.09	0.82
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.58	0.82
1:A:435:ILE:HD12	1:A:435:ILE:N	1.95	0.81
1:B:712:LYS:HD2	1:B:712:LYS:N	1.96	0.81
1:A:322:ILE:HD11	1:A:376:LEU:HD11	1.64	0.80
1:A:48:VAL:HG22	1:A:52:GLU:HG2	1.60	0.80
1:B:253:ASN:HD22	1:B:253:ASN:H	1.25	0.80
1:B:169:LYS:HD2	1:B:533:GLN:NE2	1.97	0.80
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.62	0.79
1:A:648:GLU:HB2	1:A:651:GLU:HG3	1.65	0.79
1:A:346:ARG:HD2	1:A:346:ARG:N	1.95	0.79
1:B:510:ARG:N	1:B:522:GLN:HE21	1.76	0.79
1:B:48:VAL:HG21	1:B:133:SER:HB3	1.63	0.79
1:A:46:ILE:HG22	1:A:83:ILE:HB	1.65	0.78
1:A:563:GLN:NE2	1:A:585:PHE:H	1.81	0.78
1:B:304:LYS:CE	1:B:304:LYS:H	1.98	0.77
1:B:677:LEU:HD11	3:B:2001:GM6:HAI2	1.67	0.77
1:B:712:LYS:CD	1:B:712:LYS:H	1.93	0.76
1:A:677:LEU:HD11	3:A:1001:GM6:HAI2	1.68	0.75
1:B:126:GLU:N	1:B:127:PRO:HD3	2.00	0.75
1:B:39:ILE:O	1:B:43:ILE:HG12	1.86	0.75
1:B:748:ASP:OD2	1:B:751:GLU:HG2	1.87	0.74
1:B:693:ASP:OD2	1:B:708:VAL:HG12	1.86	0.74
1:A:721:GLU:HA	1:A:724:ASN:ND2	2.03	0.74
1:A:704:GLN:HG2	1:A:705:SER:N	2.02	0.74
1:B:121:ALA:HB2	1:B:129:LEU:HD23	1.70	0.74
1:A:268:TYR:HB3	1:B:125:TYR:CE2	2.23	0.73
1:B:34:GLU:O	1:B:37:LYS:N	2.21	0.73
1:B:88:ILE:HD11	1:B:118:TYR:C	2.10	0.73
1:A:62:LEU:HD21	1:A:147:VAL:HG11	1.69	0.72
1:A:741:PHE:O	1:A:745:HIS:HD2	1.72	0.72
1:B:104:ILE:HG22	1:B:105:LYS:H	1.54	0.72
1:A:439:GLU:HB2	1:A:486:VAL:HG12	1.72	0.72
1:B:320:LYS:HB3	1:B:356:LEU:HD21	1.71	0.71
1:A:268:TYR:HB3	1:B:125:TYR:CZ	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LYS:HD2	1:B:82:TYR:HE2	1.56	0.71
1:A:322:ILE:CD1	1:A:376:LEU:HD11	2.21	0.71
1:A:317:GLU:HA	1:A:320:LYS:HE3	1.73	0.70
1:A:346:ARG:HD2	1:A:346:ARG:H	1.53	0.70
1:B:97:LEU:HD12	1:B:102:LYS:HG3	1.72	0.70
1:B:104:ILE:HG22	1:B:105:LYS:N	2.06	0.70
1:B:346:ARG:HH12	1:B:357:LEU:HD13	1.56	0.70
1:A:676:GLU:HA	1:A:676:GLU:OE1	1.92	0.70
1:B:169:LYS:HD2	1:B:533:GLN:HE22	1.57	0.69
1:A:55:LYS:HG2	1:A:133:SER:OG	1.93	0.69
1:A:275:LYS:NZ	1:A:279:GLN:HE22	1.90	0.69
1:A:103:LYS:HD2	1:A:111:ASP:HB3	1.73	0.69
1:A:753:LEU:O	1:A:756:GLN:HB3	1.93	0.69
1:A:675:VAL:HG22	3:A:1001:GM6:HAJ1	1.74	0.68
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.59	0.68
1:B:312:SER:OG	1:B:315:GLU:HG3	1.94	0.68
1:B:611:GLN:NE2	1:B:613:ASP:HB2	2.08	0.67
1:A:48:VAL:HG23	1:A:52:GLU:CG	2.18	0.67
1:A:349:LEU:O	1:A:352:GLU:HG2	1.95	0.67
1:B:643:TYR:HA	1:B:646:GLN:HG3	1.76	0.67
1:A:611:GLN:NE2	1:A:770:ILE:HG21	2.11	0.66
1:A:123:GLU:HG2	1:A:124:GLY:H	1.61	0.66
1:B:107:ILE:O	1:B:107:ILE:HD13	1.96	0.66
1:B:98:SER:O	1:B:101:LYS:HG3	1.96	0.66
1:B:677:LEU:HD11	3:B:2001:GM6:CAI	2.26	0.66
1:B:563:GLN:NE2	1:B:585:PHE:H	1.94	0.66
1:A:316:LYS:O	1:A:320:LYS:HG3	1.97	0.65
1:B:48:VAL:HG13	1:B:85:ASP:OD2	1.97	0.65
1:B:45:LYS:HD2	1:B:82:TYR:CE2	2.31	0.65
1:A:496:ASN:C	1:A:496:ASN:HD22	1.99	0.65
1:A:57:GLU:O	1:A:61:LYS:HG2	1.96	0.65
1:B:40:MET:O	1:B:44:VAL:HB	1.97	0.65
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.32	0.65
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.79	0.65
1:B:496:ASN:N	1:B:496:ASN:HD22	1.94	0.64
1:B:706:ASP:N	1:B:706:ASP:OD1	2.30	0.64
1:A:437:LEU:HD12	1:A:505:LEU:HD11	1.78	0.64
1:A:83:ILE:HD12	1:A:83:ILE:N	2.12	0.64
1:A:182:ASP:OD2	1:A:184:ASP:HB2	1.98	0.64
1:B:331:SER:OG	1:B:334:GLU:HG3	1.98	0.64
1:A:728:TYR:CE2	3:A:1001:GM6:HAH	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:HA	1:A:178:LYS:HG2	1.80	0.64
1:B:480:SER:HB3	1:B:525:ILE:HG22	1.78	0.64
1:A:312:SER:HB3	1:A:315:GLU:HG3	1.80	0.64
1:A:98:SER:O	1:A:102:LYS:HG3	1.98	0.63
1:A:48:VAL:HG22	1:A:52:GLU:CG	2.25	0.63
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.27	0.63
1:B:662:GLU:H	1:B:662:GLU:CD	2.02	0.63
1:B:496:ASN:H	1:B:496:ASN:HD22	1.47	0.63
