



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 07:47 AM EDT

PDB ID : 3VB9  
Title : Crystal structure of VPA0735 from *Vibrio parahaemolyticus* in monoclinic form, NorthEast Structural Genomics target VpR109  
Authors : Seetharaman, J.; Neely, H.; Cunningham, K.; Ciccocanti, C.; Bjelic, S.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2011-12-31  
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

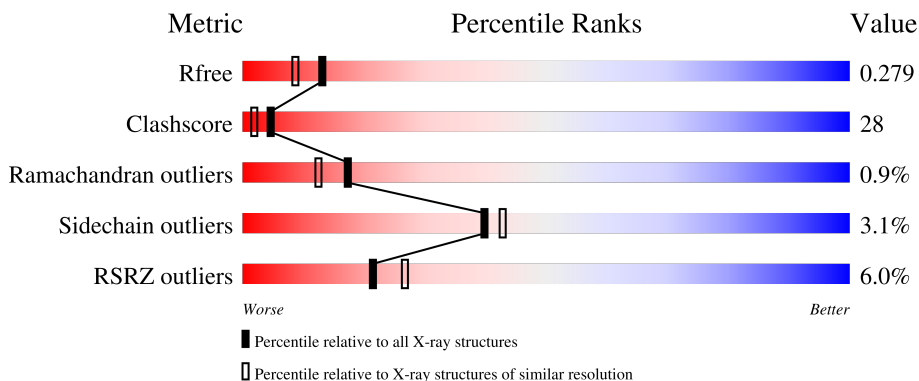
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	483	 5% 52% 41% • 5%
1	B	483	 9% 51% 42% • •
1	C	483	 5% 56% 36% • 5%
1	D	483	 4% 61% 33% • 5%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15733 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 Uncharacterized protein VPA0735.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	460	3717	2382	623	698	14	0	0	0
1	B	462	3736	2393	627	702	14	0	0	0
1	C	460	3717	2382	623	698	14	0	0	0
1	D	460	3717	2382	623	698	14	0	0	0

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

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

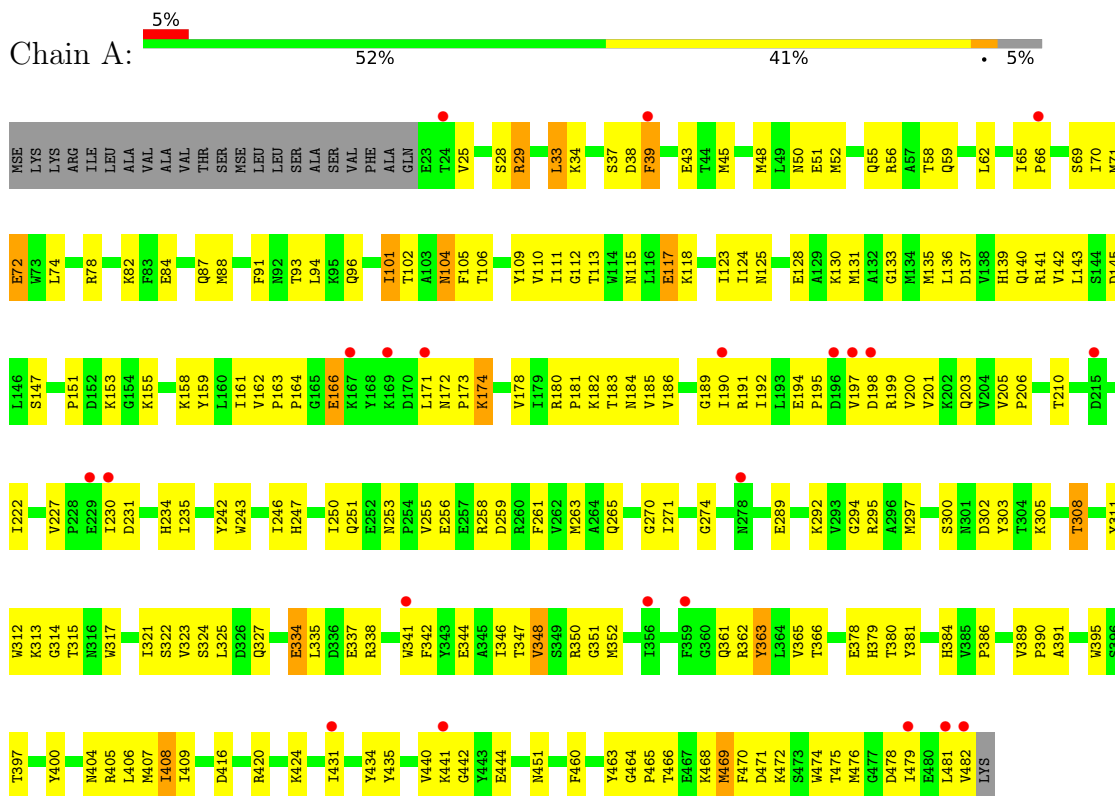
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total 197	O 197	0	0
3	B	217	Total 217	O 217	0	0
3	C	190	Total 190	O 190	0	0
3	D	235	Total 235	O 235	0	0

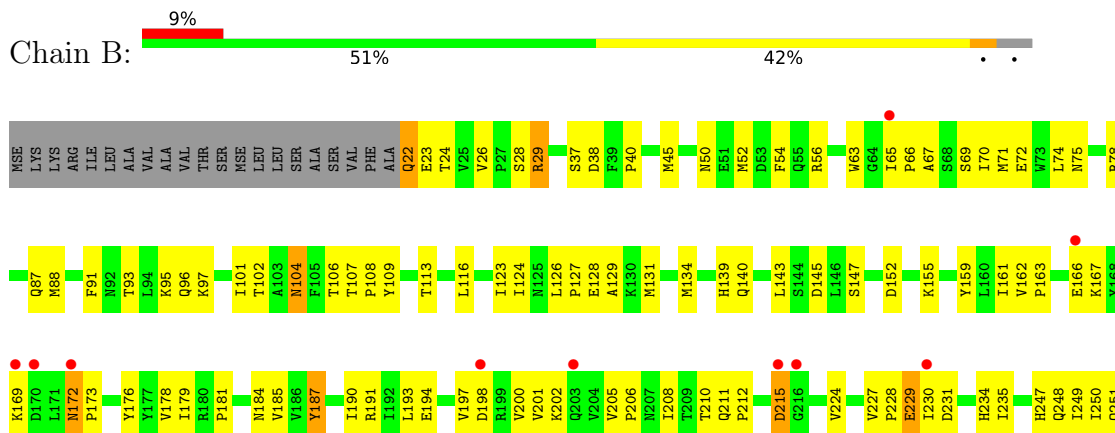
### 3 Residue-property plots

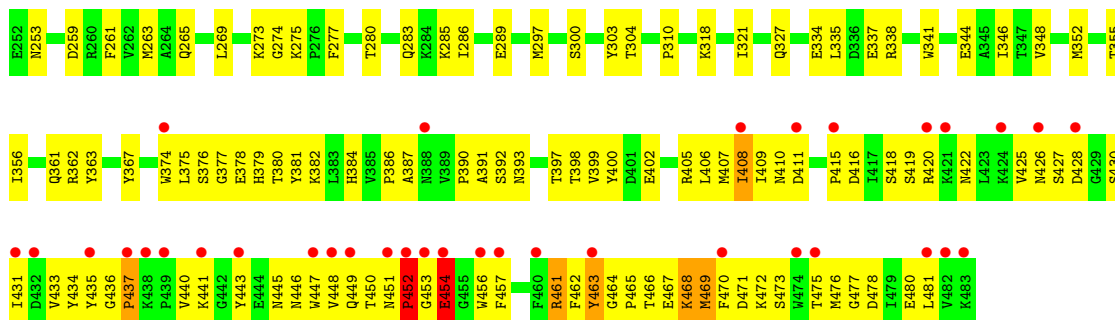
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uncharacterized protein VPA0735

