



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 10:12 AM JST

PDB ID : 21FP / pdb\_000021fp  
Title : Chloramphenicol-bound MexB  
Authors : Ueda, Y.; Yonehara, R.; Nakagawa, A.; Yamashita, E.  
Deposited on : 2025-12-11  
Resolution : 2.89 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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

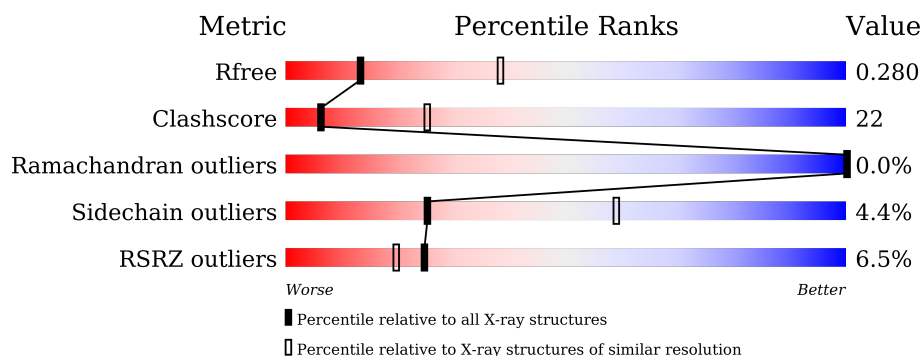
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	1054	<div> <div>6%</div> <div>61% 35% ..</div> </div>
1	B	1054	<div> <div>9%</div> <div>54% 42% ..</div> </div>
1	C	1054	<div> <div>4%</div> <div>56% 40% ..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23408 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 Multidrug resistance protein MexB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0	0
			7764	4998	1289	1437	40			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			

There are 24 discrepancies between the modelled and reference sequences:

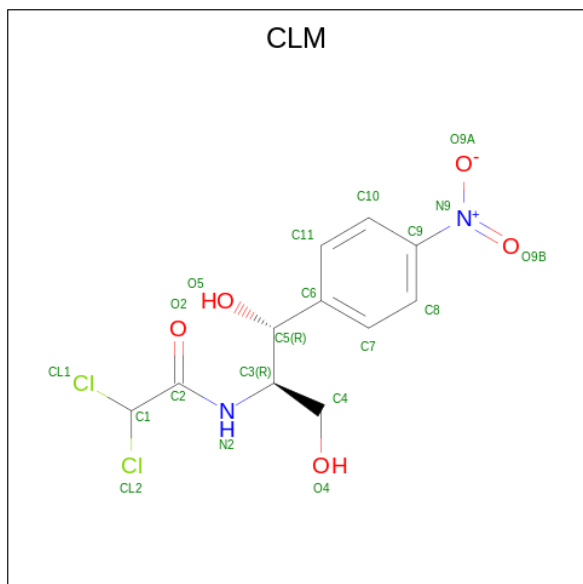
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	LEU	-	expression tag	UNP P52002
A	1048	GLU	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
A	1053	HIS	-	expression tag	UNP P52002
A	1054	HIS	-	expression tag	UNP P52002
B	1047	LEU	-	expression tag	UNP P52002
B	1048	GLU	-	expression tag	UNP P52002
B	1049	HIS	-	expression tag	UNP P52002
B	1050	HIS	-	expression tag	UNP P52002
B	1051	HIS	-	expression tag	UNP P52002
B	1052	HIS	-	expression tag	UNP P52002
B	1053	HIS	-	expression tag	UNP P52002
B	1054	HIS	-	expression tag	UNP P52002
C	1047	LEU	-	expression tag	UNP P52002
C	1048	GLU	-	expression tag	UNP P52002
C	1049	HIS	-	expression tag	UNP P52002
C	1050	HIS	-	expression tag	UNP P52002
C	1051	HIS	-	expression tag	UNP P52002
C	1052	HIS	-	expression tag	UNP P52002
C	1053	HIS	-	expression tag	UNP P52002

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P52002

- Molecule 2 is CHLORAMPHENICOL (CCD ID: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ) (labeled as "Ligand of Interest" by depositor).