1:B:474:ASN:HB3	1:B:597:GLU:HG3	1.80	0.63
1:A:268:TYR:HB3	1:B:125:TYR:OH	1.99	0.62
1:A:314:GLU:O	1:A:317:GLU:HB2	1.99	0.62
1:A:564:LEU:O	1:A:568:GLN:HG3	1.99	0.62
1:A:474:ASN:HB3	1:A:597:GLU:HG3	1.81	0.62
1:B:401:SER:OG	1:B:638:ASN:ND2	2.28	0.62
1:A:655:SER:HB2	3:A:1001:GM6:OAL	2.00	0.62
1:B:48:VAL:HG22	1:B:84:VAL:HA	1.78	0.62
1:B:126:GLU:N	1:B:127:PRO:CD	2.63	0.62
1:B:70:VAL:HG13	1:B:155:LEU:HD13	1.81	0.62
1:A:48:VAL:HG22	1:A:52:GLU:OE2	2.00	0.62
1:A:500:LYS:HE2	1:A:537:GLN:NE2	2.15	0.61
1:B:89:THR:HG22	1:B:95:GLU:HG2	1.82	0.61
1:B:655:SER:HB2	3:B:2001:GM6:OAL	1.99	0.61
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.35	0.61
1:A:535:ILE:HD13	1:A:544:ARG:HB2	1.83	0.61
1:B:167:TYR:CZ	1:B:203:VAL:HG21	2.36	0.61
1:B:249:GLU:O	1:B:250:GLN:HG3	2.00	0.61
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.31	0.61
1:B:578:LYS:O	1:B:579:TYR:HB2	2.01	0.61
1:B:34:GLU:O	1:B:36:LEU:N	2.34	0.61
1:B:98:SER:O	1:B:101:LYS:CG	2.49	0.60
1:A:322:ILE:HD11	1:A:376:LEU:CD1	2.30	0.60
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.66	0.60
1:B:48:VAL:HG23	1:B:84:VAL:CA	2.28	0.60
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.81	0.60
1:B:662:GLU:N	1:B:662:GLU:OE2	2.24	0.60
1:B:373:LYS:HG2	1:B:377:LYS:HE3	1.84	0.60
1:A:244:MET:HA	1:A:244:MET:HE3	1.83	0.60
1:B:608:ASN:C	1:B:609:ASN:HD22	2.05	0.60
1:A:263:ARG:HB2	1:A:266:SER:HB2	1.84	0.60
1:A:49:LYS:NZ	1:A:49:LYS:HB2	2.17	0.60
1:B:304:LYS:HE3	1:B:304:LYS:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:HB3	1:A:45:LYS:NZ	2.17	0.59
1:A:99:GLU:OE2	1:A:102:LYS:HE3	2.02	0.59
1:A:759:ALA:N	1:A:760:PRO:HD3	2.18	0.59
1:A:647:ASP:HB2	1:A:651:GLU:OE1	2.02	0.59
1:B:741:PHE:O	1:B:745:HIS:HD2	1.85	0.59
1:B:97:LEU:HD12	1:B:102:LYS:CG	2.32	0.59
1:A:715:ILE:O	1:A:719:LYS:HG3	2.02	0.59
1:B:97:LEU:HD12	1:B:102:LYS:CE	2.33	0.59
1:A:84:VAL:HG11	1:A:91:HIS:HD2	1.68	0.58
1:B:449:THR:HA	1:B:673:LYS:HD3	1.85	0.58
1:A:424:HIS:O	1:A:510:ARG:HD2	2.03	0.58
1:B:102:LYS:HA	1:B:114:LEU:CD1	2.34	0.58
1:A:103:LYS:HE3	1:A:113:LEU:CD2	2.33	0.58
1:A:737:PHE:CE1	1:A:766:ILE:HG12	2.39	0.58
1:A:107:ILE:HG12	1:A:149:TYR:CG	2.38	0.58
1:B:446:LEU:HG	1:B:591:TYR:HB2	1.85	0.58
1:B:97:LEU:HD12	1:B:102:LYS:HE3	1.85	0.58
1:B:264:MET:O	1:B:268:TYR:HD1	1.87	0.58
1:A:40:MET:HE3	1:A:63:LEU:HD12	1.84	0.58
1:A:97:LEU:HD23	1:A:98:SER:N	2.18	0.58
1:A:657:GLY:O	3:A:1001:GM6:HAC2	2.03	0.58
1:A:677:LEU:HD11	3:A:1001:GM6:CAI	2.33	0.58
1:A:696:ALA:HB2	1:A:773:ILE:HD11	1.86	0.58
1:B:35:HIS:O	1:B:39:ILE:HG13	2.04	0.58
1:A:767:ASN:O	1:A:771:LYS:HG3	2.03	0.58
1:A:691:ALA:O	1:A:694:ASP:HB3	2.04	0.57
1:B:104:ILE:CD1	1:B:114:LEU:CD2	2.40	0.57
1:A:119:VAL:HG12	1:A:131:ILE:HG12	1.84	0.57
1:A:35:HIS:HD2	1:A:68:SER:OG	1.87	0.57
1:A:577:PRO:O	1:A:580:THR:CG2	2.51	0.57
1:A:169:LYS:NZ	1:A:251:GLU:OE2	2.37	0.57
1:A:301:GLU:HG3	1:A:302:PRO:HD2	1.86	0.57
1:B:48:VAL:HG23	1:B:83:ILE:O	2.05	0.57
1:B:140:ASN:HD22	1:B:140:ASN:C	2.08	0.57
1:B:45:LYS:HB2	1:B:82:TYR:CD2	2.40	0.56
1:B:723:SER:CB	1:B:730:ARG:HD3	2.36	0.56
1:B:765:PHE:O	1:B:769:GLN:HG2	2.05	0.56
1:B:496:ASN:H	1:B:496:ASN:ND2	2.04	0.56
1:A:104:ILE:HG13	1:A:120:TYR:HE1	1.71	0.56
1:B:319:LEU:HD23	1:B:345:ILE:HG13	1.86	0.56
1:A:107:ILE:HG12	1:A:149:TYR:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:HIS:ND1	1:B:118:TYR:CD1	2.74	0.56
1:B:563:GLN:HE21	1:B:585:PHE:HB2	1.71	0.56
1:B:639:ILE:HG22	1:B:641:GLU:H	1.71	0.56
1:B:34:GLU:C	1:B:36:LEU:N	2.59	0.56
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.05	0.56
1:A:435:ILE:CD1	1:A:435:ILE:N	2.62	0.55
1:B:516:ASN:ND2	1:B:516:ASN:H	2.04	0.55
1:A:312:SER:HB3	1:A:315:GLU:CG	2.35	0.55
1:A:577:PRO:O	1:A:580:THR:HG23	2.07	0.55
1:A:348:SER:O	1:A:349:LEU:HB2	2.06	0.55
1:B:34:GLU:O	1:B:35:HIS:C	2.44	0.55