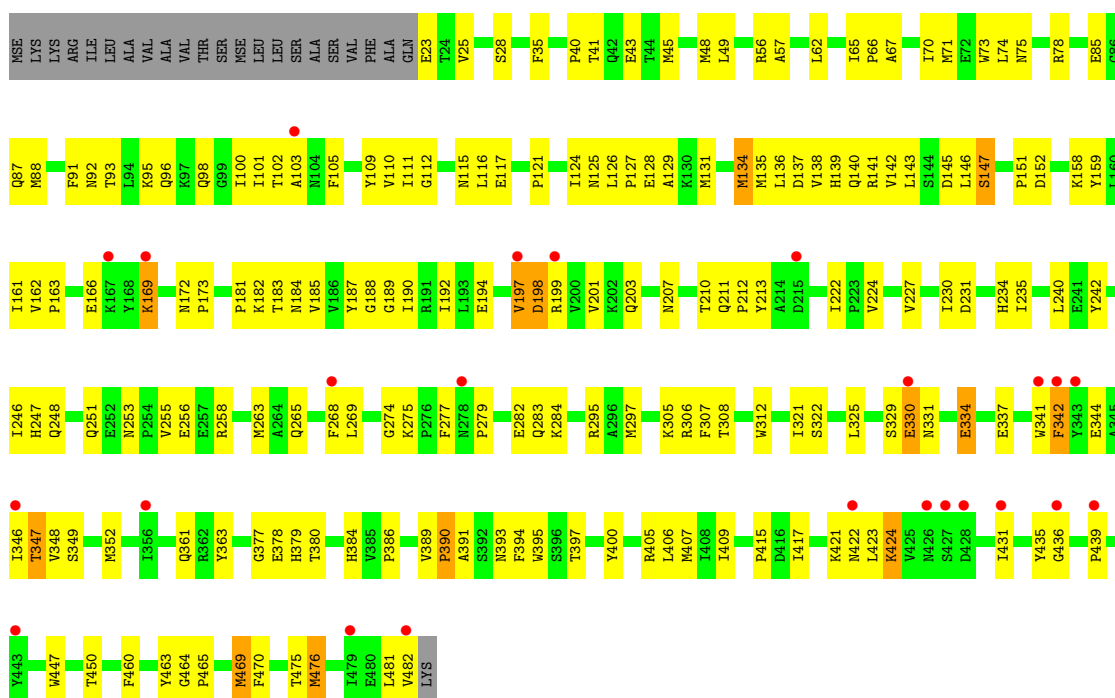


#### • Molecule 1: Uncharacterized protein VPA0735

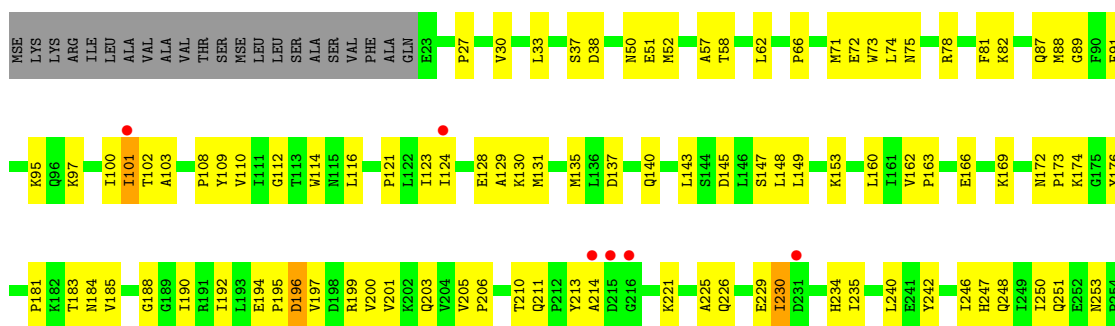


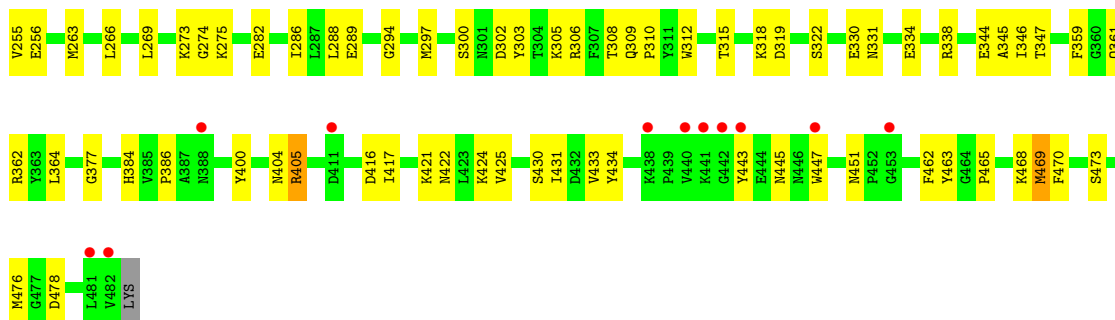


• Molecule 1: Uncharacterized protein VPA0735



• Molecule 1: Uncharacterized protein VPA0735





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.27Å 106.93Å 157.18Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	39.99 – 2.10 39.99 – 2.09	Depositor EDS
% Data completeness (in resolution range)	89.9 (39.99-2.10) 95.8 (39.99-2.09)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.08Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.224 , 0.274 0.224 , 0.279	Depositor DCC
$R_{free}$ test set	19578 reflections (8.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtrriage
Anisotropy	0.831	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3721e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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: 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	0.35	0/3803	0.63	3/5137 (0.1%)
1	B	0.36	0/3822	0.61	0/5160
1	C	0.34	0/3803	0.59	0/5137
1	D	0.35	0/3803	0.62	0/5137
All	All	0.35	0/15231	0.61	3/20571 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	MSE	N-CA-CB	-9.13	94.17	110.60
1	A	351	GLY	N-CA-C	7.81	132.62	113.10
1	A	352	MSE	N-CA-C	-5.48	96.21	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	3717	0	3643	244	0
1	B	3736	0	3664	280	0
1	C	3717	0	3643	208	0
1	D	3717	0	3643	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	197	0	0	12	0
3	B	217	0	0	18	0
3	C	190	0	0	11	0
3	D	235	0	0	9	0
All	All	15733	0	14593	830	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 28.