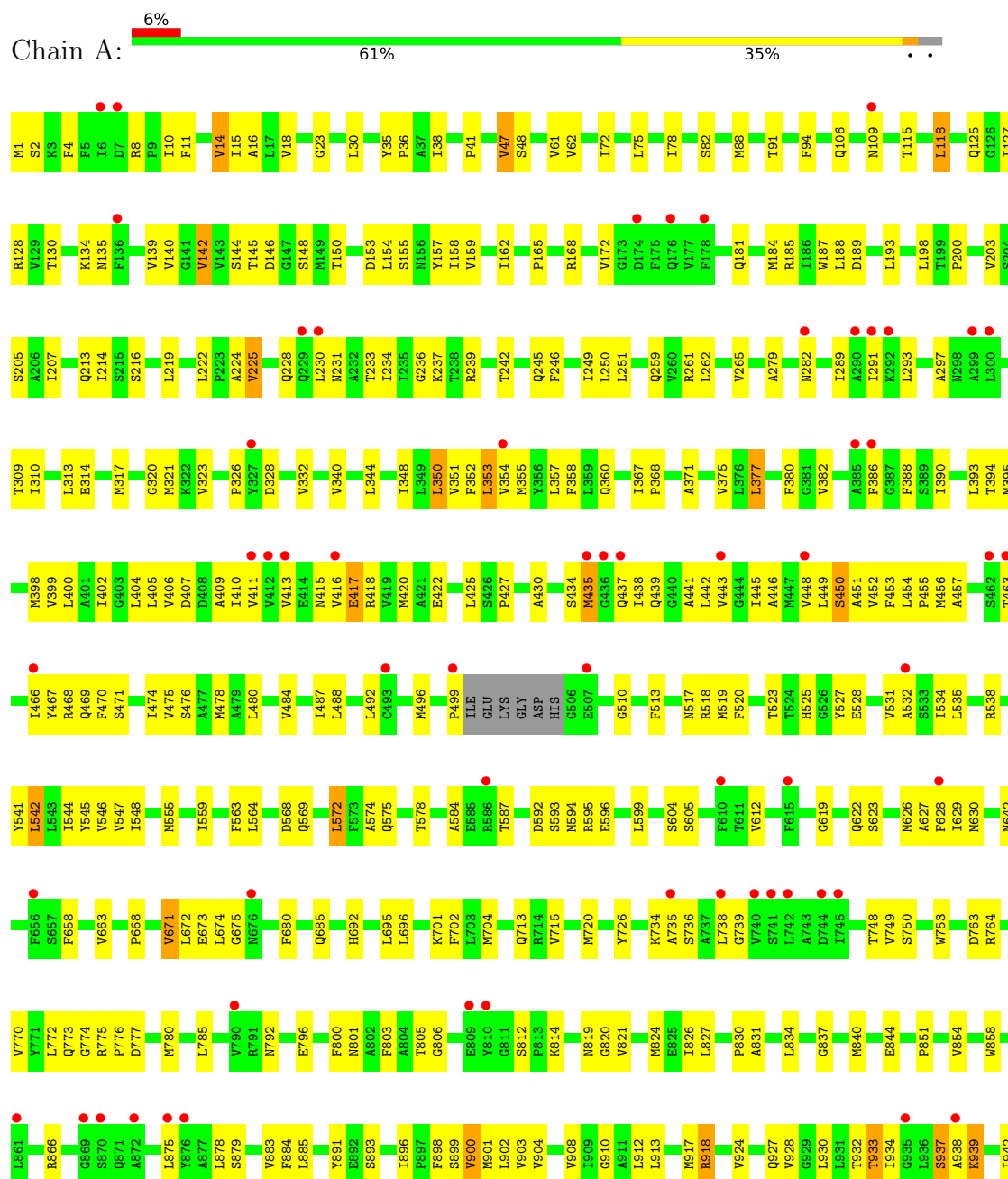


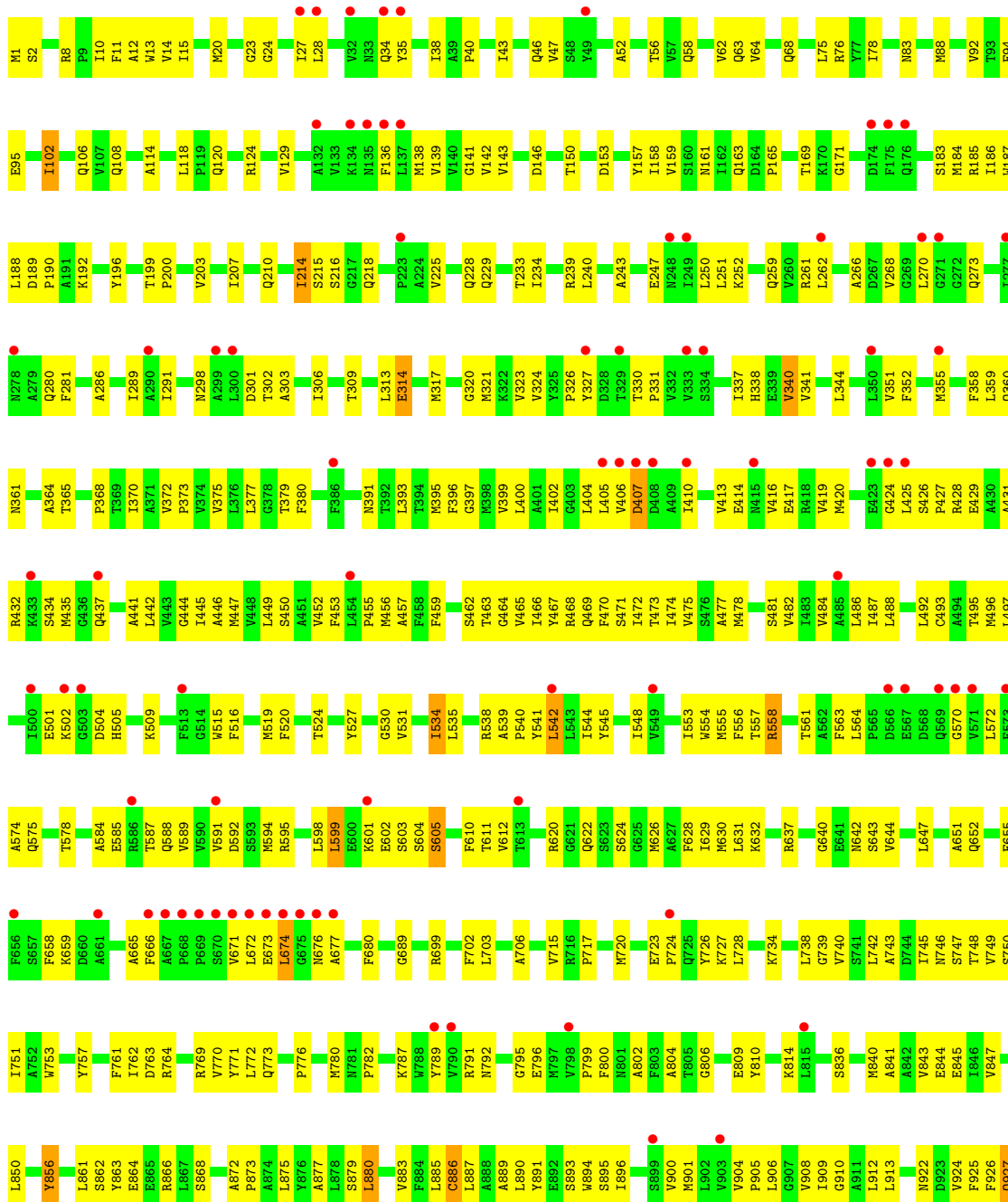
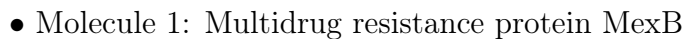
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

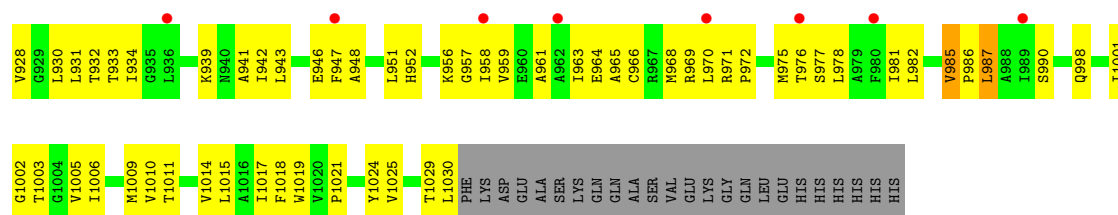
### 3 Residue-property plots

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.

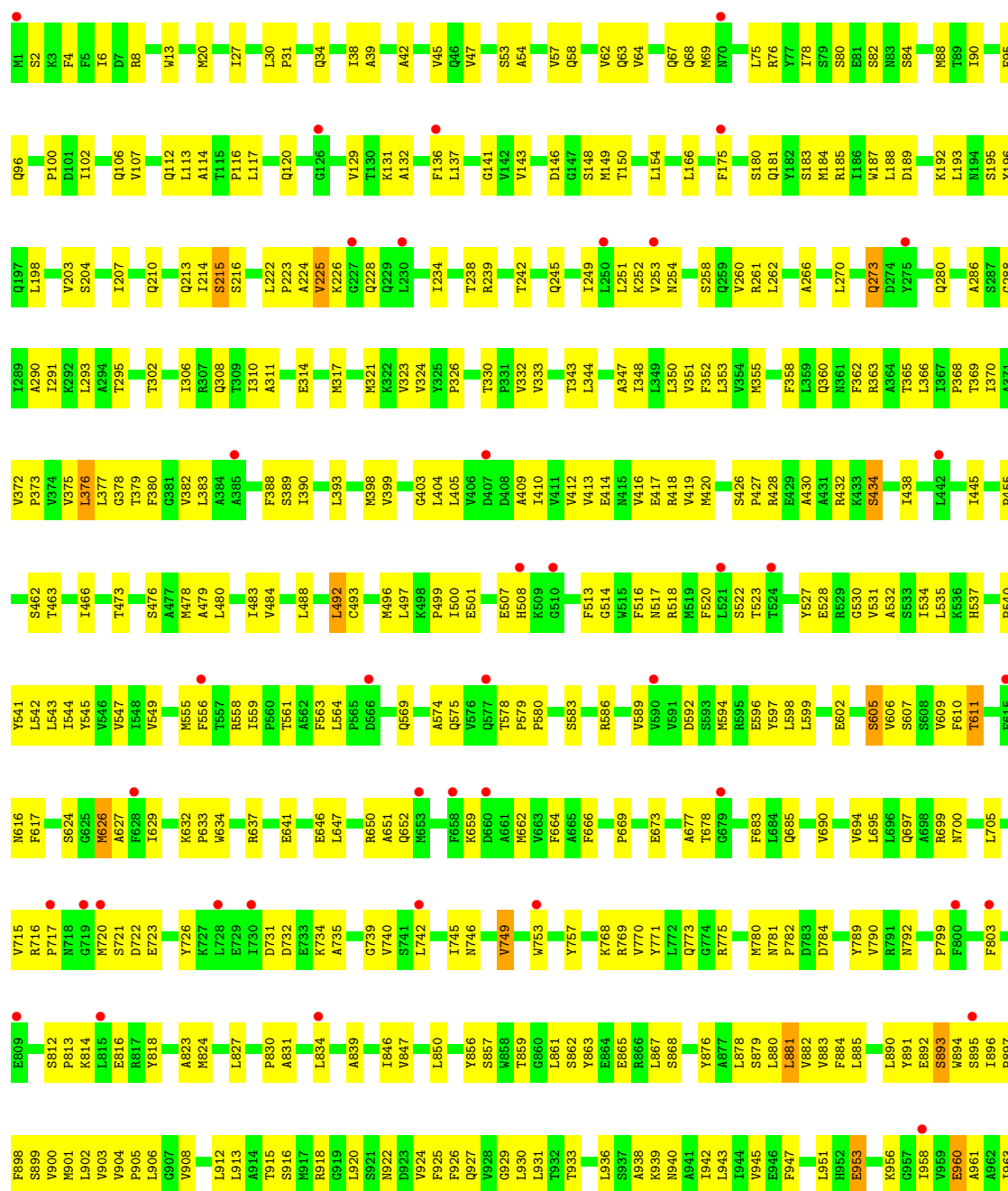
#### • Molecule 1: Multidrug resistance protein MexB