1:A:371:LYS:H	1:A:371:LYS:HD3	1.71	0.55
1:A:712:LYS:CD	1:A:713:LYS:H	2.17	0.55
1:B:339:LYS:O	1:B:343:ILE:HG12	2.06	0.55
1:B:440:ASN:HD21	1:B:500:LYS:NZ	2.05	0.55
1:A:675:VAL:CG2	3:A:1001:GM6:HAJ1	2.36	0.55
1:B:675:VAL:HG13	1:B:675:VAL:O	2.07	0.55
1:A:322:ILE:HD13	1:A:376:LEU:HD21	1.89	0.55
1:A:500:LYS:HE2	1:A:537:GLN:HE22	1.69	0.55
1:B:516:ASN:HD22	1:B:516:ASN:N	2.05	0.55
1:B:277:HIS:CD2	1:B:429:SER:HB2	2.42	0.55
1:A:84:VAL:HG11	1:A:91:HIS:CD2	2.42	0.54
1:B:186:GLN:HE21	1:B:195:LYS:HG2	1.72	0.54
1:A:420:ASP:OD1	1:A:523:ARG:HD3	2.07	0.54
1:B:332:THR:O	1:B:336:GLU:HG2	2.07	0.54
1:B:322:ILE:HD13	1:B:376:LEU:HD21	1.90	0.54
1:B:155:LEU:HA	1:B:159:ILE:HG13	1.89	0.54
1:A:65:LYS:HE2	1:A:227:PRO:HG2	1.88	0.54
1:A:618:VAL:O	1:A:622:LEU:HG	2.08	0.54
1:B:149:TYR:HA	1:B:222:ALA:HB2	1.89	0.54
1:B:440:ASN:ND2	1:B:500:LYS:HG2	2.23	0.54
1:A:352:GLU:HA	1:A:355:GLU:HG2	1.90	0.54
1:B:304:LYS:HE3	1:B:304:LYS:N	2.22	0.54
1:A:104:ILE:HG13	1:A:120:TYR:CE1	2.43	0.54
1:A:675:VAL:O	1:A:675:VAL:HG23	2.08	0.54
1:B:79:GLY:HA2	1:B:127:PRO:HB2	1.90	0.54
1:A:107:ILE:HG21	1:A:145:LEU:HD12	1.88	0.54
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.90	0.54
3:A:1001:GM6:HAJ2	3:A:1001:GM6:CAK	2.38	0.53
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.42	0.53
1:B:611:GLN:NE2	1:B:774:ILE:HD13	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LYS:O	1:B:320:LYS:HG3	2.08	0.53
1:A:379:LEU:O	1:A:383:ILE:HG12	2.08	0.53
1:A:178:LYS:HG3	1:A:179:ASN:N	2.23	0.53
1:B:516:ASN:ND2	1:B:516:ASN:N	2.57	0.53
1:A:48:VAL:HG11	1:A:55:LYS:HD3	1.90	0.53
1:A:584:THR:HG23	1:A:630:VAL:HG22	1.91	0.53
1:A:204:GLU:H	1:A:204:GLU:CD	2.11	0.53
1:B:37:LYS:O	1:B:41:LYS:N	2.42	0.53
1:A:662:GLU:OE2	1:A:662:GLU:N	2.29	0.53
1:B:46:ILE:HD11	1:B:56:LYS:HG3	1.90	0.53
1:A:614:LEU:O	1:A:618:VAL:HG23	2.09	0.53
3:B:2001:GM6:CAK	3:B:2001:GM6:HAJ2	2.39	0.52
1:B:347:ASP:O	1:B:347:ASP:OD1	2.28	0.52
1:B:392:LEU:HD21	1:B:416:ILE:HD13	1.91	0.52
1:A:675:VAL:HG13	3:A:1001:GM6:OAZ	2.08	0.52
1:A:67:PRO:HG2	1:A:248:ASN:OD1	2.10	0.52
1:B:726:THR:OG1	1:B:739:GLU:HG2	2.09	0.52
1:A:97:LEU:HD23	1:A:98:SER:H	1.75	0.52
1:A:268:TYR:CB	1:B:125:TYR:CE2	2.93	0.52
1:A:244:MET:HE2	1:A:248:ASN:HD21	1.74	0.52
1:A:768:ASP:HA	1:A:771:LYS:HE2	1.91	0.52
1:B:346:ARG:NH1	1:B:357:LEU:HD13	2.24	0.52
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.25	0.52
1:B:733:GLU:CD	1:B:733:GLU:H	2.11	0.52
1:A:70:VAL:HG12	1:A:252:ILE:HD11	1.91	0.52
1:A:658:LEU:HD22	1:A:659:TYR:N	2.25	0.52
1:B:749:HIS:HA	1:B:752:ARG:HD2	1.91	0.52
1:B:297:GLN:O	1:B:298:ILE:HD13	2.09	0.52
1:B:424:HIS:HA	1:B:510:ARG:HD2	1.92	0.52
1:B:723:SER:HA	1:B:730:ARG:CG	2.39	0.52
1:B:153:LYS:O	1:B:157:ARG:HB3	2.10	0.52
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.39	0.52
1:A:364:SER:O	1:A:365:SER:HB2	2.09	0.52
1:A:712:LYS:HD2	1:A:713:LYS:N	2.20	0.52
1:B:46:ILE:CD1	1:B:56:LYS:HG3	2.40	0.52
1:B:156:SER:HB3	1:B:217:PHE:CD2	2.45	0.52
1:A:612:SER:O	1:A:616:LYS:HG3	2.09	0.52
1:B:250:GLN:O	1:B:253:ASN:ND2	2.43	0.52
1:B:140:ASN:HD22	1:B:142:GLU:H	1.57	0.52
1:A:443:ILE:HD12	1:A:454:LEU:HD22	1.92	0.52
1:A:126:GLU:N	1:A:127:PRO:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:HG13	1:A:165:GLN:HG3	1.91	0.52
1:B:253:ASN:ND2	1:B:253:ASN:H	2.02	0.52
1:A:456:ASP:HB3	1:A:459:ASP:O	2.10	0.52
1:A:679:ASN:H	1:A:679:ASN:HD22	1.58	0.52
1:B:711:SER:O	1:B:715:ILE:HG13	2.10	0.51
1:B:726:THR:HG23	1:B:743:LEU:HD11	1.93	0.51
1:A:695:TYR:O	1:A:698:TYR:HB3	2.10	0.51
1:B:221:PHE:O	1:B:225:ILE:HG12	2.11	0.51
1:B:645:HIS:CD2	1:B:663:SER:HB3	2.45	0.51
1:A:45:LYS:HD2	1:A:82:TYR:CE2	2.46	0.51
1:A:412:TYR:O	1:A:416:ILE:HG13	2.11	0.51
1:B:564:LEU:O	1:B:568:GLN:HG3	2.10	0.51
1:B:104:ILE:CG2	1:B:105:LYS:N	2.74	0.51