All (830) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:HA	1:B:45:MSE:HE2	1.18	1.14
1:C:105:PHE:HB2	1:C:407:MSE:HE1	1.32	1.11
1:C:135:MSE:HE3	1:C:146:LEU:HD11	1.32	1.10
1:A:303:TYR:HB2	1:B:45:MSE:HE1	1.30	1.09
1:C:45:MSE:HE1	1:D:303:TYR:HB2	1.24	1.09
1:A:105:PHE:HB2	1:A:407:MSE:HE1	1.33	1.07
1:A:297:MSE:HB3	1:B:52:MSE:HE3	1.36	1.07
1:B:378:GLU:HB3	1:B:452:PRO:HD3	1.34	1.07
1:C:45:MSE:HE2	1:D:300:SER:HA	1.34	1.06
1:C:66:PRO:HA	1:C:342:PHE:CD2	1.92	1.02
1:B:392:SER:HB3	1:B:463:TYR:HB3	1.38	1.01
1:C:66:PRO:HA	1:C:342:PHE:HD2	1.26	1.01
1:D:88:MSE:HE3	1:D:210:THR:HG21	1.48	0.95
1:D:140:GLN:HE22	1:D:347:THR:H	1.17	0.92
1:B:251:GLN:HE22	1:B:274:GLY:H	1.13	0.92
1:A:251:GLN:HE22	1:A:274:GLY:H	1.18	0.91
1:C:330:GLU:HB3	3:C:603:HOH:O	1.68	0.91
1:B:415:PRO:HA	1:B:447:TRP:HZ3	1.36	0.91
1:A:70:ILE:HD11	1:A:140:GLN:HG2	1.52	0.90
1:C:397:THR:HG21	1:C:435:TYR:OH	1.72	0.90
1:C:49:LEU:HD13	1:D:306:ARG:HD2	1.50	0.90
1:D:57:ALA:HB2	1:D:269:LEU:HD21	1.53	0.89
1:D:308:THR:HG22	1:D:309:GLN:H	1.39	0.88
1:C:141:ARG:HD2	1:C:182:LYS:NZ	1.89	0.88
1:A:297:MSE:HB3	1:B:52:MSE:CE	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:VAL:HG13	1:C:198:ASP:H	1.39	0.86
1:C:140:GLN:HG2	1:C:140:GLN:O	1.75	0.86
1:C:62:LEU:HD11	1:C:297:MSE:CE	2.06	0.85
1:D:62:LEU:HD11	1:D:297:MSE:HE3	1.56	0.85
1:A:52:MSE:HE2	1:B:297:MSE:HB3	1.58	0.84
1:C:92:ASN:H	1:C:96:GLN:NE2	1.74	0.84
1:C:344:GLU:HA	1:C:405:ARG:HD2	1.60	0.84
1:A:62:LEU:HD11	1:B:52:MSE:HE2	1.60	0.83
1:A:294:GLY:HA2	1:A:297:MSE:HE2	1.58	0.83
1:A:45:MSE:HE1	1:B:303:TYR:HB2	1.61	0.83
1:A:397:THR:HG21	1:A:435:TYR:OH	1.77	0.83
1:B:134:MSE:CE	1:B:352:MSE:HE1	2.09	0.82
1:A:62:LEU:CD1	1:B:52:MSE:HE2	2.09	0.82
1:A:62:LEU:HD11	1:A:297:MSE:HE3	1.62	0.81
1:D:101:ILE:H	1:D:234:HIS:HE1	1.27	0.81
1:B:375:LEU:O	1:B:454:GLU:HG2	1.78	0.81
1:A:66:PRO:HG2	1:A:338:ARG:HG2	1.61	0.81
1:A:325:LEU:HD12	1:A:350:ARG:HH21	1.45	0.80
1:D:184:ASN:H	1:D:253:ASN:HD22	1.27	0.80
1:B:29:ARG:HH11	1:B:29:ARG:HB3	1.44	0.80
1:D:282:GLU:HG3	3:D:811:HOH:O	1.81	0.79
1:B:71:MSE:HB2	1:B:249:ILE:HD11	1.63	0.79
1:C:307:PHE:HD1	1:C:308:THR:HG23	1.46	0.79
1:D:251:GLN:HE22	1:D:274:GLY:H	1.29	0.79
1:C:263:MSE:HE1	3:C:679:HOH:O	1.83	0.79
1:A:88:MSE:HE3	1:A:210:THR:HG21	1.64	0.79
1:B:191:ARG:HH22	1:B:352:MSE:CE	1.96	0.78
1:B:390:PRO:C	1:B:465:PRO:HD2	2.04	0.78
1:B:402:GLU:HB2	1:B:454:GLU:OE2	1.84	0.78
1:C:143:LEU:HD13	1:C:181:PRO:HG3	1.66	0.78
1:A:104:ASN:C	1:A:104:ASN:HD22	1.87	0.78
1:A:184:ASN:H	1:A:253:ASN:HD22	1.32	0.77
1:B:430:SER:HB3	3:B:796:HOH:O	1.84	0.77
1:D:140:GLN:NE2	1:D:347:THR:H	1.82	0.77
1:B:397:THR:HG21	1:B:434:TYR:OH	1.85	0.76
1:B:468:LYS:HZ3	1:B:468:LYS:HB2	1.50	0.76
1:B:74:LEU:O	1:B:78:ARG:HG2	1.85	0.76
1:C:251:GLN:HE22	1:C:274:GLY:H	1.33	0.76
1:A:395:TRP:HZ2	1:A:431:ILE:HD12	1.48	0.76
1:B:435:TYR:CE2	1:B:437:PRO:HD2	2.21	0.76
1:A:300:SER:CA	1:B:45:MSE:HE2	2.08	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:MSE:SE	1:B:477:GLY:H	2.18	0.76
1:D:101:ILE:H	1:D:234:HIS:CE1	2.04	0.75
1:C:139:HIS:CD2	1:C:258:ARG:HH22	2.04	0.75
1:C:134:MSE:HE2	1:C:134:MSE:O	1.84	0.75
1:C:469:MSE:HE2	1:C:470:PHE:CD1	2.22	0.75
1:A:37:SER:HB3	1:B:454:GLU:HB3	1.68	0.75
1:A:481:LEU:HD22	1:A:482:VAL:HG23	1.67	0.74
1:C:342:PHE:HE1	1:C:347:THR:H	1.35	0.74
1:B:88:MSE:HE3	1:B:210:THR:HG21	1.69	0.74
1:A:37:SER:HB3	1:B:454:GLU:CB	2.18	0.74
1:D:294:GLY:HA2	1:D:297:MSE:HE2	1.69	0.74
1:B:215:ASP:CG	1:D:289:GLU:HG2	2.08	0.74
1:B:95:LYS:HG2	1:B:229:GLU:HG3	1.68	0.74
1:B:134:MSE:HE2	1:B:352:MSE:HE1	1.70	0.73
1:C:62:LEU:HD11	1:C:297:MSE:HE3	1.70	0.73
1:D:108:PRO:HG2	1:D:197:VAL:HG13	1.69	0.73
1:B:184:ASN:H	1:B:253:ASN:HD22	1.36	0.73
1:C:65:ILE:HB	1:C:66:PRO:HD3	1.70	0.73
1:B:390:PRO:O	1:B:465:PRO:HD2	1.87	0.73
1:B:462:PHE:O	1:B:463:TYR:HB2	1.89	0.73
1:B:415:PRO:HA	1:B:447:TRP:CZ3	2.21	0.73
1:A:45:MSE:CE	1:B:303:TYR:HB2	2.19	0.72
1:B:411:ASP:OD2	1:B:448:VAL:HG21	1.89	0.72
1:A:182:LYS:HE3	1:A:258:ARG:HH21	1.53	0.72
1:A:65:ILE:HB	1:A:66:PRO:HD3	1.72	0.72
1:C:141:ARG:CD	1:C:182:LYS:NZ	2.53	0.72
1:A:469:MSE:HE2	1:A:470:PHE:HD1	1.54	0.72
1:A:481:LEU:HD23	1:A:482:VAL:H	1.54	0.71
1:A:321:ILE:N	1:A:321:ILE:HD12	2.05	0.71
1:A:37:SER:O	1:B:454:GLU:HB3	1.90	0.71
1:C:137:ASP:OD2	1:C:182:LYS:HE2	1.90	0.71
1:D:308:THR:HG22	1:D:309:GLN:N	2.05	0.71
1:B:376:SER:HA	1:B:454:GLU:HA	1.72	0.71
1:A:481:LEU:HD23	1:A:482:VAL:N	2.05	0.71
1:B:104:ASN:HD22	1:B:104:ASN:C	1.95	0.71
1:A:45:MSE:CE	1:B:300:SER:HA	2.21	0.70
1:B:71:MSE:HB2	1:B:249:ILE:CD1	2.20	0.70
1:B:104:ASN:ND2	1:B:106:THR:H	1.89	0.70
1:A:109:TYR:HB3	1:A:111:ILE:CD1	2.21	0.70
1:B:338:ARG:CZ	3:B:601:HOH:O	2.40	0.70
1:C:199:ARG:HH11	1:C:199:ARG:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:HD22	1:B:106:THR:H	1.39	0.70
1:B:185:VAL:H	1:B:253:ASN:HD21	1.39	0.70
1:C:247:HIS:O	1:C:251:GLN:HG2	1.90	0.70
1:A:124:ILE:HD13	1:A:210:THR:HG22	1.74	0.69
1:C:45:MSE:HE1	1:D:303:TYR:CB	2.13	0.69
1:C:141:ARG:HD2	1:C:182:LYS:HZ1	1.56	0.69
1:B:161:ILE:HD12	1:B:161:ILE:N	2.07	0.69
1:B:380:THR:HG23	1:B:435:TYR:HB2	1.75	0.69
1:C:92:ASN:H	1:C:96:GLN:HE21	1.40	0.69
1:C:307:PHE:CD1	1:C:308:THR:HG23	2.28	0.69
1:C:105:PHE:HB2	1:C:407:MSE:CE	2.18	0.69
1:B:197:VAL:O	1:B:201:VAL:HG12	1.93	0.68
1:C:101:ILE:H	1:C:234:HIS:HE1	1.39	0.68
1:B:247:HIS:O	1:B:251:GLN:HG2	1.93	0.68
1:B:286:ILE:HD12	3:B:729:HOH:O	1.93	0.68
1:B:420:ARG:HB2	3:B:707:HOH:O	1.93	0.68
1:A:45:MSE:HE2	1:B:300:SER:O	1.94	0.68
1:D:75:ASN:HD21	1:D:248:GLN:HE22	1.40	0.68
1:A:185:VAL:H	1:A:253:ASN:HD21	1.43	0.67
1:A:201:VAL:O	1:A:205:VAL:HG22	1.93	0.67
1:A:235:ILE:HD11	1:A:406:LEU:HD21	1.75	0.67
1:B:65:ILE:HB	1:B:66:PRO:HD3	1.75	0.67
1:C:62:LEU:HD11	1:C:297:MSE:HE2	1.74	0.67
1:C:469:MSE:HE2	1:C:470:PHE:HD1	1.58	0.67
1:A:182:LYS:HG2	3:A:718:HOH:O	1.94	0.67
1:A:110:VAL:C	1:A:111:ILE:HD12	2.14	0.67
1:B:382:LYS:HB2	1:B:481:LEU:HD11	1.77	0.67
1:D:101:ILE:HD11	1:D:405:ARG:HB2	1.77	0.67
1:A:109:TYR:HB3	1:A:111:ILE:HD13	1.76	0.67
1:B:40:PRO:CG	1:B:45:MSE:HE3	2.25	0.66
1:B:29:ARG:HB3	1:B:29:ARG:NH1	2.09	0.66
1:A:250:ILE:HD12	1:A:263:MSE:SE	2.45	0.66
1:A:71:MSE:HE1	1:A:74:LEU:HD23	1.77	0.66
1:A:205:VAL:CG2	1:A:206:PRO:HD3	2.25	0.66
1:C:184:ASN:H	1:C:253:ASN:HD22	1.42	0.66
1:A:93:THR:OG1	1:A:96:GLN:HG3	1.95	0.66
1:B:393:ASN:H	1:B:463:TYR:HB2	1.61	0.65
1:B:440:VAL:HA	1:B:443:TYR:HE1	1.61	0.65
1:D:282:GLU:O	1:D:286:ILE:HD13	1.96	0.65
1:A:303:TYR:CB	1:B:45:MSE:HE1	2.18	0.65
1:D:185:VAL:H	1:D:253:ASN:HD21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ILE:HD12	1:C:231:ASP:H	1.61	0.65
1:C:395:TRP:HZ2	1:C:431:ILE:HD12	1.61	0.65
1:D:130:LYS:HG3	1:D:148:LEU:HD11	1.78	0.65
1:D:66:PRO:HG2	3:D:610:HOH:O	1.96	0.65
1:B:451:ASN:HB3	1:B:452:PRO:HD2	1.77	0.65
1:C:475:THR:HG22	1:C:476:MSE:N	2.12	0.64
1:B:191:ARG:HH22	1:B:352:MSE:HE2	1.61	0.64
1:B:470:PHE:CD2	1:B:472:LYS:HE3	2.33	0.64
1:B:344:GLU:HA	1:B:405:ARG:HD2	1.80	0.64
1:A:101:ILE:H	1:A:234:HIS:HE1	1.44	0.64
1:C:93:THR:H	1:C:96:GLN:HE21	1.44	0.64
1:A:153:LYS:HB2	1:A:155:LYS:HE2	1.80	0.64
1:C:349:SER:OG	1:C:352:MSE:HE3	1.98	0.64
1:B:440:VAL:HA	1:B:443:TYR:CE1	2.33	0.64
1:A:45:MSE:HE3	1:B:300:SER:HA	1.80	0.64
1:B:335:LEU:HA	1:B:338:ARG:HH11	1.62	0.64
1:B:382:LYS:HE3	1:B:431:ILE:HD13	1.80	0.64
1:C:139:HIS:O	1:C:140:GLN:HB3	1.98	0.64
1:D:465:PRO:HB2	1:D:469:MSE:HG2	1.79	0.64
1:B:391:ALA:HA	1:B:465:PRO:HD3	1.80	0.64
1:B:397:THR:O	1:B:416:ASP:HB2	1.98	0.63
1:C:93:THR:H	1:C:96:GLN:NE2	1.97	0.63
1:C:101:ILE:HA	1:C:406:LEU:HD23	1.78	0.63
1:C:334:GLU:HB3	1:C:337:GLU:HB2	1.80	0.63
1:C:469:MSE:HE3	1:C:470:PHE:HA	1.81	0.63
1:D:250:ILE:HD12	1:D:263:MSE:SE	2.48	0.63
1:D:184:ASN:H	1:D:253:ASN:ND2	1.97	0.63
1:B:250:ILE:O	1:B:273:LYS:HD3	1.99	0.63
1:B:435:TYR:CD2	1:B:437:PRO:HD2	2.34	0.63
1:A:469:MSE:HE2	1:A:470:PHE:CD1	2.32	0.62
1:B:468:LYS:HG3	1:B:469:MSE:N	2.12	0.62
1:A:104:ASN:ND2	1:A:106:THR:H	1.97	0.62
1:B:215:ASP:OD1	1:D:289:GLU:HG2	1.99	0.62
1:C:116:LEU:HD21	1:C:161:ILE:HG22	1.81	0.62
1:D:253:ASN:O	1:D:273:LYS:HE3	2.00	0.62
1:A:131:MSE:SE	1:A:190:ILE:HG21	2.49	0.62
1:A:289:GLU:HG3	1:B:29:ARG:HG3	1.82	0.62
1:B:193:LEU:HD13	1:B:463:TYR:HE1	1.65	0.62
1:A:258:ARG:NH1	3:A:601:HOH:O	2.32	0.61
1:A:39:PHE:HD1	1:B:374:TRP:HB3	1.65	0.61
1:B:29:ARG:HH11	1:B:29:ARG:CB	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:CD1	1:A:140:GLN:HG2	2.28	0.61
1:A:205:VAL:HG22	1:A:206:PRO:HD3	1.83	0.61
1:B:191:ARG:NH2	1:B:352:MSE:HE2	2.15	0.61
1:A:125:ASN:HD22	1:A:158:LYS:HG2	1.66	0.61
1:C:297:MSE:HE3	1:D:52:MSE:HG3	1.81	0.61
1:C:88:MSE:HB2	1:C:224:VAL:HG22	1.83	0.61
1:D:81:PHE:HE1	1:D:230:ILE:HD11	1.66	0.61
1:B:399:VAL:HG12	1:B:408:ILE:HG21	1.83	0.60
1:C:135:MSE:HE2	1:C:188:GLY:HA2	1.83	0.60
1:C:377:GLY:O	1:C:450:THR:HG23	2.00	0.60
1:D:95:LYS:HG2	1:D:229:GLU:OE2	2.01	0.60
1:C:124:ILE:HD13	1:C:210:THR:HG22	1.84	0.60
1:C:341:TRP:CZ3	1:C:347:THR:O	2.54	0.60
1:B:172:ASN:HD22	1:B:178:VAL:HG21	1.66	0.60
1:C:242:TYR:CE2	1:C:246:ILE:HD11	2.35	0.60
1:D:183:THR:HG22	1:D:256:GLU:OE2	2.02	0.60
1:C:125:ASN:HD22	1:C:158:LYS:HG2	1.67	0.60
1:A:270:GLY:C	1:A:271:ILE:HD12	2.22	0.60
1:A:300:SER:HA	1:B:45:MSE:CE	2.12	0.60
1:A:71:MSE:CE	1:A:74:LEU:HD23	2.32	0.60