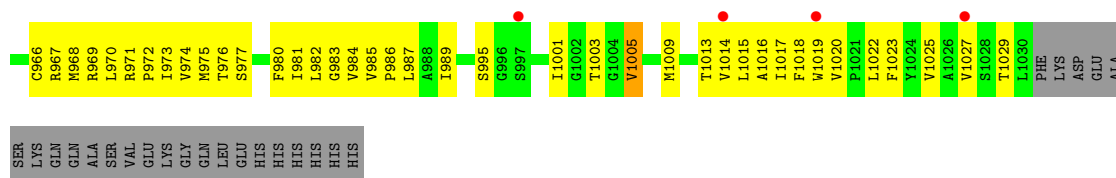






• Molecule 1: Multidrug resistance protein MexB







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.87Å 169.17Å 171.93Å 90.00° 102.16° 90.00°	Depositor
Resolution (Å)	51.02 – 2.89 51.02 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (51.02-2.89) 99.3 (51.02-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419+SVN	Depositor
R, $R_{free}$	0.224 , 0.280 0.226 , 0.280	Depositor DCC
$R_{free}$ test set	6472 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.6	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 78.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.46	2/7921 (0.0%)	0.68	0/10765
1	B	0.39	3/7971 (0.0%)	0.62	1/10833 (0.0%)
1	C	0.39	0/7971	0.63	0/10833
All	All	0.42	5/23863 (0.0%)	0.64	1/32431 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	985	VAL	CA-CB	6.05	1.57	1.54
1	B	46	GLN	C-N	-5.46	1.28	1.33
1	A	1020	VAL	CA-CB	-5.13	1.51	1.54
1	B	985	VAL	C-N	5.04	1.38	1.33
1	B	314	GLU	C-N	5.03	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	VAL	N-CA-C	-6.32	107.13	113.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7764	0	7899	313	0
1	B	7812	0	7944	430	0
1	C	7812	0	7944	353	0
2	B	20	0	11	1	0
All	All	23408	0	23798	1050	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 22.