1:B:726:THR:CG2	1:B:743:LEU:HD11	2.41	0.51
1:A:739:GLU:HA	1:A:739:GLU:OE1	2.11	0.51
1:B:104:ILE:CG2	1:B:105:LYS:H	2.22	0.51
1:B:88:ILE:HD11	1:B:118:TYR:CA	2.40	0.51
1:B:304:LYS:HE2	1:B:304:LYS:H	1.74	0.51
1:A:101:LYS:C	1:A:103:LYS:H	2.14	0.51
1:A:616:LYS:O	1:A:620:ASN:HB2	2.11	0.51
1:A:160:LEU:HB3	1:A:165:GLN:HB2	1.93	0.51
1:A:118:TYR:N	1:A:118:TYR:CD1	2.79	0.51
1:A:634:ILE:HD11	1:A:639:ILE:HD12	1.92	0.50
1:B:632:THR:OG1	1:B:634:ILE:HG12	2.11	0.50
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.11	0.50
1:A:119:VAL:HG11	1:A:147:VAL:HG22	1.92	0.50
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.45	0.50
1:A:43:ILE:HD11	1:A:71:LEU:HG	1.93	0.50
1:B:88:ILE:HG23	1:B:130:VAL:CG1	2.42	0.50
1:B:338:LEU:HD22	1:B:379:LEU:HD13	1.94	0.50
1:A:98:SER:HB2	1:A:100:ASP:OD1	2.11	0.50
1:A:656:LYS:O	1:A:656:LYS:HD3	2.11	0.50
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.76	0.50
1:A:441:MET:O	1:A:499:LEU:HB2	2.11	0.50
1:B:212:GLU:O	1:B:216:VAL:HG23	2.12	0.50
1:A:675:VAL:HG22	3:A:1001:GM6:CAJ	2.40	0.49
1:A:99:GLU:HA	1:A:102:LYS:CE	2.42	0.49
1:B:741:PHE:O	1:B:745:HIS:CD2	2.65	0.49
1:B:721:GLU:OE1	1:B:761:LYS:HG2	2.12	0.49
1:B:117:HIS:ND1	1:B:118:TYR:N	2.54	0.49
1:B:500:LYS:HE3	1:B:537:GLN:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HD21	1:B:68:SER:OG	2.12	0.49
1:B:67:PRO:HB2	1:B:70:VAL:HG23	1.95	0.49
1:A:187:ASP:HA	1:A:195:LYS:NZ	2.28	0.49
1:B:244:MET:CE	1:B:248:ASN:HD21	2.26	0.49
1:A:333:GLU:OE2	1:A:333:GLU:HA	2.12	0.49
1:B:723:SER:HB3	1:B:730:ARG:HD3	1.95	0.49
1:B:440:ASN:HD21	1:B:500:LYS:HZ2	1.60	0.49
1:B:129:LEU:HD11	1:B:131:ILE:HD11	1.95	0.48
1:B:55:LYS:O	1:B:58:ALA:HB3	2.12	0.48
1:A:313:GLN:H	1:A:313:GLN:CD	2.17	0.48
1:A:171:LEU:HD21	1:A:201:PHE:HB2	1.95	0.48
1:B:33:GLU:HA	1:B:36:LEU:HB2	1.95	0.48
1:B:303:LYS:HB2	1:B:306:ASP:OD2	2.13	0.48
1:A:354:LYS:HD2	1:A:358:ASN:OD1	2.14	0.48
1:A:101:LYS:O	1:A:103:LYS:N	2.46	0.48
1:A:40:MET:O	1:A:44:VAL:HB	2.14	0.48
1:B:145:LEU:HD23	1:B:222:ALA:HB1	1.95	0.48
1:A:730:ARG:HG2	1:A:730:ARG:O	2.13	0.48
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.48	0.48
1:B:723:SER:HA	1:B:730:ARG:HG2	1.95	0.48
1:A:394:ASP:O	1:A:634:ILE:HB	2.13	0.48
1:B:609:ASN:N	1:B:609:ASN:HD22	2.11	0.48
1:A:67:PRO:HB2	1:A:70:VAL:HG13	1.95	0.48
1:A:323:GLN:HG2	1:A:325:ASP:H	1.78	0.48
1:B:36:LEU:O	1:B:40:MET:HG3	2.14	0.48
1:B:45:LYS:HB2	1:B:82:TYR:CE2	2.49	0.48
1:A:48:VAL:HG22	1:A:52:GLU:CD	2.34	0.48
1:A:87:ASP:OD2	1:A:115:HIS:HA	2.15	0.47
1:B:186:GLN:HG3	1:B:190:PHE:CD1	2.48	0.47
1:A:307:ILE:HG21	1:A:341:LEU:CD1	2.45	0.47
1:B:645:HIS:NE2	1:B:663:SER:HB3	2.30	0.47
1:A:94:LEU:HD22	1:A:97:LEU:HD12	1.97	0.47
1:A:437:LEU:HD12	1:A:505:LEU:CD1	2.44	0.47
1:A:490:GLU:OE2	1:A:500:LYS:HE3	2.15	0.47
1:B:381:LEU:HD11	1:B:650:TYR:HA	1.96	0.47
1:B:696:ALA:HB2	1:B:773:ILE:HD11	1.96	0.47
1:B:33:GLU:C	1:B:36:LEU:HB2	2.36	0.47
1:B:759:ALA:N	1:B:760:PRO:HD3	2.30	0.47
1:A:536:LYS:HG3	1:A:537:GLN:N	2.29	0.47
1:A:437:LEU:CD1	1:A:505:LEU:HD11	2.45	0.46
1:B:769:GLN:NE2	1:B:769:GLN:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LYS:O	1:A:307:ILE:HG12	2.15	0.46
1:B:253:ASN:N	1:B:253:ASN:HD22	2.00	0.46
1:A:369:SER:OG	1:A:372:GLU:HG2	2.14	0.46
1:B:50:GLY:O	1:B:55:LYS:NZ	2.48	0.46
1:A:366:ASN:N	1:A:367:PRO:CD	2.79	0.46
1:B:210:SER:O	1:B:214:GLN:HG3	2.16	0.46
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.96	0.46
1:A:501:TRP:HB3	1:A:503:ILE:CD1	2.40	0.46
1:B:149:TYR:HE1	1:B:219:LYS:HG3	1.81	0.46
1:A:660:VAL:HG12	1:A:663:SER:H	1.81	0.46
1:B:420:ASP:OD2	1:B:523:ARG:NH1	2.49	0.46
1:B:87:ASP:OD2	1:B:115:HIS:HA	2.16	0.46
1:B:578:LYS:O	1:B:579:TYR:CB	2.64	0.46
1:B:38:GLU:OE1	1:B:42:HIS:HB2	2.16	0.46
1:A:313:GLN:O	1:A:317:GLU:HG3	2.16	0.45
1:A:301:GLU:HG3	1:A:302:PRO:CD	2.46	0.45