1:D:87:GLN:C	1:D:88:MSE:HE2	2.22	0.60
1:D:330:GLU:HB3	3:D:656:HOH:O	2.02	0.59
1:C:182:LYS:HG2	3:C:728:HOH:O	2.02	0.59
1:A:59:GLN:NE2	1:B:56:ARG:HE	2.00	0.59
1:A:341:TRP:CZ3	1:A:347:THR:O	2.55	0.59
1:D:108:PRO:HB2	1:D:192:ILE:HD13	1.84	0.59
1:B:87:GLN:C	1:B:88:MSE:HE2	2.23	0.59
1:B:387:ALA:CB	1:B:428:ASP:HB3	2.33	0.59
1:C:436:GLY:C	1:C:450:THR:HG22	2.22	0.59
1:D:101:ILE:HD13	1:D:405:ARG:O	2.02	0.59
1:A:182:LYS:CE	1:A:258:ARG:HH21	2.15	0.59
1:D:81:PHE:CE1	1:D:230:ILE:HD11	2.36	0.59
1:A:141:ARG:CD	1:A:182:LYS:NZ	2.66	0.59
1:C:45:MSE:HE2	1:D:300:SER:CA	2.23	0.59
1:D:197:VAL:O	1:D:201:VAL:HG23	2.03	0.59
1:D:310:PRO:HA	1:D:318:LYS:HG2	1.84	0.59
1:B:338:ARG:NE	3:B:601:HOH:O	2.36	0.59
1:A:407:MSE:O	1:A:409:ILE:HD12	2.02	0.59
1:C:101:ILE:H	1:C:234:HIS:CE1	2.21	0.59
1:B:247:HIS:HE1	1:B:275:LYS:O	1.86	0.58
1:B:418:SER:O	1:B:420:ARG:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:GLY:HA3	1:D:451:ASN:O	2.03	0.58
1:C:185:VAL:H	1:C:253:ASN:HD21	1.51	0.58
1:D:88:MSE:SE	1:D:112:GLY:HA3	2.53	0.58
1:C:102:THR:HA	1:C:400:TYR:CE1	2.38	0.58
1:A:84:GLU:H	1:A:87:GLN:HE21	1.51	0.58
1:A:235:ILE:HD11	1:A:406:LEU:CD2	2.32	0.58
1:C:197:VAL:HG13	1:C:198:ASP:N	2.15	0.58
1:C:141:ARG:CD	1:C:182:LYS:HZ3	2.17	0.58
1:A:174:LYS:NZ	1:A:174:LYS:HB3	2.19	0.58
1:B:377:GLY:HA3	1:B:450:THR:O	2.03	0.58
1:A:113:THR:HG23	1:A:186:VAL:O	2.04	0.58
1:B:410:ASN:ND2	1:B:448:VAL:HG13	2.18	0.58
1:B:235:ILE:HD11	1:B:406:LEU:HG	1.86	0.58
1:D:101:ILE:HD11	1:D:405:ARG:HG3	1.85	0.58
1:A:104:ASN:C	1:A:104:ASN:ND2	2.56	0.58
1:C:78:ARG:NE	1:C:85:GLU:OE2	2.31	0.58
1:A:271:ILE:HD12	1:A:271:ILE:N	2.19	0.58
1:C:199:ARG:HG3	1:C:203:GLN:HE22	1.68	0.58
1:C:124:ILE:HB	1:C:159:TYR:HB2	1.86	0.57
1:C:141:ARG:NH1	1:C:258:ARG:CZ	2.67	0.57
1:A:50:ASN:ND2	1:B:29:ARG:HH21	2.02	0.57
1:B:67:ALA:HB1	1:B:249:ILE:HD12	1.86	0.57
1:C:75:ASN:HD21	1:C:248:GLN:HE22	1.50	0.57
1:B:50:ASN:ND2	1:B:286:ILE:HD11	2.20	0.57
1:B:374:TRP:NE1	3:B:753:HOH:O	2.21	0.57
1:C:136:LEU:HD11	1:C:347:THR:OG1	2.04	0.57
1:A:246:ILE:O	1:A:250:ILE:HG12	2.04	0.57
1:D:110:VAL:HB	1:D:190:ILE:HB	1.87	0.57
1:A:172:ASN:HD22	1:A:178:VAL:HG21	1.70	0.57
1:C:325:LEU:HD12	1:C:325:LEU:H	1.70	0.57
1:A:29:ARG:HD2	1:B:54:PHE:CE2	2.40	0.57
1:B:128:GLU:HG3	1:B:155:LYS:HA	1.87	0.57
1:A:102:THR:HA	1:A:400:TYR:CE1	2.40	0.57
1:B:230:ILE:HG13	1:B:231:ASP:N	2.20	0.56
1:B:466:THR:HG23	1:B:470:PHE:CE1	2.38	0.56
1:C:424:LYS:HB2	1:C:424:LYS:NZ	2.20	0.56
1:A:39:PHE:CD2	1:B:402:GLU:HG3	2.40	0.56
1:A:58:THR:HG22	1:A:297:MSE:HE1	1.85	0.56
1:D:71:MSE:HE3	1:D:71:MSE:HA	1.87	0.56
1:D:121:PRO:HB2	1:D:213:TYR:HB3	1.86	0.56
1:A:222:ILE:HD11	3:A:777:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PHE:CD2	1:C:227:VAL:HG21	2.41	0.56
1:D:417:ILE:CD1	1:D:433:VAL:HG13	2.36	0.56
1:A:56:ARG:HD3	1:A:265:GLN:HB3	1.88	0.56
1:B:410:ASN:CG	1:B:448:VAL:HG13	2.26	0.56
1:C:141:ARG:CD	1:C:182:LYS:HZ1	2.17	0.56
1:C:222:ILE:HD11	3:C:659:HOH:O	2.06	0.56
1:A:424:LYS:HE3	1:A:442:GLY:O	2.06	0.56
1:B:101:ILE:HA	1:B:406:LEU:HD23	1.87	0.56
1:B:131:MSE:SE	1:B:190:ILE:HG21	2.55	0.56
1:D:58:THR:HG22	1:D:297:MSE:HE1	1.87	0.56
1:D:404:ASN:O	1:D:405:ARG:HG2	2.05	0.56
1:B:334:GLU:HB3	1:B:337:GLU:HB2	1.88	0.56
1:C:135:MSE:HE3	1:C:146:LEU:CD1	2.21	0.56
1:D:315:THR:HA	1:D:478:ASP:OD2	2.05	0.56
1:A:465:PRO:HB2	1:A:469:MSE:HG2	1.86	0.55
1:C:62:LEU:CD1	1:C:297:MSE:CE	2.82	0.55
1:A:172:ASN:N	1:A:173:PRO:HD3	2.19	0.55
1:B:155:LYS:HB2	1:B:155:LYS:NZ	2.21	0.55
1:B:102:THR:HA	1:B:400:TYR:CE1	2.41	0.55
1:B:425:VAL:HG12	1:B:426:ASN:N	2.21	0.55
1:C:41:THR:OG1	1:C:43:GLU:HG2	2.06	0.55
1:A:101:ILE:HD12	1:A:344:GLU:O	2.07	0.55
1:A:141:ARG:HD2	1:A:182:LYS:NZ	2.22	0.55
1:A:341:TRP:CZ3	1:A:348:VAL:HG13	2.41	0.55
1:D:131:MSE:SE	1:D:190:ILE:HG21	2.57	0.55
1:A:479:ILE:HD12	1:A:479:ILE:N	2.22	0.55
1:B:104:ASN:HD21	1:B:107:THR:H	1.52	0.55
1:C:111:ILE:HD13	1:C:187:TYR:OH	2.07	0.55
1:C:161:ILE:HD12	1:C:161:ILE:N	2.22	0.55
1:C:282:GLU:HG3	1:C:283:GLN:N	2.22	0.55
1:C:450:THR:HG21	3:C:663:HOH:O	2.07	0.55
1:B:194:GLU:HB2	1:B:200:VAL:HG21	1.88	0.55
1:A:475:THR:HG22	1:A:476:MSE:N	2.22	0.55
1:B:327:GLN:HA	1:B:334:GLU:OE1	2.07	0.55
1:C:169:LYS:HE2	3:C:788:HOH:O	2.07	0.55
1:A:194:GLU:HG2	3:A:768:HOH:O	2.07	0.54
1:C:199:ARG:HB2	1:C:199:ARG:NH1	2.22	0.54
1:D:78:ARG:O	1:D:82:LYS:HA	2.07	0.54
1:B:235:ILE:HD11	1:B:406:LEU:CG	2.37	0.54
1:B:398:THR:O	1:B:457:PHE:CB	2.55	0.54
1:B:440:VAL:O	1:B:441:LYS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:PHE:CB	1:C:407:MSE:HE1	2.23	0.54
1:D:246:ILE:O	1:D:250:ILE:HG12	2.07	0.54
1:C:56:ARG:HD3	1:C:265:GLN:HB3	1.88	0.54
1:B:91:PHE:HB2	1:B:109:TYR:HB2	1.90	0.54
1:B:93:THR:OG1	1:B:96:GLN:HG3	2.06	0.54
1:A:28:SER:HB3	1:A:33:LEU:HD21	1.90	0.54
1:A:62:LEU:HD13	1:B:52:MSE:HE2	1.87	0.54
1:B:408:ILE:HG23	1:B:447:TRP:CH2	2.43	0.54
1:C:141:ARG:NH1	1:C:258:ARG:NH2	2.56	0.54
1:A:62:LEU:HD11	1:A:297:MSE:CE	2.35	0.54
1:A:295:ARG:NE	3:A:635:HOH:O	2.41	0.54
1:C:341:TRP:CH2	1:C:347:THR:O	2.60	0.54
1:D:58:THR:HG22	1:D:297:MSE:CE	2.37	0.54
1:A:78:ARG:NH2	1:A:118:LYS:HE2	2.23	0.54
1:D:30:VAL:HG11	1:D:51:GLU:HG2	1.88	0.54
1:B:97:LYS:HE2	1:B:109:TYR:CD2	2.43	0.54
1:B:102:THR:HG21	1:B:456:TRP:CH2	2.43	0.54
1:C:135:MSE:CE	1:C:188:GLY:HA2	2.37	0.54
1:A:128:GLU:HG3	1:A:155:LYS:HA	1.91	0.53
1:B:172:ASN:ND2	1:B:178:VAL:HG21	2.24	0.53
1:B:185:VAL:H	1:B:253:ASN:ND2	2.06	0.53
1:B:408:ILE:HG12	1:B:447:TRP:HZ2	1.72	0.53
1:D:308:THR:CG2	1:D:309:GLN:H	2.18	0.53
1:A:104:ASN:HD22	1:A:106:THR:H	1.55	0.53
1:B:78:ARG:HD2	3:B:728:HOH:O	2.08	0.53
1:D:247:HIS:HE1	1:D:275:LYS:O	1.91	0.53
1:A:166:GLU:H	1:A:166:GLU:CD	2.12	0.53
1:C:378:GLU:HG2	1:C:379:HIS:CD2	2.44	0.53
1:A:469:MSE:HG3	1:A:470:PHE:N	2.23	0.53
1:B:381:TYR:HD2	1:B:449:GLN:HE22	1.56	0.53
1:D:135:MSE:HE2	1:D:188:GLY:CA	2.38	0.53
1:D:425:VAL:HA	1:D:431:ILE:CD1	2.38	0.53
1:A:45:MSE:HE2	1:B:300:SER:HA	1.90	0.53
1:A:161:ILE:N	1:A:161:ILE:HD12	2.24	0.53
1:C:135:MSE:HE2	1:C:135:MSE:HA	1.91	0.53
1:A:242:TYR:CE1	1:A:246:ILE:HD11	2.43	0.53
1:A:315:THR:HA	1:A:478:ASP:OD2	2.09	0.53
1:B:191:ARG:HH22	1:B:352:MSE:HE1	1.72	0.53
1:B:382:LYS:HG3	1:B:431:ILE:HG23	1.89	0.53
1:B:468:LYS:HE2	3:B:677:HOH:O	2.08	0.53
1:C:361:GLN:HG2	1:C:463:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:MSE:SE	1:D:190:ILE:CG2	3.07	0.53
1:B:104:ASN:C	1:B:104:ASN:ND2	2.60	0.53
1:D:101:ILE:CD1	1:D:405:ARG:HB2	2.39	0.53
1:B:102:THR:HG21	1:B:456:TRP:HH2	1.74	0.52
1:B:285:LYS:HB2	3:B:729:HOH:O	2.10	0.52
1:A:334:GLU:O	1:A:338:ARG:HB2	2.08	0.52
1:D:101:ILE:HD12	1:D:344:GLU:O	2.10	0.52
1:A:378:GLU:HG2	1:A:379:HIS:ND1	2.24	0.52
1:B:101:ILE:H	1:B:234:HIS:CE1	2.28	0.52
1:A:137:ASP:OD2	1:A:182:LYS:HE2	2.09	0.52
1:D:417:ILE:HD13	1:D:433:VAL:HG13	1.92	0.52
1:A:87:GLN:C	1:A:88:MSE:HE2	2.29	0.52
1:C:331:ASN:HB3	1:D:255:VAL:HG21	1.90	0.52
1:D:172:ASN:N	1:D:173:PRO:HD3	2.25	0.52
1:A:39:PHE:CD1	1:B:374:TRP:HB3	2.45	0.52
1:C:347:THR:HG23	1:C:352:MSE:HE1	1.91	0.52
1:B:40:PRO:HG2	1:B:45:MSE:HE3	1.91	0.52
1:D:114:TRP:HE1	1:D:116:LEU:HD23	1.74	0.52
1:A:72:GLU:OE1	1:A:72:GLU:HA	2.09	0.52
1:C:475:THR:CG2	1:C:476:MSE:N	2.72	0.52
1:C:182:LYS:HE3	1:C:258:ARG:HH21	1.75	0.52
1:D:199:ARG:O	1:D:203:GLN:HG3	2.10	0.52
1:A:101:ILE:HD13	1:A:405:ARG:O	2.11	0.51
1:B:29:ARG:HD2	3:B:762:HOH:O	2.10	0.51
1:B:187:TYR:CD1	1:B:187:TYR:C	2.83	0.51
1:A:66:PRO:CG	1:A:338:ARG:HG2	2.36	0.51
1:C:131:MSE:HE2	1:C:190:ILE:HG22	1.91	0.51
1:D:108:PRO:CG	1:D:197:VAL:HG13	2.39	0.51
1:A:101:ILE:H	1:A:234:HIS:CE1	2.26	0.51
1:D:101:ILE:HG23	1:D:345:ALA:HA	1.92	0.51
1:A:111:ILE:HD12	1:A:111:ILE:N	2.25	0.51
1:A:468:LYS:HD3	3:A:693:HOH:O	2.09	0.51
1:B:387:ALA:HB1	1:B:428:ASP:HB3	1.93	0.51
1:B:451:ASN:O	1:B:453:GLY:N	2.42	0.51
1:D:361:GLN:HG2	1:D:463:TYR:CZ	2.45	0.51
1:A:441:LYS:HG3	1:A:441:LYS:O	2.11	0.51
1:B:129:ALA:HB3	1:B:131:MSE:HE2	1.93	0.51
1:B:321:ILE:HD12	1:B:321:ILE:N	2.25	0.51
1:B:341:TRP:HE1	1:B:348:VAL:CG1	2.24	0.51
1:C:295:ARG:HG3	1:C:295:ARG:HH11	1.76	0.51
1:D:57:ALA:HB2	1:D:269:LEU:CD2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ILE:H	1:B:234:HIS:HE1	1.59	0.51
1:C:116:LEU:HD21	1:C:161:ILE:CG2	2.39	0.51
1:B:172:ASN:N	1:B:173:PRO:HD3	2.25	0.51
1:B:335:LEU:HD12	1:B:338:ARG:NH1	2.26	0.51
1:D:30:VAL:HG12	1:D:30:VAL:O	2.09	0.51
1:B:147:SER:HA	1:B:152:ASP:OD1	2.11	0.51
1:C:126:LEU:HD21	1:C:190:ILE:CD1	2.40	0.51
1:D:101:ILE:HD11	1:D:405:ARG:CG	2.40	0.51
1:A:140:GLN:NE2	1:A:346:ILE:HD12	2.26	0.50
1:A:305:LYS:HE3	3:A:733:HOH:O	2.11	0.50
1:A:313:LYS:HZ2	1:A:314:GLY:CA	2.24	0.50
1:C:140:GLN:CD	1:C:342:PHE:CD1	2.85	0.50
1:B:285:LYS:O	1:B:289:GLU:HG3	2.09	0.50
1:B:467:GLU:HA	1:B:472:LYS:HD2	1.93	0.50
1:A:302:ASP:O	1:A:305:LYS:HG3	2.11	0.50
1:B:40:PRO:HG3	1:B:45:MSE:HE3	1.92	0.50
1:B:335:LEU:HA	1:B:338:ARG:NH1	2.26	0.50
1:C:45:MSE:CE	1:D:303:TYR:HB2	2.17	0.50
1:C:230:ILE:HD12	1:C:231:ASP:N	2.25	0.50
1:D:240:LEU:HG	1:D:288:LEU:HD21	1.92	0.50
1:D:404:ASN:C	1:D:405:ARG:HG2	2.31	0.50
1:A:29:ARG:NH1	1:A:29:ARG:HG3	2.26	0.50
1:C:390:PRO:HB2	1:C:469:MSE:HB3	1.92	0.50
1:A:185:VAL:H	1:A:253:ASN:ND2	2.09	0.50
1:B:408:ILE:HG12	1:B:447:TRP:CZ2	2.47	0.50
1:B:464:GLY:N	3:B:783:HOH:O	2.40	0.50