All (1050) 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:158:ILE:HG21	1:B:289:ILE:HD11	1.32	1.08
1:A:445:ILE:HD13	1:A:939:LYS:HZ1	1.15	1.07
1:C:884:PHE:HB2	1:C:901:MET:HE2	1.45	0.97
1:C:350:LEU:HB3	1:C:982:LEU:HD12	1.48	0.95
1:B:417:GLU:HA	1:B:420:MET:HB2	1.47	0.95
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.49	0.95
1:A:937:SER:HB2	1:A:1012:ALA:HB1	1.48	0.93
1:A:696:LEU:HA	1:A:824:MET:HE1	1.48	0.92
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.52	0.91
1:B:108:GLN:HB2	1:C:112:GLN:HE22	1.34	0.89
1:A:492:LEU:HD22	1:A:496:MET:HE1	1.60	0.84
1:A:619:GLY:HA3	1:A:720:MET:HE2	1.59	0.82
1:B:400:LEU:HD11	1:B:1001:ILE:HD13	1.59	0.82
1:C:830:PRO:HB3	1:C:839:ALA:HB2	1.60	0.80
1:B:981:ILE:HD11	1:B:1009:MET:HG3	1.63	0.80
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.62	0.80
1:A:407:ASP:OD2	1:A:939:LYS:HD3	1.82	0.79
1:A:780:MET:HE1	1:C:224:ALA:HB1	1.63	0.79
1:A:958:ILE:HG13	1:A:959:VAL:H	1.48	0.79
1:C:940:ASN:HD21	1:C:1013:THR:HG22	1.46	0.79
1:B:800:PHE:HD1	1:B:804:ALA:HB2	1.47	0.78
1:A:355:MET:HE1	1:A:368:PRO:HD2	1.66	0.78
1:A:780:MET:HE2	1:C:225:VAL:H	1.48	0.78
1:C:203:VAL:HG13	1:C:262:LEU:HD11	1.65	0.78
1:C:561:THR:HG22	1:C:922:ASN:HB3	1.66	0.78
1:C:555:MET:HE2	1:C:913:LEU:HD22	1.64	0.77
1:B:904:VAL:HG13	1:B:905:PRO:HD3	1.67	0.77
1:B:584:ALA:H	1:B:622:GLN:HE21	1.32	0.77
1:C:314:GLU:HA	1:C:317:MET:HE3	1.65	0.76
1:B:658:PHE:HD1	1:B:659:LYS:H	1.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD11	1:A:1001:ILE:HD11	1.65	0.76
1:A:441:ALA:O	1:A:445:ILE:HG13	1.85	0.76
1:B:449:LEU:HB2	1:B:478:MET:HE3	1.67	0.76
1:B:584:ALA:H	1:B:622:GLN:NE2	1.84	0.75
1:B:68:GLN:HG3	1:B:114:ALA:HB2	1.69	0.74
1:A:146:ASP:HB2	1:A:320:GLY:HA3	1.69	0.74
1:B:555:MET:HE2	1:B:913:LEU:HD22	1.68	0.74
1:C:428:ARG:HH22	1:C:432:ARG:HH11	1.32	0.74
1:B:38:ILE:HD12	1:B:671:VAL:HG21	1.68	0.73
1:B:585:GLU:HA	1:B:588:GLN:HB3	1.70	0.73
1:A:470:PHE:CE2	1:A:928:VAL:HG13	2.24	0.73
1:B:441:ALA:HA	1:B:890:LEU:HD11	1.69	0.73
1:C:662:MET:HB3	1:C:664:PHE:HE2	1.53	0.72
1:C:188:LEU:HD23	1:C:266:ALA:HB2	1.70	0.72
1:B:52:ALA:HB1	1:B:56:THR:HB	1.71	0.72
1:C:534:ILE:HG23	1:C:541:TYR:HD2	1.54	0.72
1:B:444:GLY:HA3	1:B:890:LEU:HD13	1.71	0.72
1:C:332:VAL:HG22	1:C:634:TRP:HZ2	1.54	0.71
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.72	0.71
1:A:140:VAL:HG11	1:A:310:ILE:HD11	1.73	0.71
1:B:591:VAL:HG22	1:B:611:THR:HB	1.71	0.71
1:A:413:VAL:HA	1:A:416:VAL:HG12	1.73	0.70
1:B:400:LEU:HB3	1:B:932:THR:HG21	1.73	0.70
1:B:981:ILE:CD1	1:B:1009:MET:HG3	2.20	0.70
1:B:939:LYS:HA	1:B:942:ILE:HB	1.74	0.70
1:A:574:ALA:HB3	1:A:627:ALA:HB3	1.72	0.70
1:A:545:TYR:HB2	1:A:1019:TRP:CZ3	2.27	0.70
1:C:75:LEU:HD11	1:C:78:ILE:HD11	1.73	0.69
1:A:420:MET:HE3	1:A:430:ALA:HB3	1.74	0.69
1:B:703:LEU:HD21	1:B:717:PRO:HD3	1.75	0.69
1:B:624:SER:OG	1:B:720:MET:HE1	1.91	0.69
1:C:358:PHE:HB2	1:C:975:MET:HE3	1.73	0.69
1:B:572:LEU:HG	1:B:629:ILE:HD12	1.73	0.69
1:B:933:THR:HG21	1:B:1005:VAL:HA	1.74	0.68
1:B:981:ILE:HD11	1:B:1009:MET:HB3	1.75	0.68
1:A:242:THR:HG23	1:A:245:GLN:H	1.58	0.68
1:A:225:VAL:HG22	1:B:776:PRO:HB2	1.74	0.68
1:A:488:LEU:HG	1:A:492:LEU:HG	1.76	0.68
1:A:445:ILE:HD13	1:A:939:LYS:NZ	2.01	0.68
1:B:344:LEU:HD13	1:B:402:ILE:HD11	1.75	0.68
1:C:938:ALA:O	1:C:942:ILE:HG12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:VAL:HB	1:A:674:LEU:HG	1.75	0.68
1:B:186:ILE:HD13	1:B:262:LEU:HD21	1.77	0.67
1:C:881:LEU:O	1:C:885:LEU:HD12	1.93	0.67
1:A:47:VAL:HG12	1:A:88:MET:HE3	1.75	0.67
1:C:940:ASN:ND2	1:C:1013:THR:HG22	2.09	0.67
1:B:344:LEU:HD21	1:B:399:VAL:HG12	1.76	0.67
1:C:428:ARG:HH12	1:C:432:ARG:HD2	1.59	0.67
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.76	0.67
1:A:900:VAL:HG21	1:A:942:ILE:HG12	1.77	0.67
1:A:938:ALA:O	1:A:942:ILE:HG13	1.95	0.67
1:B:14:VAL:HG13	1:C:885:LEU:HB3	1.77	0.67
1:C:545:TYR:HB2	1:C:1019:TRP:CZ3	2.30	0.67
1:A:445:ILE:CD1	1:A:939:LYS:HZ1	2.00	0.66
1:C:690:VAL:HG12	1:C:694:VAL:CG2	2.24	0.66
1:C:908:VAL:HG12	1:C:912:LEU:HD11	1.75	0.66
1:C:970:LEU:O	1:C:974:VAL:HG23	1.96	0.66
1:B:515:TRP:CH2	1:B:519:MET:HB2	2.31	0.66
1:C:943:LEU:HD13	1:C:973:ILE:HG12	1.77	0.66
1:C:1016:ALA:O	1:C:1020:VAL:HG23	1.95	0.66
1:A:958:ILE:HG13	1:A:959:VAL:N	2.11	0.66
1:B:456:MET:HE1	1:B:928:VAL:HG12	1.76	0.66
1:B:449:LEU:O	1:B:453:PHE:HD1	1.79	0.66
1:C:981:ILE:O	1:C:985:VAL:HG23	1.95	0.66
1:A:780:MET:CE	1:C:225:VAL:H	2.08	0.66
1:B:108:GLN:CD	1:C:112:GLN:NE2	2.54	0.66
1:A:467:TYR:CE2	1:A:924:VAL:HG23	2.31	0.66
1:B:447:MET:HB3	1:B:886:CYS:SG	2.36	0.66
1:B:792:ASN:HB3	1:B:795:GLY:H	1.60	0.66
1:C:463:THR:HG21	1:C:868:SER:HB2	1.77	0.66
1:B:416:VAL:HA	1:B:434:SER:OG	1.95	0.65
1:B:847:VAL:HA	1:B:850:LEU:HD13	1.76	0.65
1:B:981:ILE:HG23	1:B:1006:ILE:HG13	1.76	0.65
1:C:915:THR:HG23	1:C:920:LEU:HB2	1.78	0.65
1:A:386:PHE:HB3	1:A:388:PHE:HE1	1.61	0.65