1:B:57:GLU:HA	1:B:60:GLU:HB3	1.97	0.45
1:A:95:GLU:C	1:A:97:LEU:H	2.20	0.45
1:A:360:ILE:O	1:A:364:SER:HB2	2.16	0.45
1:B:612:SER:O	1:B:616:LYS:HD3	2.16	0.45
1:B:559:ILE:HD13	1:B:587:VAL:HB	1.98	0.45
1:A:94:LEU:O	1:A:97:LEU:HB2	2.16	0.45
1:B:118:TYR:HA	1:B:132:GLN:HG3	1.98	0.45
1:A:721:GLU:CA	1:A:724:ASN:HD22	2.19	0.45
1:A:103:LYS:HE3	1:A:113:LEU:HD23	1.98	0.45
1:A:679:ASN:ND2	1:A:682:GLU:H	2.14	0.45
1:B:639:ILE:CG2	1:B:641:GLU:H	2.30	0.45
1:B:666:ILE:HD12	1:B:687:CYS:HB3	1.98	0.45
1:A:446:LEU:HG	1:A:591:TYR:HB2	1.98	0.45
1:B:104:ILE:HD11	1:B:114:LEU:CG	2.39	0.45
1:B:122:LYS:HB3	1:B:128:VAL:HG22	1.98	0.45
1:B:614:LEU:O	1:B:618:VAL:HG23	2.17	0.45
1:B:84:VAL:HG22	1:B:85:ASP:N	2.32	0.45
1:A:354:LYS:NZ	1:A:357:LEU:HD23	2.32	0.45
1:B:77:ILE:HD13	1:B:259:LEU:HD21	1.98	0.45
1:B:77:ILE:CG2	1:B:127:PRO:HG2	2.46	0.45
1:B:501:TRP:HB3	1:B:503:ILE:CD1	2.46	0.45
1:A:45:LYS:HB3	1:A:45:LYS:HZ3	1.80	0.45
1:B:350:SER:O	1:B:353:GLU:N	2.50	0.45
1:A:480:SER:OG	1:A:484:MET:HG3	2.17	0.45
1:B:117:HIS:CE1	1:B:118:TYR:CE1	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:PRO:HB2	1:A:580:THR:HG22	1.98	0.45
1:B:149:TYR:CZ	1:B:153:LYS:HE3	2.52	0.45
1:B:659:TYR:HD1	1:B:666:ILE:HD13	1.82	0.45
1:B:231:ASP:O	1:B:235:LEU:HB2	2.17	0.45
1:B:122:LYS:HE2	1:B:128:VAL:HG22	1.99	0.45
1:A:443:ILE:CD1	1:A:454:LEU:HD22	2.47	0.45
1:A:437:LEU:CD1	1:A:519:LEU:HD12	2.47	0.45
1:A:90:LYS:HG2	1:A:90:LYS:O	2.17	0.45
1:A:741:PHE:O	1:A:745:HIS:CD2	2.62	0.44
1:A:329:PHE:CD1	1:A:330:LEU:HG	2.52	0.44
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.17	0.44
1:A:204:GLU:O	1:A:208:GLN:HG2	2.18	0.44
1:B:387:ASP:HB3	1:B:390:GLN:HB3	1.98	0.44
1:B:48:VAL:CG2	1:B:84:VAL:CA	2.83	0.44
1:A:167:TYR:OH	1:A:536:LYS:HE2	2.18	0.44
1:A:40:MET:CE	1:A:63:LEU:HD12	2.47	0.44
1:A:118:TYR:CE2	1:A:143:LYS:HA	2.53	0.44
1:B:97:LEU:HD12	1:B:102:LYS:CD	2.47	0.44
1:B:143:LYS:O	1:B:147:VAL:HG23	2.17	0.44
1:B:606:TRP:CH2	1:B:615:ILE:HG23	2.51	0.44
1:A:686:HIS:HB2	1:A:742:ARG:HD3	1.99	0.44
1:A:598:SER:O	1:A:602:ILE:HG13	2.17	0.44
1:B:123:GLU:CD	1:B:157:ARG:HD2	2.38	0.44
1:A:215:GLU:HG3	1:A:219:LYS:HE3	1.98	0.44
1:A:323:GLN:NE2	1:A:325:ASP:HB2	2.31	0.44
1:B:51:GLU:OE2	1:B:53:ALA:CB	2.54	0.44
1:B:81:ILE:HG23	1:B:129:LEU:HD12	1.99	0.44
1:B:609:ASN:C	1:B:610:ILE:HG13	2.38	0.44
1:A:149:TYR:HA	1:A:222:ALA:HB2	1.98	0.44
1:B:769:GLN:HE21	1:B:769:GLN:HA	1.83	0.44
1:A:371:LYS:H	1:A:371:LYS:CD	2.31	0.44
1:B:38:GLU:O	1:B:38:GLU:OE1	2.35	0.44
1:B:97:LEU:CD1	1:B:114:LEU:HD12	2.48	0.44
1:A:677:LEU:O	1:A:678:ARG:C	2.56	0.44
1:A:566:ILE:HD13	1:A:583:ILE:HG21	2.00	0.44
1:B:33:GLU:CA	1:B:36:LEU:HB2	2.48	0.44
1:A:225:ILE:O	1:A:227:PRO:HD3	2.18	0.44
1:B:123:GLU:HG3	1:B:157:ARG:NE	2.33	0.44
1:A:637:PRO:HD3	1:A:654:HIS:HB2	2.00	0.44
1:B:136:ASP:HB2	1:B:143:LYS:HD2	1.99	0.44
1:B:513:TYR:HA	1:B:519:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:TYR:HA	1:A:646:GLN:HG3	2.00	0.43
1:B:104:ILE:CG1	1:B:114:LEU:CD2	2.96	0.43
1:B:37:LYS:O	1:B:41:LYS:CB	2.66	0.43
1:B:43:ILE:HA	1:B:80:LYS:HD3	1.99	0.43
1:A:437:LEU:HD11	1:A:519:LEU:HD12	2.00	0.43
1:A:94:LEU:HD21	1:A:122:LYS:HB2	1.99	0.43
1:A:433:ASN:O	1:A:435:ILE:HG13	2.17	0.43
1:A:46:ILE:O	1:A:46:ILE:HD12	2.18	0.43
1:A:693:ASP:HB2	1:A:737:PHE:CD2	2.54	0.43
1:B:343:ILE:O	1:B:347:ASP:HB2	2.19	0.43
1:B:104:ILE:HD11	1:B:114:LEU:HD23	0.60	0.43
1:B:48:VAL:CG2	1:B:133:SER:HB3	2.41	0.43
1:A:315:GLU:O	1:A:318:LEU:N	2.51	0.43
1:B:126:GLU:O	1:B:128:VAL:HG13	2.19	0.43
1:A:354:LYS:HD2	1:A:358:ASN:HD21	1.82	0.43
1:B:33:GLU:HA	1:B:36:LEU:HD12	2.01	0.43
1:A:275:LYS:HZ2	1:A:279:GLN:HE22	1.62	0.43
1:A:366:ASN:O	1:A:367:PRO:O	2.36	0.43
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.53	0.43
1:B:712:LYS:HA	1:B:715:ILE:HD12	1.99	0.43