1:D:425:VAL:HG22	1:D:431:ILE:HD11	1.93	0.50
1:C:146:LEU:O	1:C:147:SER:HB3	2.12	0.50
1:C:73:TRP:CZ3	1:C:346:ILE:HD13	2.46	0.50
1:C:88:MSE:HE3	1:C:210:THR:HG21	1.93	0.50
1:A:28:SER:HB3	1:A:33:LEU:CD2	2.41	0.50
1:A:341:TRP:HZ3	1:A:348:VAL:HG13	1.77	0.50
1:B:230:ILE:HD12	1:B:231:ASP:H	1.75	0.50
1:B:467:GLU:HG3	3:B:724:HOH:O	2.11	0.50
1:D:192:ILE:N	1:D:192:ILE:HD12	2.27	0.50
1:A:91:PHE:CD2	1:A:227:VAL:HG21	2.47	0.49
1:A:139:HIS:CD2	1:A:258:ARG:HH22	2.30	0.49
1:C:182:LYS:HG3	1:C:183:THR:HG23	1.94	0.49
1:D:230:ILE:HD13	1:D:230:ILE:H	1.76	0.49
1:D:123:ILE:HD13	1:D:160:LEU:HD13	1.94	0.49
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LYS:NZ	3:A:764:HOH:O	2.45	0.49
1:C:40:PRO:CG	1:C:45:MSE:HE3	2.43	0.49
1:C:71:MSE:HE1	1:C:74:LEU:HD23	1.95	0.49
1:A:235:ILE:HD11	1:A:406:LEU:CG	2.42	0.49
1:B:356:ILE:N	1:B:356:ILE:HD12	2.27	0.49
1:C:91:PHE:HB2	1:C:109:TYR:HB2	1.94	0.49
1:D:302:ASP:O	1:D:305:LYS:HG3	2.13	0.49
1:A:408:ILE:HD13	1:A:409:ILE:N	2.28	0.49
1:C:166:GLU:HA	1:C:166:GLU:OE1	2.11	0.49
1:A:37:SER:O	1:A:38:ASP:HB2	2.13	0.49
1:A:133:GLY:HA3	1:A:190:ILE:HD13	1.95	0.49
1:B:215:ASP:HB2	1:C:28:SER:C	2.33	0.49
1:D:123:ILE:HG22	1:D:124:ILE:N	2.28	0.49
1:D:123:ILE:CD1	1:D:160:LEU:HD13	2.42	0.49
1:A:37:SER:HB3	1:B:454:GLU:HB2	1.91	0.49
1:C:141:ARG:HD2	1:C:182:LYS:CE	2.42	0.49
1:D:102:THR:HA	1:D:400:TYR:CE1	2.47	0.49
1:D:430:SER:O	1:D:431:ILE:HD13	2.13	0.49
1:A:243:TRP:CZ3	1:A:246:ILE:HD12	2.48	0.49
1:B:230:ILE:CG1	1:B:231:ASP:N	2.76	0.49
1:C:141:ARG:CZ	1:C:182:LYS:HZ1	2.25	0.49
1:A:197:VAL:HG23	1:A:198:ASP:N	2.28	0.48
1:A:363:TYR:CD1	1:A:363:TYR:N	2.81	0.48
1:B:194:GLU:CB	1:B:200:VAL:HG21	2.43	0.48
1:B:398:THR:HA	1:B:416:ASP:HB3	1.94	0.48
1:B:476:MSE:CG	1:B:477:GLY:N	2.76	0.48
1:D:196:ASP:HB2	3:D:807:HOH:O	2.13	0.48
1:A:141:ARG:NH1	1:A:258:ARG:CZ	2.77	0.48
1:B:69:SER:OG	1:B:346:ILE:HD13	2.12	0.48
1:A:303:TYR:HB2	1:B:45:MSE:CE	2.23	0.48
1:A:380:THR:O	1:A:482:VAL:N	2.46	0.48
1:A:444:GLU:CD	1:A:444:GLU:H	2.17	0.48
1:B:341:TRP:HE1	1:B:348:VAL:HG13	1.77	0.48
1:C:111:ILE:HG12	1:C:189:GLY:HA2	1.96	0.48
1:C:199:ARG:HG3	1:C:203:GLN:NE2	2.27	0.48
1:A:341:TRP:HZ3	1:A:347:THR:O	1.97	0.48
1:A:381:TYR:HB3	1:A:479:ILE:CG2	2.44	0.48
1:B:63:TRP:HA	1:B:335:LEU:HD11	1.96	0.48
1:B:134:MSE:HE1	1:B:352:MSE:HE1	1.92	0.48
1:C:322:SER:HB2	3:C:660:HOH:O	2.13	0.48
1:A:43:GLU:HG2	3:A:790:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MSE:O	1:A:56:ARG:HG3	2.14	0.48
1:A:141:ARG:CD	1:A:182:LYS:HZ3	2.26	0.48
1:B:251:GLN:O	1:B:273:LYS:HE3	2.13	0.48
1:C:405:ARG:NH1	3:C:680:HOH:O	2.46	0.48
1:C:255:VAL:HG21	1:D:331:ASN:HB3	1.95	0.48
1:D:205:VAL:HB	1:D:206:PRO:HD3	1.95	0.48
1:B:335:LEU:CD1	1:B:338:ARG:HH12	2.27	0.48
1:C:182:LYS:CE	1:C:258:ARG:HH21	2.27	0.48
1:D:266:LEU:HD23	1:D:269:LEU:HD22	1.94	0.48
1:A:141:ARG:CZ	1:A:182:LYS:HZ1	2.27	0.48
1:B:139:HIS:HD2	3:B:633:HOH:O	1.96	0.48
1:D:100:ILE:HB	1:D:103:ALA:HB2	1.95	0.48
1:C:121:PRO:HB2	1:C:213:TYR:O	2.14	0.47
1:C:235:ILE:HD11	1:C:406:LEU:HG	1.95	0.47
1:C:321:ILE:HD12	1:C:341:TRP:CZ2	2.49	0.47
1:D:143:LEU:HD11	1:D:181:PRO:HB3	1.96	0.47
1:B:390:PRO:HB2	1:B:468:LYS:HB3	1.96	0.47
1:A:115:ASN:OD1	1:A:117:GLU:HB3	2.14	0.47
1:D:87:GLN:NE2	1:D:225:ALA:HB2	2.29	0.47
1:D:101:ILE:HD11	1:D:405:ARG:CB	2.44	0.47
1:C:143:LEU:CD1	1:C:181:PRO:HG3	2.43	0.47
1:D:27:PRO:HB3	3:D:645:HOH:O	2.15	0.47
1:A:51:GLU:O	1:A:55:GLN:HG3	2.14	0.47
1:A:192:ILE:HD12	1:A:192:ILE:N	2.29	0.47
1:A:289:GLU:HG3	1:B:29:ARG:HD2	1.96	0.47
1:A:395:TRP:CZ2	1:A:431:ILE:HD12	2.39	0.47
1:B:140:GLN:NE2	1:B:346:ILE:HD12	2.30	0.47
1:C:70:ILE:HD13	1:C:346:ILE:HD11	1.97	0.47
1:D:226:GLN:HG2	3:D:718:HOH:O	2.14	0.47
1:D:247:HIS:O	1:D:251:GLN:HG2	2.14	0.47
1:A:420:ARG:HG2	1:A:420:ARG:HH11	1.80	0.47
1:B:37:SER:O	1:B:38:ASP:HB2	2.14	0.47
1:C:100:ILE:HB	1:C:103:ALA:HB2	1.96	0.47
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.15	0.47
1:B:392:SER:HB3	1:B:463:TYR:CB	2.27	0.47
1:A:78:ARG:O	1:A:82:LYS:HA	2.14	0.47
1:B:435:TYR:O	1:B:448:VAL:HA	2.14	0.47
1:B:461:ARG:CG	1:B:461:ARG:HH11	2.28	0.47
1:D:62:LEU:CD1	1:D:297:MSE:HE3	2.35	0.47
1:A:182:LYS:HD2	1:A:256:GLU:OE1	2.13	0.46
1:B:215:ASP:OD2	1:D:289:GLU:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASN:HD21	1:D:248:GLN:NE2	2.11	0.46
1:A:460:PHE:CD2	1:A:476:MSE:HE1	2.51	0.46
1:B:310:PRO:HA	1:B:318:LYS:HG2	1.96	0.46
1:C:197:VAL:O	1:C:201:VAL:HG23	2.15	0.46
1:A:184:ASN:H	1:A:253:ASN:ND2	2.07	0.46
1:C:66:PRO:CA	1:C:342:PHE:CD2	2.83	0.46
1:B:108:PRO:CG	1:B:197:VAL:HG13	2.45	0.46
1:B:184:ASN:H	1:B:253:ASN:ND2	2.07	0.46
1:D:50:ASN:ND2	1:D:286:ILE:HD11	2.30	0.46
1:A:469:MSE:HE3	1:A:470:PHE:HA	1.97	0.46
1:B:22:GLN:HE21	1:B:22:GLN:HB2	1.59	0.46
1:B:434:TYR:HB3	1:B:447:TRP:HD1	1.81	0.46
1:A:135:MSE:HE2	1:A:161:ILE:HG12	1.97	0.46
1:B:201:VAL:HG23	1:B:205:VAL:HG21	1.96	0.46
1:C:111:ILE:CG2	1:C:112:GLY:N	2.79	0.46
1:D:124:ILE:CD1	1:D:210:THR:HG22	2.45	0.46
1:C:67:ALA:HA	1:C:138:VAL:O	2.15	0.46
1:C:363:TYR:CD1	1:C:363:TYR:N	2.83	0.46
1:D:424:LYS:HD3	1:D:443:TYR:CE1	2.51	0.46
1:B:70:ILE:CD1	1:B:346:ILE:HD11	2.46	0.46
1:B:387:ALA:HB2	1:B:428:ASP:HB3	1.96	0.46
1:B:435:TYR:N	1:B:449:GLN:HG3	2.30	0.46
1:D:72:GLU:OE1	1:D:72:GLU:HA	2.15	0.46
1:A:235:ILE:HD13	1:A:404:ASN:O	2.16	0.46
1:A:335:LEU:HD21	3:A:657:HOH:O	2.16	0.46
1:A:365:VAL:HG22	1:A:366:THR:N	2.30	0.46
1:B:355:THR:H	1:B:356:ILE:HD12	1.81	0.46
1:B:377:GLY:HA2	1:B:449:GLN:HB3	1.96	0.46
1:B:457:PHE:HZ	1:B:478:ASP:CG	2.19	0.46
1:A:312:TRP:CZ3	1:A:476:MSE:HB3	2.51	0.46
1:A:366:THR:HG21	1:A:479:ILE:CD1	2.46	0.46
1:B:75:ASN:HD21	1:B:248:GLN:HE22	1.63	0.46
1:B:251:GLN:HE22	1:B:274:GLY:N	1.96	0.46
1:D:322:SER:HB2	3:D:626:HOH:O	2.14	0.46
1:B:468:LYS:HZ3	1:B:468:LYS:CB	2.24	0.45
1:A:84:GLU:H	1:A:87:GLN:NE2	2.13	0.45
1:A:182:LYS:CD	1:A:256:GLU:OE1	2.64	0.45
1:B:229:GLU:HG2	3:B:770:HOH:O	2.15	0.45
1:B:384:HIS:O	1:B:386:PRO:HD3	2.16	0.45
1:C:235:ILE:HD11	1:C:406:LEU:CG	2.46	0.45
1:C:417:ILE:HG23	1:C:423:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HD13	1:A:102:THR:N	2.32	0.45
1:A:183:THR:CG2	1:A:256:GLU:OE2	2.64	0.45
1:A:199:ARG:O	1:A:203:GLN:HG3	2.15	0.45
1:B:390:PRO:C	1:B:465:PRO:CD	2.81	0.45
1:C:128:GLU:O	1:C:129:ALA:HB2	2.17	0.45
1:C:279:PRO:HB2	1:C:284:LYS:CG	2.46	0.45
1:B:434:TYR:HB3	1:B:449:GLN:HE21	1.82	0.45
1:D:71:MSE:HE1	1:D:74:LEU:HD23	1.98	0.45
1:A:91:PHE:HB2	1:A:109:TYR:HB2	1.99	0.45
1:C:342:PHE:CZ	1:C:346:ILE:HG13	2.51	0.45
1:A:171:LEU:O	1:A:180:ARG:NH2	2.49	0.45
1:D:149:LEU:HD21	1:D:359:PHE:HB3	1.98	0.45
1:D:201:VAL:HG13	1:D:205:VAL:HG21	1.98	0.45
1:D:468:LYS:HG2	1:D:473:SER:OG	2.16	0.45
1:A:261:PHE:O	1:A:265:GLN:HG3	2.17	0.45
1:C:48:MSE:HE2	1:C:48:MSE:HA	1.99	0.45
1:C:308:THR:HG21	1:C:322:SER:OG	2.16	0.45
1:A:194:GLU:CB	1:A:200:VAL:HG21	2.47	0.45
1:B:108:PRO:HG2	1:B:197:VAL:HG13	1.98	0.45
1:B:198:ASP:OD1	1:B:202:LYS:HE3	2.16	0.45
1:B:352:MSE:HG2	1:B:363:TYR:CE1	2.51	0.45
1:C:279:PRO:HB2	1:C:284:LYS:HG3	1.98	0.45
1:A:136:LEU:HD11	1:A:347:THR:HA	1.99	0.45
1:A:142:VAL:HG21	1:A:325:LEU:HD22	1.99	0.45
1:A:164:PRO:HD2	3:A:627:HOH:O	2.16	0.45
1:B:104:ASN:HB2	3:B:808:HOH:O	2.16	0.45
1:B:470:PHE:O	1:B:471:ASP:HB2	2.17	0.45
1:C:131:MSE:SE	1:C:190:ILE:HG21	2.67	0.45
1:C:115:ASN:OD1	1:C:117:GLU:HB3	2.17	0.45
1:C:141:ARG:NE	1:C:182:LYS:HZ1	2.15	0.45
1:A:308:THR:HG21	1:A:322:SER:OG	2.16	0.44
1:B:261:PHE:O	1:B:265:GLN:HG3	2.16	0.44
1:B:361:GLN:HA	1:B:461:ARG:O	2.17	0.44
1:D:416:ASP:O	1:D:417:ILE:HG13	2.17	0.44
1:A:255:VAL:HG22	1:A:263:MSE:HE3	1.99	0.44
1:C:305:LYS:HG2	1:C:307:PHE:CE1	2.53	0.44
1:D:184:ASN:N	1:D:253:ASN:HD22	2.04	0.44
1:D:421:LYS:HE2	1:D:445:ASN:HB3	1.99	0.44
1:A:39:PHE:CD1	1:B:454:GLU:HG3	2.53	0.44
1:A:111:ILE:HG13	1:A:189:GLY:HA2	1.99	0.44
1:A:361:GLN:HG2	1:A:463:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:SER:O	1:B:428:ASP:CB	2.66	0.44
1:B:457:PHE:HZ	1:B:478:ASP:OD2	2.00	0.44
1:A:194:GLU:HB2	1:A:200:VAL:HG21	1.99	0.44
1:A:361:GLN:HG2	1:A:463:TYR:CZ	2.51	0.44
1:B:126:LEU:HA	1:B:127:PRO:HD3	1.86	0.44
1:B:390:PRO:HG2	1:B:473:SER:HB3	1.99	0.44
1:C:393:ASN:O	1:C:394:PHE:HB3	2.16	0.44
1:A:292:LYS:HD3	1:B:26:VAL:HG12	2.00	0.44
1:B:159:TYR:HD2	1:B:179:ILE:HD11	1.81	0.44
1:B:362:ARG:HD2	1:B:362:ARG:HA	1.85	0.44
1:B:475:THR:HG22	1:B:476:MSE:N	2.32	0.44
1:C:151:PRO:HG2	1:C:159:TYR:OH	2.18	0.44
1:A:366:THR:HG21	1:A:479:ILE:HD13	2.00	0.44
1:A:481:LEU:CD2	1:A:482:VAL:HG23	2.41	0.44
1:B:280:THR:OG1	1:B:283:GLN:HG3	2.17	0.44
1:C:136:LEU:HD11	1:C:347:THR:HA	1.99	0.44
1:C:183:THR:CG2	1:C:256:GLU:OE2	2.66	0.44
1:C:277:PHE:CE1	1:C:279:PRO:HG3	2.52	0.44
1:C:347:THR:HG23	1:C:352:MSE:SE	2.67	0.44
1:D:319:ASP:HA	1:D:364:LEU:HD23	2.00	0.44
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.86	0.44
1:A:346:ILE:C	1:A:347:THR:HG23	2.38	0.44
1:B:215:ASP:HB2	1:C:28:SER:HA	1.99	0.44
1:B:341:TRP:NE1	1:B:348:VAL:CG1	2.80	0.44
1:B:457:PHE:CZ	1:B:478:ASP:OD2	2.71	0.44
1:D:73:TRP:CZ3	1:D:346:ILE:HD13	2.53	0.44
1:D:27:PRO:HB2	3:D:835:HOH:O	2.18	0.44
1:A:111:ILE:CG2	1:A:112:GLY:N	2.81	0.44
1:B:378:GLU:CB	1:B:452:PRO:HD3	2.24	0.44
1:B:399:VAL:HA	1:B:457:PHE:HB3	2.00	0.44
1:B:476:MSE:HG3	1:B:477:GLY:N	2.33	0.44
1:C:71:MSE:CE	1:C:74:LEU:HD23	2.47	0.44