1:A:584:ALA:HB2	1:A:622:GLN:HG2	1.79	0.65
1:A:454:LEU:HG	1:A:475:VAL:HG21	1.77	0.65
1:C:310:ILE:HG21	1:C:323:VAL:HG11	1.77	0.65
1:B:108:GLN:OE1	1:C:112:GLN:NE2	2.28	0.65
1:C:757:TYR:CE1	1:C:769:ARG:HB3	2.31	0.65
1:B:108:GLN:HB2	1:C:112:GLN:NE2	2.09	0.65
1:B:544:ILE:O	1:B:548:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:THR:HG22	1:B:970:LEU:HD23	1.79	0.65
1:B:38:ILE:HG22	1:B:462:SER:HB3	1.78	0.65
1:B:200:PRO:HG2	1:B:748:THR:HG22	1.79	0.65
1:B:344:LEU:HD22	1:B:402:ILE:HG13	1.78	0.65
1:C:63:GLN:O	1:C:67:GLN:HG2	1.97	0.65
1:C:527:TYR:CE1	1:C:966:CYS:HB3	2.31	0.65
1:A:62:VAL:HG22	1:A:88:MET:HG3	1.78	0.65
1:B:925:PHE:HB3	1:B:1001:ILE:HG13	1.78	0.65
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.79	0.65
1:A:913:LEU:O	1:A:917:MET:HG3	1.97	0.64
1:B:987:LEU:HD22	1:B:998:GLN:HB3	1.79	0.64
1:A:972:PRO:HA	1:A:975:MET:HB2	1.80	0.64
1:B:535:LEU:HD12	1:B:959:VAL:HG13	1.79	0.64
1:B:280:GLN:HE21	1:B:588:GLN:HE22	1.45	0.64
1:A:837:GLY:HA2	1:A:840:MET:HG3	1.79	0.64
1:C:154:LEU:HD22	1:C:321:MET:HE3	1.80	0.64
1:B:453:PHE:HD2	1:B:474:ILE:HD11	1.63	0.64
1:B:971:ARG:O	1:B:975:MET:HG3	1.98	0.64
1:B:495:THR:HG23	1:B:496:MET:HG2	1.79	0.63
1:B:563:PHE:HB3	1:B:677:ALA:HB1	1.79	0.63
1:C:38:ILE:HG23	1:C:462:SER:HB2	1.80	0.63
1:C:900:VAL:HA	1:C:903:VAL:HG22	1.80	0.63
1:A:4:PHE:HE1	1:A:8:ARG:HD2	1.61	0.63
1:B:556:PHE:HD1	1:B:912:LEU:HD21	1.64	0.63
1:A:144:SER:HA	1:A:321:MET:HA	1.79	0.63
1:B:742:LEU:HA	1:B:745:ILE:HD12	1.79	0.63
1:B:225:VAL:HG12	1:C:780:MET:HG3	1.79	0.63
1:B:239:ARG:HB2	1:B:762:ILE:HG12	1.79	0.63
1:C:609:VAL:HG12	1:C:611:THR:HG22	1.80	0.63
1:B:416:VAL:HG21	1:B:493:CYS:HB3	1.80	0.63
1:C:607:SER:HB2	1:C:632:LYS:HG2	1.80	0.63
1:A:467:TYR:HE2	1:A:924:VAL:HG23	1.64	0.63
1:A:527:TYR:O	1:A:531:VAL:HG23	1.99	0.63
1:B:158:ILE:HG21	1:B:289:ILE:CD1	2.21	0.63
1:C:428:ARG:HH12	1:C:432:ARG:CD	2.11	0.62
1:A:407:ASP:O	1:A:411:VAL:HG22	1.99	0.62
1:A:898:PHE:O	1:A:902:LEU:HD23	1.99	0.62
1:A:203:VAL:O	1:A:207:ILE:HG13	1.99	0.62
1:A:222:LEU:HD11	1:B:622:GLN:NE2	2.14	0.62
1:A:702:PHE:CE1	1:A:826:ILE:HG21	2.35	0.62
1:B:158:ILE:HD13	1:B:289:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:PHE:HA	1:B:928:VAL:HG22	1.82	0.62
1:A:48:SER:O	1:A:125:GLN:HG3	1.99	0.62
1:B:699:ARG:O	1:B:703:LEU:HD12	1.98	0.62
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.82	0.62
1:A:150:THR:HG22	1:A:153:ASP:CG	2.24	0.62
1:A:399:VAL:HG11	1:A:987:LEU:HD11	1.82	0.62
1:C:983:GLY:O	1:C:986:PRO:HD2	1.98	0.62
1:C:137:LEU:HD22	1:C:293:LEU:HD13	1.80	0.62
1:C:332:VAL:HG11	1:C:569:GLN:HG2	1.81	0.62
1:B:904:VAL:O	1:B:908:VAL:HG13	2.00	0.61
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.82	0.61
1:C:430:ALA:O	1:C:434:SER:HB2	2.00	0.61
1:B:800:PHE:CD1	1:B:804:ALA:HB2	2.33	0.61
1:B:910:GLY:H	1:B:1011:THR:HG21	1.66	0.61
1:C:38:ILE:CG2	1:C:462:SER:HB2	2.30	0.61
1:C:306:ILE:O	1:C:310:ILE:HG12	2.00	0.61
1:C:968:MET:HE2	1:C:968:MET:H	1.64	0.61
1:A:115:THR:HA	1:A:118:LEU:HD12	1.81	0.61
1:B:492:LEU:HA	1:B:495:THR:HG22	1.82	0.61
1:C:971:ARG:O	1:C:975:MET:HG3	1.99	0.61
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.83	0.61
1:A:594:MET:HG3	1:A:595:ARG:N	2.14	0.61
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.83	0.61
1:B:706:ALA:HB1	1:B:715:VAL:HG21	1.82	0.61
1:C:166:LEU:HD13	1:C:291:ILE:HD11	1.82	0.61
1:A:400:LEU:HD13	1:A:932:THR:HG21	1.82	0.61
1:A:726:TYR:CZ	1:A:806:GLY:HA3	2.36	0.61
1:A:983:GLY:O	1:A:986:PRO:HD2	2.00	0.61
1:C:507:GLU:HG2	1:C:508:HIS:H	1.65	0.61
1:A:450:SER:O	1:A:454:LEU:HB2	2.01	0.60
1:B:453:PHE:CD2	1:B:474:ILE:HD11	2.36	0.60
1:C:532:ALA:HA	1:C:535:LEU:HD12	1.81	0.60
1:C:958:ILE:H	1:C:958:ILE:HD12	1.65	0.60
1:B:856:TYR:H	1:B:856:TYR:HD2	1.49	0.60
1:B:1002:GLY:O	1:B:1006:ILE:HG22	2.01	0.60
1:B:745:ILE:O	1:B:749:VAL:HG23	2.00	0.60
1:B:964:GLU:HG3	1:B:968:MET:HE2	1.83	0.60
1:A:332:VAL:HG21	1:A:569:GLN:HG2	1.81	0.60
1:C:480:LEU:O	1:C:484:VAL:HG23	2.02	0.60
1:A:470:PHE:CD2	1:A:928:VAL:HG13	2.37	0.60
1:C:641:GLU:HA	1:C:646:GLU:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:MET:HE2	1:C:225:VAL:HG13	1.82	0.60
1:B:640:GLY:HA2	1:B:643:SER:HB3	1.84	0.60
1:C:507:GLU:HG2	1:C:508:HIS:N	2.17	0.60
1:A:593:SER:HB3	1:A:658:PHE:HZ	1.66	0.60
1:B:250:LEU:HA	1:B:261:ARG:HG2	1.84	0.60
1:C:351:VAL:O	1:C:355:MET:HG3	2.01	0.60
1:C:403:GLY:HA3	1:C:980:PHE:HA	1.83	0.60
1:A:445:ILE:HD12	1:A:446:ALA:N	2.15	0.60
1:A:317:MET:HE1	1:A:323:VAL:HG23	1.84	0.60
1:A:435:MET:HE2	1:A:435:MET:HA	1.82	0.60
1:B:38:ILE:HD12	1:B:671:VAL:CG2	2.31	0.60
1:C:416:VAL:HA	1:C:419:VAL:HG12	1.84	0.60
1:B:368:PRO:O	1:B:372:VAL:HG22	2.02	0.59
1:A:159:VAL:HG11	1:A:181:GLN:HB3	1.84	0.59
1:B:216:SER:HB2	1:B:234:ILE:O	2.01	0.59
1:B:605:SER:HB2	1:B:647:LEU:HD22	1.84	0.59
1:B:303:ALA:HB2	1:B:330:THR:HG21	1.84	0.59
1:B:922:ASN:HA	1:B:926:PHE:HD1	1.67	0.59