1:A:107:ILE:HG22	1:A:108:TYR:CD1	2.52	0.43
1:A:686:HIS:ND1	1:A:739:GLU:OE1	2.47	0.43
1:A:637:PRO:CD	1:A:654:HIS:HB2	2.48	0.43
1:A:192:ASN:HA	1:A:195:LYS:HB2	2.00	0.43
1:A:293:LEU:HD22	1:A:520:ILE:HD12	2.01	0.43
1:B:197:HIS:HA	1:B:198:PRO:HD3	1.87	0.43
1:B:226:GLU:OE1	1:B:228:GLN:HB2	2.18	0.43
1:B:184:ASP:HB3	1:B:236:TYR:HD1	1.84	0.43
1:A:176:THR:O	1:A:180:ALA:HB2	2.19	0.42
1:B:391:ARG:HG3	1:B:412:TYR:CE1	2.54	0.42
1:A:145:LEU:O	1:A:145:LEU:HD13	2.19	0.42
1:B:739:GLU:OE2	1:B:739:GLU:HA	2.19	0.42
1:A:121:ALA:HB2	1:A:150:GLU:HG3	2.01	0.42
1:A:563:GLN:HE21	1:A:585:PHE:N	1.93	0.42
1:A:496:ASN:C	1:A:496:ASN:ND2	2.70	0.42
1:B:69:ASP:O	1:B:73:MET:HG3	2.19	0.42
1:B:84:VAL:O	1:B:132:GLN:HA	2.19	0.42
1:A:372:GLU:O	1:A:375:PHE:HB3	2.20	0.42
1:A:655:SER:HB2	3:A:1001:GM6:CAK	2.50	0.42
1:B:89:THR:C	1:B:91:HIS:H	2.23	0.42
1:B:293:LEU:HD21	1:B:422:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LEU:CD2	1:B:742:ARG:CZ	2.97	0.42
1:B:398:LEU:O	1:B:401:SER:HB3	2.19	0.42
1:A:107:ILE:HG13	1:A:145:LEU:CD1	2.49	0.42
1:A:771:LYS:C	1:A:773:ILE:H	2.23	0.42
1:A:399:ILE:HD12	1:A:413:LYS:HG3	2.01	0.42
1:A:298:ILE:HG13	1:A:298:ILE:O	2.19	0.42
1:B:65:LYS:HB2	1:B:148:TYR:OH	2.19	0.42
1:B:655:SER:HB2	3:B:2001:GM6:CAK	2.50	0.42
1:A:307:ILE:HG21	1:A:341:LEU:HD11	2.02	0.42
1:A:292:LEU:HD22	1:A:419:ILE:HD11	2.02	0.42
1:B:104:ILE:O	1:B:111:ASP:HA	2.19	0.42
1:A:352:GLU:O	1:A:355:GLU:HG2	2.19	0.42
1:B:278:TYR:CE2	1:B:425:GLN:HB3	2.54	0.42
1:A:83:ILE:CD1	1:A:83:ILE:N	2.82	0.42
1:A:415:ASP:O	1:A:419:ILE:HG13	2.20	0.42
1:A:679:ASN:N	1:A:679:ASN:HD22	2.17	0.42
1:B:278:TYR:HE2	1:B:425:GLN:HB3	1.85	0.42
1:A:119:VAL:CG1	1:A:147:VAL:HG22	2.49	0.41
1:B:229:HIS:O	1:B:232:VAL:HB	2.20	0.41
1:B:34:GLU:C	1:B:36:LEU:H	2.24	0.41
1:B:186:GLN:O	1:B:190:PHE:HB2	2.20	0.41
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.34	0.41
1:B:296:LEU:HD23	1:B:520:ILE:HD12	2.01	0.41
1:B:269:GLU:HG3	1:B:273:LYS:HE3	2.02	0.41
1:B:657:GLY:O	1:B:658:LEU:HB2	2.19	0.41
1:B:762:THR:O	1:B:763:PHE:C	2.59	0.41
1:B:314:GLU:O	1:B:318:LEU:HD13	2.20	0.41
1:A:187:ASP:HA	1:A:195:LYS:CE	2.50	0.41
1:A:30:LYS:CD	1:A:33:GLU:HG3	2.36	0.41
1:B:140:ASN:OD1	1:B:143:LYS:HG3	2.19	0.41
1:B:57:GLU:HG2	1:B:57:GLU:O	2.21	0.41
1:A:135:GLU:O	1:A:135:GLU:HG2	2.20	0.41
1:B:50:GLY:O	1:B:55:LYS:CE	2.68	0.41
1:A:173:VAL:O	1:A:177:ILE:HG12	2.20	0.41
1:B:59:ALA:O	1:B:62:LEU:HB3	2.20	0.41
1:B:713:LYS:HE3	1:B:713:LYS:HB2	1.90	0.41
1:A:323:GLN:HA	1:A:324:ILE:HD12	2.01	0.41
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.34	0.41
1:B:145:LEU:CD2	1:B:222:ALA:HB1	2.50	0.41
1:A:187:ASP:HA	1:A:195:LYS:HE2	2.03	0.41
1:A:627:GLY:HA3	1:A:664:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:NE2	1:A:193:GLN:HA	2.35	0.41
1:A:324:ILE:CD1	1:A:324:ILE:N	2.50	0.41
1:B:88:ILE:HG23	1:B:130:VAL:HG11	2.01	0.41
1:A:753:LEU:O	1:A:756:GLN:N	2.53	0.41
1:A:749:HIS:O	1:A:752:ARG:HB2	2.21	0.41
1:A:321:ARG:HD2	1:A:321:ARG:HA	1.85	0.41
1:A:243:TYR:C	1:A:243:TYR:CD1	2.93	0.41
1:A:701:ASP:HB3	1:A:703:ASN:OD1	2.21	0.41
1:A:322:ILE:CD1	1:A:376:LEU:CD1	2.95	0.41
1:B:169:LYS:O	1:B:172:ASP:HB2	2.21	0.41
1:B:320:LYS:HG2	1:B:345:ILE:CG2	2.51	0.41
1:B:713:LYS:O	1:B:717:ILE:HG12	2.20	0.41
1:A:92:ILE:HG13	1:A:92:ILE:H	1.55	0.41
1:B:554:LYS:HA	1:B:554:LYS:HD2	1.79	0.41
1:B:609:ASN:N	1:B:609:ASN:ND2	2.68	0.41
1:A:404:ILE:HD13	1:A:404:ILE:N	2.35	0.41
1:B:436:TYR:HA	1:B:503:ILE:O	2.21	0.40
1:A:640:ALA:C	1:A:642:GLN:N	2.75	0.40
1:B:135:GLU:O	1:B:135:GLU:HG3	2.21	0.40
1:A:681:SER:O	1:A:682:GLU:C	2.59	0.40
1:A:639:ILE:HG23	1:A:641:GLU:OE1	2.21	0.40
1:A:174:LEU:HD11	1:A:213:VAL:HG13	2.02	0.40
1:B:118:TYR:CD1	1:B:118:TYR:N	2.89	0.40
1:B:48:VAL:HG23	1:B:83:ILE:C	2.42	0.40