1:C:213:TYR:CD1	1:C:213:TYR:C	2.91	0.44
1:C:389:VAL:HA	1:C:390:PRO:HD3	1.87	0.44
1:C:464:GLY:N	1:C:465:PRO:CD	2.81	0.44
1:C:235:ILE:HD11	1:C:406:LEU:HD21	1.99	0.43
1:C:312:TRP:CG	1:C:475:THR:HG23	2.53	0.43
1:B:230:ILE:CD1	1:B:231:ASP:H	2.30	0.43
1:B:425:VAL:HG12	1:B:426:ASN:H	1.82	0.43
1:C:141:ARG:HH12	1:C:258:ARG:CZ	2.31	0.43
1:A:25:VAL:HG22	1:A:34:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASN:HD21	1:B:286:ILE:HD11	1.83	0.43
1:C:87:GLN:C	1:C:88:MSE:HE2	2.38	0.43
1:C:341:TRP:HZ3	1:C:348:VAL:HB	1.83	0.43
1:C:436:GLY:CA	1:C:450:THR:HG22	2.48	0.43
1:D:211:GLN:CD	1:D:221:LYS:HD3	2.39	0.43
1:A:235:ILE:HD11	1:A:406:LEU:HG	1.99	0.43
1:A:342:PHE:HZ	1:A:348:VAL:CG2	2.31	0.43
1:B:375:LEU:HD13	1:B:457:PHE:CE1	2.53	0.43
1:C:182:LYS:HD2	1:C:256:GLU:OE1	2.19	0.43
1:C:203:GLN:O	1:C:207:ASN:ND2	2.51	0.43
1:C:255:VAL:HG22	1:C:263:MSE:HE3	2.00	0.43
1:C:380:THR:HA	1:C:435:TYR:O	2.18	0.43
1:D:362:ARG:HD2	1:D:362:ARG:HA	1.76	0.43
1:A:321:ILE:HG13	1:A:341:TRP:CE2	2.53	0.43
1:A:380:THR:HA	1:A:435:TYR:O	2.18	0.43
1:B:379:HIS:HB3	1:B:480:GLU:OE2	2.19	0.43
1:D:91:PHE:HB2	1:D:109:TYR:HB2	2.00	0.43
1:D:425:VAL:HA	1:D:431:ILE:HD13	1.99	0.43
1:A:251:GLN:HE22	1:A:274:GLY:N	2.00	0.43
1:A:312:TRP:CG	1:A:475:THR:HG23	2.54	0.43
1:A:408:ILE:HD11	1:A:451:ASN:OD1	2.18	0.43
1:B:95:LYS:CG	1:B:229:GLU:HG3	2.44	0.43
1:B:104:ASN:ND2	1:B:107:THR:H	2.15	0.43
1:B:162:VAL:HA	1:B:163:PRO:HD3	1.86	0.43
1:B:410:ASN:CB	1:B:448:VAL:HG13	2.49	0.43
1:D:469:MSE:HG3	1:D:470:PHE:N	2.33	0.43
1:A:390:PRO:HD3	1:A:474:TRP:CD2	2.54	0.43
1:B:123:ILE:HD13	1:B:176:TYR:HE2	1.83	0.43
1:B:143:LEU:CD1	1:B:181:PRO:HB3	2.49	0.43
1:B:161:ILE:N	1:B:161:ILE:CD1	2.76	0.43
1:B:382:LYS:HE3	1:B:431:ILE:HG21	2.01	0.43
1:B:408:ILE:HD12	1:B:409:ILE:N	2.34	0.43
1:C:40:PRO:HG2	1:C:45:MSE:HE3	2.01	0.43
1:C:384:HIS:O	1:C:386:PRO:HD3	2.18	0.43
1:C:481:LEU:HD13	1:C:481:LEU:C	2.39	0.43
1:D:97:LYS:HE2	1:D:109:TYR:CD2	2.54	0.43
1:D:194:GLU:HA	1:D:195:PRO:HD3	1.83	0.43
1:A:130:LYS:HD2	1:A:194:GLU:CD	2.39	0.43
1:B:124:ILE:CD1	1:B:210:THR:HG22	2.49	0.43
1:B:193:LEU:HD13	1:B:463:TYR:CE1	2.51	0.43
1:C:147:SER:HA	1:C:152:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLU:HG3	3:C:686:HOH:O	2.18	0.43
1:A:475:THR:CG2	1:A:476:MSE:N	2.81	0.43
1:C:73:TRP:HZ3	1:C:346:ILE:HD13	1.83	0.43
1:C:421:LYS:HG2	1:C:422:ASN:N	2.34	0.43
1:C:439:PRO:HG3	1:C:447:TRP:CZ3	2.54	0.42
1:D:148:LEU:O	1:D:153:LYS:HA	2.19	0.42
1:D:174:LYS:HG3	3:D:780:HOH:O	2.19	0.42
1:B:467:GLU:HG2	1:B:472:LYS:HD2	2.00	0.42
1:C:172:ASN:N	1:C:173:PRO:HD3	2.34	0.42
1:A:195:PRO:HD2	3:A:741:HOH:O	2.19	0.42
1:A:247:HIS:O	1:A:251:GLN:HG2	2.19	0.42
1:A:391:ALA:HA	1:A:464:GLY:O	2.19	0.42
1:B:205:VAL:HB	1:B:206:PRO:HD3	2.00	0.42
1:B:382:LYS:HE3	1:B:431:ILE:CG2	2.49	0.42
1:B:461:ARG:CG	1:B:461:ARG:NH1	2.83	0.42
1:C:56:ARG:HB3	1:C:265:GLN:HB3	2.01	0.42
1:C:91:PHE:CE2	1:C:227:VAL:HG21	2.54	0.42
1:D:135:MSE:HE2	1:D:188:GLY:HA3	2.00	0.42
1:A:342:PHE:CZ	1:A:348:VAL:HG22	2.55	0.42
1:B:211:GLN:HA	1:B:212:PRO:HD3	1.93	0.42
1:C:57:ALA:HB2	1:C:269:LEU:CD1	2.50	0.42
1:C:211:GLN:HA	1:C:212:PRO:HD3	1.83	0.42
1:C:475:THR:CG2	1:C:476:MSE:H	2.33	0.42
1:D:166:GLU:OE2	1:D:169:LYS:HD2	2.19	0.42
1:D:230:ILE:HD13	1:D:230:ILE:N	2.34	0.42
1:D:462:PHE:CE2	1:D:469:MSE:HE3	2.54	0.42
1:A:45:MSE:HE1	1:B:304:THR:N	2.34	0.42
1:A:48:MSE:HE2	1:A:48:MSE:HA	2.02	0.42
1:A:143:LEU:HD11	1:A:181:PRO:HB3	2.02	0.42
1:B:70:ILE:HD13	1:B:346:ILE:HD11	2.00	0.42
1:B:468:LYS:C	1:B:468:LYS:HZ2	2.22	0.42
1:A:205:VAL:HG23	1:A:206:PRO:HD3	1.98	0.42
1:D:384:HIS:O	1:D:386:PRO:HD3	2.20	0.42
1:A:69:SER:OG	1:A:346:ILE:HD13	2.19	0.42
1:A:197:VAL:O	1:A:201:VAL:HG23	2.20	0.42
1:C:110:VAL:HB	1:C:190:ILE:HB	2.02	0.42
1:C:247:HIS:HE1	1:C:275:LYS:O	2.03	0.42
1:C:268:PHE:HE2	1:D:306:ARG:HD3	1.85	0.42
1:C:389:VAL:C	1:C:391:ALA:H	2.23	0.42
1:A:88:MSE:HE2	1:A:88:MSE:N	2.34	0.42
1:A:317:TRP:CZ2	1:A:479:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PHE:HZ	1:A:348:VAL:HG22	1.84	0.42
1:B:71:MSE:CB	1:B:249:ILE:HD11	2.44	0.42
1:B:361:GLN:HG2	1:B:462:PHE:CZ	2.55	0.42
1:C:131:MSE:HE3	1:C:192:ILE:HG12	2.02	0.42
1:C:349:SER:CB	1:C:352:MSE:HE3	2.50	0.42
1:D:162:VAL:HA	1:D:163:PRO:HD3	1.96	0.42
1:D:421:LYS:HG2	1:D:422:ASN:N	2.34	0.42
1:B:88:MSE:HG2	3:B:688:HOH:O	2.19	0.41
1:C:139:HIS:O	1:C:140:GLN:CB	2.66	0.41
1:D:196:ASP:O	1:D:200:VAL:HG22	2.20	0.41
1:A:141:ARG:NE	1:A:182:LYS:HZ1	2.18	0.41
1:A:183:THR:HG22	1:A:256:GLU:OE2	2.19	0.41
1:A:230:ILE:HG12	1:A:231:ASP:N	2.34	0.41
1:C:23:GLU:HA	1:C:35:PHE:O	2.20	0.41
1:D:101:ILE:HG12	1:D:235:ILE:HG22	2.00	0.41
1:A:141:ARG:NH1	1:A:258:ARG:NH2	2.68	0.41
1:A:258:ARG:NH1	1:A:259:ASP:OD2	2.54	0.41
1:B:375:LEU:O	1:B:454:GLU:CG	2.59	0.41
1:D:462:PHE:CD2	1:D:469:MSE:HE3	2.55	0.41
1:A:323:VAL:HG22	1:A:324:SER:O	2.20	0.41
1:B:408:ILE:HD13	3:B:756:HOH:O	2.19	0.41
1:C:162:VAL:O	1:C:181:PRO:HD2	2.19	0.41
1:C:247:HIS:CE1	1:C:275:LYS:O	2.74	0.41
1:C:407:MSE:HE2	1:C:415:PRO:HG2	2.01	0.41
1:C:460:PHE:CZ	1:C:476:MSE:HE1	2.56	0.41
1:D:128:GLU:O	1:D:129:ALA:HB2	2.20	0.41
1:A:251:GLN:NE2	1:A:274:GLY:H	2.01	0.41
1:C:162:VAL:HA	1:C:163:PRO:HD3	1.89	0.41
1:D:286:ILE:HD12	1:D:286:ILE:N	2.36	0.41
1:B:227:VAL:HA	1:B:228:PRO:HD3	1.87	0.41
1:C:182:LYS:CD	1:C:256:GLU:OE1	2.69	0.41
1:D:66:PRO:HG3	1:D:338:ARG:HG2	2.01	0.41
1:A:190:ILE:HG22	1:A:191:ARG:N	2.35	0.41
1:B:167:LYS:HE3	1:C:25:VAL:O	2.19	0.41
1:B:378:GLU:O	1:B:435:TYR:HE1	2.04	0.41
1:C:98:GLN:OE1	1:C:409:ILE:HD11	2.21	0.41
1:A:101:ILE:HD12	1:A:344:GLU:C	2.40	0.41
1:A:123:ILE:O	1:A:210:THR:HA	2.21	0.41
1:B:445:ASN:OD1	1:B:445:ASN:N	2.53	0.41
1:B:468:LYS:HB2	1:B:468:LYS:NZ	2.26	0.41
1:C:240:LEU:HD11	1:C:284:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:TRP:CZ3	1:D:476:MSE:HB3	2.56	0.41
1:A:56:ARG:HD3	1:A:265:GLN:CB	2.50	0.41
1:A:384:HIS:O	1:A:386:PRO:HD3	2.21	0.41
1:A:390:PRO:HB3	1:A:466:THR:OG1	2.21	0.41
1:B:335:LEU:HD12	1:B:338:ARG:HH12	1.86	0.41
1:B:382:LYS:CB	1:B:481:LEU:HD11	2.49	0.41
1:B:407:MSE:HB3	1:B:415:PRO:HB3	2.02	0.41
1:B:422:ASN:HB2	1:B:445:ASN:OD1	2.21	0.41
1:B:451:ASN:N	1:B:451:ASN:HD22	2.18	0.41
1:B:454:GLU:C	1:B:454:GLU:CD	2.80	0.41
1:B:468:LYS:CB	1:B:468:LYS:NZ	2.83	0.41
1:C:312:TRP:CZ3	1:C:476:MSE:HB3	2.56	0.41
1:D:242:TYR:O	1:D:246:ILE:HG12	2.21	0.41
1:D:434:TYR:O	1:D:447:TRP:HA	2.21	0.41
1:A:72:GLU:HB3	1:A:234:HIS:O	2.21	0.41
1:A:162:VAL:HA	1:A:163:PRO:HD3	1.93	0.41
1:A:174:LYS:HB3	1:A:174:LYS:HZ3	1.85	0.41
1:A:362:ARG:NH1	1:A:469:MSE:HE2	2.35	0.41
1:A:397:THR:O	1:A:416:ASP:HB2	2.21	0.41
1:A:471:ASP:O	1:A:472:LYS:HB2	2.21	0.41
1:B:116:LEU:HD11	1:B:161:ILE:HG22	2.02	0.41
1:B:166:GLU:HG2	1:B:169:LYS:HD3	2.03	0.41
1:B:259:ASP:O	1:B:263:MSE:HG2	2.20	0.41
1:C:88:MSE:HG2	3:C:614:HOH:O	2.20	0.41
1:C:140:GLN:O	1:C:140:GLN:CG	2.56	0.41
1:C:422:ASN:HA	3:C:771:HOH:O	2.20	0.41
1:A:111:ILE:HG22	1:A:112:GLY:N	2.36	0.40
1:A:174:LYS:NZ	1:A:174:LYS:CB	2.84	0.40
1:A:205:VAL:HG23	1:A:206:PRO:CD	2.52	0.40
1:A:292:LYS:HD2	1:B:28:SER:HB3	2.02	0.40
1:A:434:TYR:CD1	1:A:440:VAL:HG21	2.56	0.40
1:B:398:THR:O	1:B:457:PHE:HB2	2.21	0.40
1:C:282:GLU:HG3	1:C:283:GLN:H	1.85	0.40
1:A:151:PRO:HD2	1:A:159:TYR:OH	2.20	0.40
1:B:208:ILE:O	1:B:224:VAL:HG23	2.20	0.40
1:B:399:VAL:HB	1:B:447:TRP:CZ2	2.56	0.40
1:D:88:MSE:HE1	1:D:114:TRP:CZ3	2.57	0.40
1:D:89:GLY:HA2	1:D:225:ALA:O	2.21	0.40
1:D:135:MSE:HE2	1:D:188:GLY:HA2	2.03	0.40
1:D:137:ASP:OD1	1:D:137:ASP:C	2.60	0.40
1:D:185:VAL:H	1:D:253:ASN:ND2	2.16	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CZ	1:B:367:TYR:HB3	2.57	0.40
1:A:66:PRO:HG2	1:A:338:ARG:CG	2.40	0.40
1:A:334:GLU:HB3	1:A:337:GLU:HB2	2.04	0.40
1:B:23:GLU:O	1:B:24:THR:HG23	2.21	0.40
1:B:74:LEU:HB2	1:B:113:THR:HG21	2.03	0.40
1:B:140:GLN:HE22	1:B:346:ILE:HD12	1.86	0.40
1:B:247:HIS:CG	1:B:277:PHE:HB2	2.57	0.40
1:B:433:VAL:HG23	1:B:446:ASN:HA	2.02	0.40
1:A:141:ARG:CZ	1:A:327:GLN:OE1	2.70	0.40
1:A:194:GLU:HA	1:A:195:PRO:HD3	1.84	0.40
1:B:435:TYR:CZ	1:B:437:PRO:HD2	2.55	0.40
1:B:436:GLY:O	1:B:448:VAL:HG23	2.20	0.40
1:C:62:LEU:CD1	1:C:297:MSE:HE2	2.45	0.40
1:C:66:PRO:O	1:C:342:PHE:CE2	2.74	0.40
1:C:126:LEU:HA	1:C:127:PRO:HD3	1.85	0.40
1:C:481:LEU:HD22	1:C:482:VAL:N	2.35	0.40
1:A:311:TYR:OH	1:A:469:MSE:HE3	2.21	0.40
1:A:389:VAL:HA	1:A:390:PRO:HD3	1.88	0.40
1:B:363:TYR:N	1:B:363:TYR:CD1	2.89	0.40
1:B:378:GLU:OE1	1:B:379:HIS:CE1	2.74	0.40
1:B:470:PHE:CG	1:B:472:LYS:HE3	2.57	0.40
1:B:477:GLY:HA3	3:B:635:HOH:O	2.20	0.40
1:C:140:GLN:OE1	1:C:342:PHE:CD1	2.75	0.40
1:C:142:VAL:CG2	1:C:348:VAL:HG13	2.52	0.40
1:D:37:SER:O	1:D:38:ASP:HB2	2.22	0.40
1:D:116:LEU:HD11	1:D:181:PRO:HG3	2.04	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	458/483 (95%)	436 (95%)	20 (4%)	2 (0%)	34	32
1	B	460/483 (95%)	428 (93%)	26 (6%)	6 (1%)	12	7
1	C	458/483 (95%)	435 (95%)	18 (4%)	5 (1%)	14	9
1	D	458/483 (95%)	432 (94%)	23 (5%)	3 (1%)	22	18
All	All	1834/1932 (95%)	1731 (94%)	87 (5%)	16 (1%)	17	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	419	SER
1	B	452	PRO
1	C	334	GLU
1	A	334	GLU
1	B	437	PRO
1	C	147	SER
1	C	197	VAL
1	B	454	GLU
1	B	463	TYR
1	D	334	GLU
1	B	215	ASP
1	D	214	ALA
1	A	147	SER
1	C	390	PRO
1	D	147	SER
1	C	330	GLU