1:B:981:ILE:HD11	1:B:1009:MET:CG	2.31	0.59
1:B:981:ILE:O	1:B:985:VAL:HG13	2.03	0.59
1:C:578:THR:HB	1:C:579:PRO:HD2	1.83	0.59
1:B:951:LEU:HD21	1:B:968:MET:HE1	1.83	0.59
1:B:887:LEU:HD13	1:B:900:VAL:HG11	1.84	0.59
1:A:626:MET:HE3	1:A:628:PHE:CE1	2.38	0.59
1:B:317:MET:HE3	1:B:321:MET:HG2	1.83	0.59
1:B:247:GLU:HG3	1:B:268:VAL:HB	1.84	0.59
1:C:881:LEU:HD23	1:C:885:LEU:HD11	1.83	0.59
1:C:203:VAL:CG1	1:C:262:LEU:HD11	2.32	0.59
1:A:1:MET:HE1	1:A:487:ILE:HG12	1.85	0.58
1:B:416:VAL:HG22	1:B:431:ALA:HA	1.85	0.58
1:C:929:GLY:O	1:C:933:THR:HG23	2.03	0.58
1:B:456:MET:HB2	1:B:471:SER:HB2	1.85	0.58
1:C:847:VAL:HA	1:C:850:LEU:HD13	1.85	0.58
1:B:933:THR:CG2	1:B:1005:VAL:HA	2.33	0.58
1:A:375:VAL:HG13	1:A:480:LEU:HB3	1.86	0.58
1:A:544:ILE:HA	1:A:547:VAL:HG12	1.84	0.58
1:C:695:LEU:CD2	1:C:824:MET:HG3	2.33	0.58
1:A:371:ALA:O	1:A:375:VAL:HG23	2.03	0.58
1:B:501:GLU:HB2	1:B:504:ASP:HB2	1.83	0.58
1:B:951:LEU:HB2	1:B:961:ALA:HB1	1.86	0.58
1:B:317:MET:HE3	1:B:321:MET:CG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LEU:HD22	1:B:481:SER:OG	2.03	0.58
1:B:302:THR:O	1:B:306:ILE:HG13	2.04	0.58
1:B:344:LEU:HD13	1:B:402:ILE:CD1	2.34	0.58
1:C:690:VAL:HG12	1:C:694:VAL:HG23	1.85	0.58
1:B:449:LEU:HB3	1:B:453:PHE:HE1	1.68	0.58
1:C:609:VAL:HG22	1:C:629:ILE:HG23	1.86	0.58
1:C:893:SER:OG	1:C:896:ILE:HD12	2.03	0.58
1:C:898:PHE:O	1:C:902:LEU:HD23	2.04	0.58
1:B:792:ASN:HB2	1:B:796:GLU:O	2.03	0.57
1:C:379:THR:HG23	1:C:476:SER:OG	2.03	0.57
1:A:544:ILE:HG13	1:A:1019:TRP:HH2	1.69	0.57
1:C:977:SER:O	1:C:981:ILE:HG13	2.04	0.57
1:B:13:TRP:HH2	1:B:370:ILE:HG21	1.68	0.57
1:B:651:ALA:HB1	1:B:655:PHE:CE2	2.39	0.57
1:B:599:LEU:O	1:B:603:SER:HB2	2.04	0.57
1:B:481:SER:HA	1:B:484:VAL:HG22	1.86	0.57
1:B:545:TYR:HB2	1:B:1019:TRP:CZ3	2.39	0.57
1:B:956:LYS:HG3	1:B:957:GLY:H	1.70	0.57
1:B:1009:MET:HE2	1:B:1009:MET:HA	1.85	0.57
1:A:470:PHE:CZ	1:A:928:VAL:HG13	2.39	0.57
1:C:740:VAL:HB	1:C:745:ILE:HD11	1.87	0.57
1:C:745:ILE:O	1:C:749:VAL:HG12	2.03	0.57
1:A:154:LEU:HD23	1:A:321:MET:HE2	1.86	0.57
1:B:188:LEU:HD23	1:B:266:ALA:HB2	1.85	0.57
1:B:672:LEU:H	1:B:672:LEU:HD12	1.69	0.57
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.69	0.57
1:B:466:ILE:HG21	1:B:924:VAL:HG21	1.86	0.57
1:B:584:ALA:HB2	1:B:622:GLN:HG2	1.87	0.57
1:C:203:VAL:O	1:C:207:ILE:HG13	2.04	0.57
1:A:445:ILE:O	1:A:449:LEU:HD12	2.05	0.57
1:A:831:ALA:HB3	1:A:834:LEU:HD13	1.85	0.57
1:A:446:ALA:O	1:A:478:MET:HE1	2.05	0.56
1:C:416:VAL:O	1:C:420:MET:HG3	2.05	0.56
1:A:840:MET:O	1:A:844:GLU:HG3	2.05	0.56
1:B:171:GLY:HA3	1:B:302:THR:HG22	1.88	0.56
1:B:414:GLU:CD	1:B:972:PRO:HD3	2.30	0.56
1:B:462:SER:CB	1:B:674:LEU:HD21	2.35	0.56
1:B:908:VAL:O	1:B:912:LEU:HD12	2.05	0.56
1:B:981:ILE:HD11	1:B:1009:MET:CB	2.34	0.56
1:C:537:HIS:O	1:C:540:PRO:HD2	2.05	0.56
1:A:409:ALA:O	1:A:413:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HD11	1:C:330:THR:HG23	1.87	0.56
1:C:428:ARG:HH22	1:C:432:ARG:NH1	2.02	0.56
1:C:347:ALA:O	1:C:351:VAL:HG12	2.06	0.56
1:A:563:PHE:O	1:A:564:LEU:HD23	2.06	0.56
1:C:136:PHE:CD1	1:C:290:ALA:HB1	2.40	0.56
1:A:157:TYR:HE2	1:A:317:MET:HG2	1.70	0.56
1:B:314:GLU:HA	1:B:317:MET:SD	2.46	0.56
1:B:637:ARG:HB2	1:B:642:ASN:HB2	1.86	0.56
1:B:726:TYR:CE1	1:B:806:GLY:HA3	2.41	0.56
1:C:534:ILE:HG12	1:C:541:TYR:CE2	2.41	0.56
1:B:218:GLN:HG2	1:B:233:THR:HA	1.88	0.56
1:B:651:ALA:HB1	1:B:655:PHE:CZ	2.41	0.56
1:C:534:ILE:HG12	1:C:541:TYR:HE2	1.71	0.56
1:C:542:LEU:HD21	1:C:1022:LEU:HD11	1.88	0.56
1:B:129:VAL:HB	1:C:112:GLN:OE1	2.05	0.56
1:C:69:MET:CE	1:C:107:VAL:HG13	2.36	0.56
1:A:142:VAL:HG22	1:A:158:ILE:HD12	1.89	0.55
1:A:780:MET:HE3	1:C:228:GLN:HB2	1.86	0.55
1:C:586:ARG:O	1:C:589:VAL:HG22	2.06	0.55
1:A:38:ILE:HD11	1:A:671:VAL:HG11	1.87	0.55
1:A:157:TYR:CE2	1:A:317:MET:HG2	2.41	0.55
1:B:505:HIS:CE1	1:B:971:ARG:HH12	2.25	0.55
1:C:445:ILE:HG23	1:C:939:LYS:HG3	1.88	0.55
1:C:884:PHE:HB2	1:C:901:MET:CE	2.30	0.55
1:B:893:SER:OG	1:B:896:ILE:HG13	2.07	0.55
1:B:927:GLN:O	1:B:931:LEU:HD23	2.06	0.55
1:A:279:ALA:HB2	1:A:612:VAL:HG22	1.89	0.55
1:C:493:CYS:O	1:C:497:LEU:HB2	2.06	0.55
1:C:890:LEU:HD12	1:C:891:TYR:CE2	2.42	0.55
1:A:78:ILE:HD11	1:A:820:GLY:N	2.20	0.55
1:A:904:VAL:HG13	1:A:934:ILE:HD13	1.87	0.55
1:B:228:GLN:OE1	1:C:780:MET:HB3	2.06	0.55
1:C:545:TYR:CZ	1:C:549:VAL:HG21	2.42	0.55
1:A:555:MET:HG3	1:A:912:LEU:HB3	1.89	0.55
1:A:404:LEU:HD13	1:A:449:LEU:HD22	1.88	0.55
1:B:404:LEU:HD13	1:B:478:MET:HB2	1.89	0.55
1:B:631:LEU:HD12	1:B:631:LEU:N	2.22	0.55
1:B:420:MET:CE	1:B:427:PRO:HA	2.38	0.54
1:C:45:VAL:HG22	1:C:129:VAL:HG22	1.89	0.54
1:B:958:ILE:HD12	1:B:958:ILE:H	1.71	0.54
1:C:720:MET:HB2	1:C:813:PRO:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:H	1:A:630:MET:HE1	1.72	0.54
1:B:969:ARG:HG2	1:B:969:ARG:HH11	1.73	0.54
1:C:597:TYR:HE2	1:C:651:ALA:HA	1.72	0.54
1:A:411:VAL:O	1:A:415:ASN:HB3	2.07	0.54