1:B:88:ILE:HG22	1:B:94:LEU:CD2	2.51	0.40
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.78	0.40
1:B:519:LEU:HD23	1:B:519:LEU:HA	1.90	0.40
1:B:99:GLU:OE1	1:B:99:GLU:HA	2.20	0.40
1:B:744:MET:HB3	1:B:744:MET:HE2	1.96	0.40
1:A:94:LEU:HD12	1:A:130:VAL:HG21	2.03	0.40
1:A:97:LEU:HD22	1:A:98:SER:O	2.21	0.40
1:B:329:PHE:HE2	1:B:373:LYS:HG3	1.86	0.40
1:A:371:LYS:HD3	1:A:371:LYS:N	2.35	0.40
1:B:602:ILE:HD11	1:B:680:ASP:HB2	2.02	0.40
1:A:244:MET:HE3	1:A:244:MET:CA	2.51	0.40
1:A:755:VAL:HG13	1:A:759:ALA:HB3	2.02	0.40
1:A:392:LEU:HD21	1:A:416:ILE:HD13	2.04	0.40
1:B:369:SER:OG	1:B:372:GLU:HG3	2.22	0.40
1:A:155:LEU:HD12	1:A:159:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	745/776 (96%)	655 (88%)	66 (9%)	24 (3%)	5	12
1	B	732/776 (94%)	659 (90%)	60 (8%)	13 (2%)	11	27
All	All	1477/1552 (95%)	1314 (89%)	126 (8%)	37 (2%)	7	18

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	367	PRO
1	A	370	GLU
1	A	473	LYS
1	B	34	GLU
1	B	51	GLU
1	B	123	GLU
1	B	350	SER
1	A	198	PRO
1	A	251	GLU
1	A	311	LEU
1	A	349	LEU
1	A	365	SER
1	A	676	GLU
1	A	723	SER
1	B	35	HIS
1	B	198	PRO
1	B	251	GLU
1	A	123	GLU
1	A	371	LYS
1	A	678	ARG
1	A	733	GLU
1	B	50	GLY
1	B	58	ALA
1	B	367	PRO

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Mol	Chain	Res	Type
1	A	36	LEU
1	A	96	ALA
1	A	346	ARG
1	A	369	SER
1	B	349	LEU
1	A	700	LEU
1	A	307	ILE
1	A	726	THR
1	A	772	PHE
1	B	250	GLN
1	B	126	GLU
1	A	675	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	686/710 (97%)	640 (93%)	46 (7%)	20	44
1	B	675/710 (95%)	641 (95%)	34 (5%)	30	60
All	All	1361/1420 (96%)	1281 (94%)	80 (6%)	24	51

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	60	GLU
1	A	107	ILE
1	A	118	TYR
1	A	119	VAL
1	A	142	GLU
1	A	171	LEU
1	A	208	GLN
1	A	233	LEU
1	A	256	LEU
1	A	259	LEU

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Mol	Chain	Res	Type
1	A	266	SER
1	A	296	LEU
1	A	301	GLU
1	A	306	ASP
1	A	319	LEU
1	A	322	ILE
1	A	324	ILE
1	A	326	SER
1	A	346	ARG
1	A	348	SER
1	A	359	ARG
1	A	371	LYS
1	A	404	ILE
1	A	411	GLN
1	A	435	ILE
1	A	446	LEU
1	A	447	THR
1	A	449	THR
1	A	494	LEU
1	A	496	ASN
1	A	499	LEU
1	A	523	ARG
1	A	564	LEU
1	A	580	THR
1	A	582	LEU
1	A	584	THR
1	A	619	THR
1	A	636	LEU
1	A	656	LYS
1	A	658	LEU
1	A	679	ASN
1	A	710	ASN
1	A	712	LYS
1	A	757	LYS
1	A	769	GLN
1	B	38	GLU
1	B	49	LYS
1	B	52	GLU
1	B	85	ASP
1	B	95	GLU
1	B	103	LYS
1	B	107	ILE

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Mol	Chain	Res	Type
1	B	118	TYR
1	B	136	ASP
1	B	140	ASN
1	B	142	GLU
1	B	145	LEU
1	B	159	ILE
1	B	231	ASP
1	B	233	LEU
1	B	253	ASN
1	B	256	LEU
1	B	304	LYS
1	B	305	ASP
1	B	348	SER
1	B	354	LYS
1	B	391	ARG
1	B	398	LEU
1	B	425	GLN
1	B	447	THR
1	B	496	ASN
1	B	516	ASN
1	B	523	ARG
1	B	611	GLN
1	B	676	GLU
1	B	679	ASN
1	B	698	TYR
1	B	706	ASP
1	B	712	LYS

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	35	HIS
1	A	42	HIS
1	A	164	ASN
1	A	193	GLN
1	A	209	ASN
1	A	214	GLN
1	A	242	ASN
1	A	248	ASN
1	A	276	GLN
1	A	277	HIS
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	313	GLN
1	A	342	GLN
1	A	496	ASN
1	A	504	GLN
1	A	524	ASN
1	A	537	GLN
1	A	563	GLN
1	A	571	ASN
1	A	588	HIS
1	A	589	ASN
1	A	608	ASN
1	A	646	GLN
1	A	652	GLN
1	A	679	ASN
1	A	710	ASN
1	A	724	ASN
1	A	745	HIS
1	A	767	ASN
1	A	769	GLN
1	B	115	HIS
1	B	164	ASN
1	B	186	GLN
1	B	193	GLN
1	B	197	HIS
1	B	214	GLN
1	B	234	GLN
1	B	242	ASN
1	B	248	ASN
1	B	253	ASN
1	B	262	GLN
1	B	277	HIS
1	B	279	GLN
1	B	297	GLN
1	B	313	GLN
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	464	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN

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Mol	Chain	Res	Type
1	B	524	ASN
1	B	533	GLN
1	B	563	GLN
1	B	571	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	638	ASN
1	B	679	ASN
1	B	710	ASN