### 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	405/408 (99%)	389 (96%)	16 (4%)	31	32
1	B	407/408 (100%)	393 (97%)	14 (3%)	37	39
1	C	405/408 (99%)	393 (97%)	12 (3%)	41	44
1	D	405/408 (99%)	397 (98%)	8 (2%)	55	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1622/1632 (99%)	1572 (97%)	50 (3%)	40 43

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	33	LEU
1	A	39	PHE
1	A	72	GLU
1	A	94	LEU
1	A	101	ILE
1	A	104	ASN
1	A	117	GLU
1	A	145	ASP
1	A	166	GLU
1	A	174	LYS
1	A	308	THR
1	A	348	VAL
1	A	363	TYR
1	A	408	ILE
1	A	469	MSE
1	B	22	GLN
1	B	29	ARG
1	B	104	ASN
1	B	145	ASP
1	B	172	ASN
1	B	187	TYR
1	B	229	GLU
1	B	269	LEU
1	B	408	ILE
1	B	452	PRO
1	B	454	GLU
1	B	461	ARG
1	B	468	LYS
1	B	469	MSE
1	C	95	LYS
1	C	134	MSE
1	C	145	ASP
1	C	169	LYS
1	C	198	ASP
1	C	306	ARG
1	C	329	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	342	PHE
1	C	347	THR
1	C	424	LYS
1	C	469	MSE
1	C	476	MSE
1	D	33	LEU
1	D	101	ILE
1	D	145	ASP
1	D	176	TYR
1	D	196	ASP
1	D	230	ILE
1	D	405	ARG
1	D	469	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	47	ASN
1	A	50	ASN
1	A	59	GLN
1	A	87	GLN
1	A	104	ASN
1	A	125	ASN
1	A	172	ASN
1	A	207	ASN
1	A	234	HIS
1	A	247	HIS
1	A	248	GLN
1	A	251	GLN
1	A	253	ASN
1	A	426	ASN
1	A	445	ASN
1	B	22	GLN
1	B	59	GLN
1	B	98	GLN
1	B	104	ASN
1	B	139	HIS
1	B	172	ASN
1	B	226	GLN
1	B	234	HIS
1	B	247	HIS
1	B	248	GLN