1:A:520:PHE:HZ	1:A:971:ARG:HA	1.73	0.54
1:B:10:ILE:HD12	1:C:893:SER:HA	1.89	0.54
1:B:544:ILE:HG23	1:B:1019:TRP:HH2	1.71	0.54
1:C:80:SER:HB3	1:C:90:ILE:HG12	1.89	0.54
1:C:332:VAL:HG22	1:C:634:TRP:CZ2	2.41	0.54
1:B:530:GLY:O	1:B:534:ILE:HG23	2.06	0.54
1:A:184:MET:HG2	1:A:246:PHE:CD2	2.43	0.54
1:B:83:ASN:ND2	1:B:620:ARG:HG3	2.23	0.54
1:A:78:ILE:HG13	1:A:819:ASN:HA	1.90	0.54
1:B:240:LEU:O	1:B:761:PHE:HB2	2.06	0.54
1:B:441:ALA:HB2	1:B:946:GLU:HG2	1.90	0.54
1:A:386:PHE:HB3	1:A:388:PHE:CE1	2.43	0.54
1:C:749:VAL:HG23	1:C:753:TRP:CE3	2.43	0.54
1:A:188:LEU:HD11	1:A:203:VAL:HG11	1.89	0.54
1:A:310:ILE:O	1:A:314:GLU:HG3	2.07	0.54
1:A:780:MET:HB3	1:C:228:GLN:OE1	2.07	0.54
1:B:379:THR:CG2	1:B:477:ALA:HA	2.38	0.54
1:C:362:PHE:CE1	1:C:366:LEU:HD22	2.42	0.54
1:A:380:PHE:CE1	1:A:395:MET:HE1	2.42	0.54
1:A:463:THR:HG22	1:A:563:PHE:CD1	2.42	0.54
1:B:982:LEU:O	1:B:985:VAL:HG22	2.07	0.54
1:C:76:ARG:HG3	1:C:95:GLU:OE2	2.08	0.54
1:C:926:PHE:CZ	1:C:930:LEU:HD21	2.43	0.54
1:A:23:GLY:HA3	1:A:377:LEU:O	2.08	0.53
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.88	0.53
1:A:826:ILE:O	1:A:827:LEU:HD23	2.08	0.53
1:B:351:VAL:HG11	1:B:406:VAL:HG13	1.90	0.53
1:C:455:PRO:HG3	1:C:882:VAL:HG21	1.89	0.53
1:B:375:VAL:O	1:B:379:THR:HG23	2.08	0.53
1:B:463:THR:HG22	1:B:563:PHE:CZ	2.44	0.53
1:C:908:VAL:O	1:C:912:LEU:HD12	2.09	0.53
1:B:463:THR:HA	1:B:563:PHE:CZ	2.44	0.53
1:B:930:LEU:O	1:B:934:ILE:HG13	2.08	0.53
1:C:780:MET:HE2	1:C:780:MET:HA	1.90	0.53
1:B:900:VAL:HG21	1:B:942:ILE:HG12	1.91	0.53
1:A:400:LEU:HD21	1:A:1005:VAL:HG21	1.89	0.53
1:A:532:ALA:HA	1:A:535:LEU:HD12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:SD	1:B:487:ILE:HD11	2.48	0.53
1:B:326:PRO:O	1:B:630:MET:HE2	2.08	0.53
1:B:379:THR:HG21	1:B:477:ALA:HA	1.91	0.53
1:B:970:LEU:HD11	1:B:1017:ILE:HD12	1.89	0.53
1:A:393:LEU:HD12	1:A:470:PHE:HB2	1.91	0.53
1:A:1014:VAL:O	1:A:1015:LEU:HD22	2.09	0.53
1:B:890:LEU:HD23	1:B:891:TYR:CE1	2.44	0.53
1:C:745:ILE:HD12	1:C:803:PHE:CE1	2.43	0.53
1:A:685:GLN:O	1:A:854:VAL:HA	2.09	0.53
1:A:981:ILE:HD11	1:A:1009:MET:HB3	1.91	0.53
1:B:520:PHE:CZ	1:B:971:ARG:HA	2.43	0.53
1:A:445:ILE:HG22	1:A:942:ILE:HD12	1.91	0.53
1:B:340:VAL:HG11	1:B:395:MET:HE3	1.90	0.53
1:B:420:MET:HE1	1:B:427:PRO:HA	1.91	0.53
1:C:881:LEU:CD2	1:C:885:LEU:HD11	2.39	0.53
1:A:11:PHE:CE2	1:B:889:ALA:HB1	2.44	0.53
1:B:610:PHE:HB3	1:B:628:PHE:HB2	1.91	0.53
1:C:344:LEU:O	1:C:348:ILE:HG13	2.09	0.53
1:B:280:GLN:NE2	1:B:588:GLN:OE1	2.42	0.52
1:B:441:ALA:O	1:B:445:ILE:HG23	2.09	0.52
1:B:452:VAL:HG13	1:B:453:PHE:CD1	2.45	0.52
1:B:572:LEU:HD12	1:B:666:PHE:O	2.09	0.52
1:B:169:THR:HG21	1:B:309:THR:OG1	2.08	0.52
1:B:738:LEU:HD22	1:B:802:ALA:HB1	1.92	0.52
1:C:956:LYS:HB3	1:C:960:GLU:HG2	1.90	0.52
1:A:417:GLU:HA	1:A:420:MET:HG3	1.90	0.52
1:C:428:ARG:NH1	1:C:432:ARG:HD2	2.24	0.52
1:C:927:GLN:O	1:C:931:LEU:HD12	2.09	0.52
1:A:259:GLN:HE21	1:A:261:ARG:HH21	1.57	0.52
1:A:535:LEU:HD23	1:A:1025:VAL:HG21	1.90	0.52
1:B:397:GLY:HA3	1:B:473:THR:CG2	2.39	0.52
1:B:676:ASN:O	1:B:861:LEU:HD12	2.09	0.52
1:C:969:ARG:HD3	1:C:972:PRO:HG2	1.91	0.52
1:A:184:MET:HB3	1:A:770:VAL:HG13	1.92	0.52
1:B:407:ASP:HB2	1:B:976:THR:CG2	2.40	0.52
1:A:466:ILE:CG2	1:A:924:VAL:HG21	2.40	0.52
1:B:14:VAL:CG1	1:C:885:LEU:HB3	2.39	0.52
1:C:369:THR:O	1:C:373:PRO:HD2	2.09	0.52
1:A:466:ILE:HG22	1:A:924:VAL:HG21	1.91	0.52
1:B:468:ARG:HA	1:B:471:SER:HB3	1.90	0.52
1:B:471:SER:O	1:B:475:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:VAL:HB	1:B:626:MET:HB3	1.92	0.52
1:B:739:GLY:O	1:B:792:ASN:HA	2.09	0.52
1:B:922:ASN:C	1:B:922:ASN:HD22	2.18	0.52
1:C:302:THR:O	1:C:306:ILE:HG13	2.10	0.52
1:C:528:GLU:OE2	1:C:967:ARG:HG3	2.09	0.52
1:C:574:ALA:HB3	1:C:627:ALA:HB3	1.91	0.52
1:B:446:ALA:HA	1:B:478:MET:CE	2.40	0.51
1:B:982:LEU:HA	1:B:985:VAL:HG13	1.92	0.51
1:C:556:PHE:HD1	1:C:912:LEU:HD21	1.75	0.51
1:B:520:PHE:HZ	1:B:971:ARG:HA	1.73	0.51
1:B:459:PHE:O	1:B:464:GLY:HA3	2.09	0.51
1:C:251:LEU:HD11	1:C:262:LEU:HD13	1.92	0.51
1:C:742:LEU:HD12	1:C:742:LEU:H	1.74	0.51
1:B:83:ASN:OD1	1:B:814:LYS:HG3	2.10	0.51
1:C:100:PRO:HB2	1:C:131:LYS:HD3	1.93	0.51
1:A:228:GLN:OE1	1:B:780:MET:HG3	2.11	0.51
1:A:451:ALA:O	1:A:879:SER:HB2	2.10	0.51
1:A:544:ILE:HG13	1:A:1019:TRP:CH2	2.45	0.51
1:A:984:VAL:HG12	1:A:1006:ILE:CD1	2.41	0.51
1:B:13:TRP:CH2	1:B:370:ILE:HG21	2.46	0.51
1:A:198:LEU:HD23	1:A:251:LEU:HD23	1.93	0.51
1:B:78:ILE:CG2	1:B:92:VAL:HG13	2.41	0.51
1:B:273:GLN:HG3	1:B:771:TYR:CE1	2.46	0.51
1:B:575:GLN:HA	1:B:626:MET:HE1	1.92	0.51
1:C:4:PHE:CE1	1:C:8:ARG:HG3	2.45	0.51
1:C:53:SER:O	1:C:57:VAL:HG23	2.11	0.51
1:B:844:GLU:O	1:B:847:VAL:HG22	2.11	0.51
1:C:616:ASN:HA	1:C:626:MET:HG2	1.92	0.51
1:A:535:LEU:O	1:A:538:ARG:HG3	2.11	0.51
1:B:38:ILE:HA	1:B:465:VAL:HG11	1.92	0.51
1:B:184:MET:HB2	1:B:770:VAL:HG22	1.93	0.51
1:C:317:MET:HG2	1:C:321:MET:SD	2.51	0.51