1	B	745	HIS
1	B	756	GLN
1	B	767	ASN
1	B	769	GLN
1	B	775	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	GM6	A	1001	2	28,29,29	1.01	1 (3%)	25,39,39	0.81	1 (4%)
3	GM6	B	2001	2	28,29,29	1.05	1 (3%)	25,39,39	0.80	1 (4%)

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	GM6	A	1001	2	-	2/27/28/28	0/2/2/2
3	GM6	B	2001	2	-	2/27/28/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	GM6	CAT-CAP	-2.86	1.33	1.38
3	A	1001	GM6	CAT-CAP	-2.61	1.33	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	GM6	CBA-NBB-CAY	-2.61	117.49	122.23
3	A	1001	GM6	CBA-NBB-CAY	-2.59	117.53	122.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	GM6	CAN-CAY-NBB-CBA
3	A	1001	GM6	CAN-CAY-NBB-CBA
3	B	2001	GM6	OAZ-CAY-NBB-CBA
3	A	1001	GM6	OAZ-CAY-NBB-CBA

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	GM6	11	0
3	B	2001	GM6	5	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	747/776 (96%)	0.47	74 (9%) <b>9</b> <b>7</b>	21, 58, 126, 154	0
1	B	736/776 (94%)	0.29	60 (8%) <b>14</b> <b>11</b>	21, 51, 120, 152	0
All	All	1483/1552 (95%)	0.38	134 (9%) <b>12</b> <b>9</b>	21, 54, 123, 154	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	ILE	10.2
1	A	362	VAL	8.6
1	B	48	VAL	8.1
1	B	356	LEU	6.7
1	A	324	ILE	6.5
1	A	356	LEU	6.1
1	A	363	ASP	5.8
1	A	367	PRO	5.8
1	B	49	LYS	5.7
1	B	84	VAL	5.5
1	A	319	LEU	5.4
1	A	322	ILE	5.3
1	B	54	VAL	5.2
1	B	34	GLU	5.2
1	B	98	SER	5.2
1	B	37	LYS	5.2
1	A	364	SER	5.1
1	B	52	GLU	5.0
1	B	88	ILE	4.8
1	A	358	ASN	4.7
1	B	50	GLY	4.7
1	A	54	VAL	4.7
1	A	180	ALA	4.7
1	B	114	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	320	LYS	4.6
1	A	48	VAL	4.6
1	B	367	PRO	4.6
1	B	353	GLU	4.5
1	A	33	GLU	4.5
1	B	53	ALA	4.4
1	A	357	LEU	4.1
1	A	368	LEU	4.1
1	A	359	ARG	4.0
1	B	352	GLU	4.0
1	B	703	ASN	4.0
1	A	30	LYS	3.9
1	B	51	GLU	3.8
1	A	53	ALA	3.8
1	B	56	LYS	3.7
1	B	350	SER	3.7
1	A	51	GLU	3.7
1	A	52	GLU	3.7
1	A	345	ILE	3.7
1	B	349	LEU	3.6
1	A	347	ASP	3.6
1	B	35	HIS	3.6
1	A	351	GLU	3.6
1	B	36	LEU	3.6
1	A	365	SER	3.5
1	A	703	ASN	3.5
1	B	355	GLU	3.5
1	A	354	LYS	3.4
1	A	318	LEU	3.4
1	A	361	GLN	3.4
1	B	94	LEU	3.4
1	A	100	ASP	3.4
1	B	46	ILE	3.3
1	A	312	SER	3.3
1	A	304	LYS	3.3
1	B	135	GLU	3.2
1	A	310	SER	3.2
1	B	354	LYS	3.2
1	A	37	LYS	3.2
1	A	49	LYS	3.2
1	A	56	LYS	3.2
1	A	309	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	36	LEU	3.1
1	A	366	ASN	3.1
1	B	345	ILE	3.1
1	A	55	LYS	3.1
1	B	321	ARG	3.0
1	A	353	GLU	3.0
1	A	341	LEU	2.9
1	B	199	THR	2.9
1	A	50	GLY	2.9
1	A	98	SER	2.9
1	B	132	GLN	2.9
1	A	303	LYS	2.9
1	A	32	GLN	2.9
1	B	351	GLU	2.8
1	A	41	LYS	2.8
1	A	306	ASP	2.8
1	A	198	PRO	2.8
1	B	113	LEU	2.8
1	B	131	ILE	2.8
1	A	346	ARG	2.8
1	B	101	LYS	2.7
1	B	357	LEU	2.7
1	B	83	ILE	2.7
1	B	324	ILE	2.7
1	A	352	GLU	2.7
1	A	313	GLN	2.6
1	B	59	ALA	2.6
1	B	139	GLU	2.6
1	A	308	ILE	2.6
1	B	704	GLN	2.6
1	B	93	SER	2.5
1	A	94	LEU	2.5
1	B	138	VAL	2.5
1	B	371	LYS	2.5
1	B	702	LYS	2.5
1	B	346	ARG	2.4
1	A	181	SER	2.4
1	A	95	GLU	2.4
1	B	60	GLU	2.3
1	A	713	LYS	2.3
1	A	327	SER	2.3
1	A	348	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	133	SER	2.3
1	B	235	LEU	2.3
1	A	321	ARG	2.3
1	B	97	LEU	2.3
1	B	82	TYR	2.3
1	A	84	VAL	2.3
1	A	97	LEU	2.2
1	A	702	LYS	2.2
1	A	701	ASP	2.2
1	A	135	GLU	2.2
1	A	330	LEU	2.2
1	A	579	TYR	2.2
1	B	45	LYS	2.2
1	A	355	GLU	2.2
1	B	40	MET	2.2
1	B	130	VAL	2.1
1	B	323	GLN	2.1
1	B	198	PRO	2.1
1	A	344	ASP	2.1
1	A	101	LYS	2.1
1	A	342	GLN	2.1
1	B	329	PHE	2.1
1	B	700	LEU	2.0
1	A	114	LEU	2.0
1	B	39	ILE	2.0
1	A	329	PHE	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	GM6	B	2001	28/28	0.87	0.30	3.19	95,98,102,103	0
3	GM6	A	1001	28/28	0.78	0.31	2.90	96,98,103,103	0
2	ZN	A	9001	1/1	0.98	0.10	-	84,84,84,84	0
2	ZN	B	9002	1/1	0.99	0.09	-	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.