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Mol	Chain	Res	Type
1	B	251	GLN
1	B	253	ASN
1	B	368	GLN
1	B	379	HIS
1	B	451	ASN
1	C	59	GLN
1	C	92	ASN
1	C	96	GLN
1	C	125	ASN
1	C	203	GLN
1	C	226	GLN
1	C	234	HIS
1	C	247	HIS
1	C	248	GLN
1	C	251	GLN
1	C	253	ASN
1	C	361	GLN
1	C	368	GLN
1	C	379	HIS
1	C	422	ASN
1	D	59	GLN
1	D	75	ASN
1	D	125	ASN
1	D	140	GLN
1	D	234	HIS
1	D	247	HIS
1	D	251	GLN
1	D	253	ASN
1	D	379	HIS
1	D	404	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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	446/483 (92%)	0.40	22 (4%) 29 35	10, 24, 45, 55	0
1	B	448/483 (92%)	0.61	45 (10%) 7 9	8, 24, 51, 68	0
1	C	446/483 (92%)	0.43	24 (5%) 25 31	8, 24, 45, 64	0
1	D	446/483 (92%)	0.32	17 (3%) 40 46	10, 21, 40, 59	0
All	All	1786/1932 (92%)	0.44	108 (6%) 21 27	8, 23, 45, 68	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	TRP	13.0
1	B	437	PRO	8.3
1	B	463	TYR	6.5
1	B	474	TRP	6.3
1	A	482	VAL	6.1
1	B	443	TYR	5.7
1	B	481	LEU	5.6
1	B	452	PRO	5.6
1	B	454	GLU	5.4
1	B	435	TYR	5.4
1	D	440	VAL	5.2
1	B	451	ASN	5.1
1	C	342	PHE	4.8
1	B	428	ASP	4.8
1	D	215	ASP	4.7
1	B	470	PHE	4.7
1	A	24	THR	4.4
1	B	215	ASP	4.4
1	C	215	ASP	4.2
1	B	457	PHE	4.1
1	B	420	ARG	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	411	ASP	3.9
1	B	441	LYS	3.9
1	A	230	ILE	3.8
1	C	482	VAL	3.7
1	B	482	VAL	3.6
1	B	456	TRP	3.5
1	A	215	ASP	3.5
1	D	447	TRP	3.5
1	C	443	TYR	3.4
1	C	341	TRP	3.4
1	D	441	LYS	3.4
1	B	388	ASN	3.3
1	D	442	GLY	3.2
1	A	341	TRP	3.2
1	B	415	PRO	3.0
1	B	374	TRP	3.0
1	D	482	VAL	3.0
1	C	330	GLU	3.0
1	A	481	LEU	2.9
1	B	483	LYS	2.9
1	B	453	GLY	2.9
1	A	441	LYS	2.9
1	A	431	ILE	2.9
1	B	203	GLN	2.8
1	B	169	LYS	2.8
1	B	439	PRO	2.8
1	D	388	ASN	2.8
1	B	421	LYS	2.8
1	A	167	LYS	2.7
1	A	359	PHE	2.7
1	B	424	LYS	2.7
1	B	426	ASN	2.7
1	A	198	ASP	2.7
1	D	443	TYR	2.7
1	A	190	ILE	2.6
1	B	408	ILE	2.6
1	B	438	LYS	2.6
1	A	356	ILE	2.6
1	A	479	ILE	2.6
1	C	278	ASN	2.6
1	C	439	PRO	2.6
1	C	422	ASN	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	346	ILE	2.5
1	B	460	PHE	2.5
1	A	169	LYS	2.5
1	D	481	LEU	2.5
1	C	199	ARG	2.5
1	C	428	ASP	2.5
1	B	448	VAL	2.4
1	D	101	ILE	2.4
1	B	198	ASP	2.4
1	A	197	VAL	2.4
1	C	103	ALA	2.3
1	B	230	ILE	2.3
1	B	166	GLU	2.3
1	C	426	ASN	2.3
1	B	216	GLY	2.3
1	C	427	SER	2.3
1	B	170	ASP	2.2
1	C	169	LYS	2.2
1	D	214	ALA	2.2
1	A	278	ASN	2.2
1	B	65	ILE	2.2
1	A	196	ASP	2.2
1	C	167	LYS	2.2
1	B	449	GLN	2.2
1	B	431	ILE	2.1
1	C	479	ILE	2.1
1	A	39	PHE	2.1
1	C	197	VAL	2.1
1	D	411	ASP	2.1
1	A	171	LEU	2.1
1	D	453	GLY	2.1
1	B	172	ASN	2.1
1	B	432	ASP	2.1
1	D	231	ASP	2.1
1	C	436	GLY	2.1
1	D	438	LYS	2.1
1	C	343	TYR	2.1
1	D	216	GLY	2.1
1	C	356	ILE	2.0
1	C	431	ILE	2.0
1	A	229	GLU	2.0
1	D	124	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	475	THR	2.0
1	C	268	PHE	2.0
1	A	66	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	502	1/1	0.97	0.42	16,16,16,16	0
2	MG	B	502	1/1	0.97	0.44	21,21,21,21	0
2	MG	D	502	1/1	0.97	0.43	20,20,20,20	0
2	MG	D	501	1/1	0.98	0.13	14,14,14,14	0
2	MG	B	501	1/1	0.98	0.20	18,18,18,18	0
2	MG	A	501	1/1	0.99	0.17	16,16,16,16	0
2	MG	C	501	1/1	0.99	0.13	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.