1:C:363:ARG:HH21	1:C:496:MET:HA	1.76	0.51
1:C:549:VAL:HG22	1:C:905:PRO:HB2	1.93	0.51
1:C:757:TYR:HB2	1:C:771:TYR:CE1	2.45	0.51
1:C:899:SER:O	1:C:903:VAL:HG13	2.10	0.51
1:A:35:TYR:CE1	1:A:564:LEU:HD13	2.45	0.51
1:B:446:ALA:O	1:B:478:MET:HE1	2.11	0.51
1:B:751:ILE:CG2	1:B:772:LEU:HD23	2.41	0.51
1:C:602:GLU:HB3	1:C:647:LEU:HD11	1.92	0.51
1:B:338:HIS:HA	1:B:341:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PHE:O	1:B:359:LEU:HD13	2.10	0.51
1:B:397:GLY:HA3	1:B:473:THR:HG21	1.92	0.51
1:B:470:PHE:CD2	1:B:928:VAL:HG11	2.46	0.51
1:C:652:GLN:NE2	1:C:664:PHE:HA	2.25	0.51
1:A:224:ALA:HB1	1:B:780:MET:HE1	1.92	0.50
1:A:425:LEU:HB2	1:A:430:ALA:HB2	1.92	0.50
1:B:337:ILE:HG22	1:B:395:MET:HE2	1.91	0.50
1:A:72:ILE:HG23	1:A:106:GLN:HB3	1.93	0.50
1:A:527:TYR:CD2	1:A:970:LEU:HG	2.47	0.50
1:A:775:ARG:HD3	1:A:777:ASP:HB2	1.93	0.50
1:B:749:VAL:HG13	1:B:753:TRP:CE3	2.46	0.50
1:A:219:LEU:HD11	1:B:726:TYR:CD2	2.47	0.50
1:A:250:LEU:HD11	1:A:259:GLN:HB2	1.92	0.50
1:A:734:LYS:HE3	1:A:738:LEU:HD11	1.92	0.50
1:C:544:ILE:HA	1:C:547:VAL:HB	1.94	0.50
1:B:143:VAL:HG23	1:B:286:ALA:HB2	1.94	0.50
1:B:214:ILE:HD12	1:B:215:SER:N	2.27	0.50
1:B:584:ALA:N	1:B:622:GLN:HE21	2.06	0.50
1:B:734:LYS:O	1:B:738:LEU:HD12	2.11	0.50
1:B:78:ILE:HG22	1:B:92:VAL:HA	1.93	0.50
1:C:414:GLU:HG2	1:C:972:PRO:HG3	1.94	0.50
1:C:859:THR:HA	1:C:863:TYR:HB2	1.92	0.50
1:A:525:HIS:HA	1:A:528:GLU:HB2	1.94	0.50
1:B:407:ASP:HB2	1:B:976:THR:HG21	1.93	0.50
1:B:424:GLY:HA3	1:B:502:LYS:HB2	1.93	0.50
1:B:505:HIS:HE1	1:B:971:ARG:HH12	1.59	0.50
1:B:841:ALA:O	1:B:845:GLU:HG2	2.12	0.50
1:A:735:ALA:HB2	1:A:803:PHE:HB2	1.94	0.50
1:A:1011:THR:O	1:A:1015:LEU:HB2	2.11	0.50
1:B:358:PHE:C	1:B:359:LEU:HD22	2.37	0.50
1:B:553:ILE:O	1:B:557:THR:HG22	2.12	0.50
1:C:13:TRP:CZ2	1:C:492:LEU:HD11	2.47	0.50
1:C:597:TYR:CE2	1:C:651:ALA:HA	2.47	0.50
1:A:127:ILE:HD12	1:A:127:ILE:H	1.76	0.50
1:A:390:ILE:HG23	1:A:395:MET:HE3	1.94	0.50
1:A:510:GLY:HA2	1:A:518:ARG:NH2	2.26	0.50
1:C:896:ILE:HB	1:C:897:PRO:HD3	1.94	0.50
1:B:289:ILE:HB	1:B:291:ILE:HD11	1.94	0.49
1:B:396:PHE:O	1:B:399:VAL:HG22	2.12	0.49
1:B:541:TYR:HA	1:B:544:ILE:HG22	1.94	0.49
1:C:183:SER:HB2	1:C:273:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ILE:HG12	1:C:501:GLU:H	1.77	0.49
1:C:715:VAL:HA	1:C:827:LEU:O	2.12	0.49
1:A:972:PRO:O	1:A:975:MET:HB2	2.12	0.49
1:B:43:ILE:HD12	1:B:94:PHE:CE1	2.47	0.49
1:B:530:GLY:HA3	1:B:1018:PHE:HE2	1.77	0.49
1:C:54:ALA:HB2	1:C:84:SER:N	2.27	0.49
1:C:69:MET:HE1	1:C:107:VAL:HG13	1.94	0.49
1:B:190:PRO:HB2	1:B:787:LYS:O	2.12	0.49
1:B:904:VAL:CG1	1:B:905:PRO:HD3	2.39	0.49
1:C:143:VAL:HG12	1:C:286:ALA:HB2	1.94	0.49
1:C:781:ASN:O	1:C:784:ASP:HB2	2.11	0.49
1:A:62:VAL:HG22	1:A:88:MET:CG	2.42	0.49
1:A:776:PRO:O	1:A:780:MET:HG2	2.12	0.49
1:B:906:LEU:HB3	1:B:1015:LEU:HD23	1.94	0.49
1:A:213:GLN:HG3	1:A:239:ARG:HG2	1.95	0.49
1:B:47:VAL:HG12	1:B:88:MET:HE2	1.93	0.49
1:B:391:ASN:O	1:B:395:MET:HG2	2.12	0.49
1:C:699:ARG:HD3	1:C:824:MET:SD	2.52	0.49
1:A:1017:ILE:HG13	1:A:1018:PHE:N	2.28	0.49
1:B:150:THR:HG22	1:B:153:ASP:OD2	2.13	0.49
1:B:465:VAL:O	1:B:469:GLN:HG2	2.11	0.49
1:B:743:ALA:O	1:B:747:SER:HB2	2.11	0.49
1:C:669:PRO:HD3	1:C:677:ALA:C	2.37	0.49
1:A:234:ILE:HG21	1:B:728:LEU:HD12	1.94	0.49
1:A:448:VAL:CG1	1:A:883:VAL:HG13	2.42	0.49
1:C:222:LEU:HA	1:C:223:PRO:C	2.37	0.49
1:C:254:ASN:HB2	1:C:258:SER:OG	2.12	0.49
1:C:951:LEU:HB2	1:C:961:ALA:CB	2.42	0.49
1:C:968:MET:HE2	1:C:968:MET:N	2.26	0.49
1:C:980:PHE:CZ	1:C:984:VAL:HG21	2.48	0.49
1:A:16:ALA:HB2	1:A:488:LEU:HD22	1.94	0.49
1:B:210:GLN:HG2	1:C:742:LEU:HD22	1.95	0.49
1:A:237:LYS:HG3	1:B:746:ASN:OD1	2.11	0.49
1:A:357:LEU:HD23	1:A:358:PHE:CE2	2.47	0.49
1:B:313:LEU:O	1:B:317:MET:HG3	2.13	0.49
1:B:531:VAL:O	1:B:534:ILE:HG13	2.13	0.49
1:B:764:ARG:O	1:B:764:ARG:HG2	2.12	0.49
1:C:399:VAL:HG11	1:C:987:LEU:HG	1.95	0.49
1:C:478:MET:HA	1:C:478:MET:HE2	1.95	0.49
1:C:940:ASN:HA	1:C:943:LEU:HD12	1.94	0.49
1:A:453:PHE:O	1:A:456:MET:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:ALA:CB	1:B:622:GLN:HE21	2.26	0.49
1:A:216:SER:OG	1:A:236:GLY:HA3	2.13	0.48
1:A:463:THR:HA	1:A:563:PHE:HE1	1.78	0.48
1:B:840:MET:O	1:B:844:GLU:HG3	2.13	0.48
1:A:184:MET:HE3	1:A:184:MET:HA	1.95	0.48
1:A:434:SER:O	1:A:438:ILE:HG12	2.13	0.48
1:A:513:PHE:O	1:A:517:ASN:HB2	2.12	0.48
1:A:884:PHE:HD1	1:A:885:LEU:HD23	1.78	0.48
1:B:229:GLN:C	1:C:583:SER:HB3	2.38	0.48
1:B:449:LEU:O	1:B:453:PHE:CD1	2.65	0.48
1:B:723:GLU:HB2	1:B:724:PRO:HD2	1.95	0.48
1:B:963:ILE:O	1:B:966:CYS:HB2	2.12	0.48
1:A:38:ILE:HG13	1:A:674:LEU:HD21	1.95	0.48
1:A:510:GLY:HA2	1:A:518:ARG:HH21	1.78	0.48
1:A:545:TYR:CE2	1:A:902:LEU:HD12	2.49	0.48
1:B:165:PRO:O	1:B:169:THR:HG23	2.14	0.48
1:B:763:ASP:OD2	1:B:764:ARG:HB3	2.12	0.48
1:C:378:GLY:O	1:C:382:VAL:HG23	2.13	0.48
1:C:563:PHE:HB2	1:C:865:GLU:HG3	1.96	0.48
1:C:1014:VAL:HG12	1:C:1015:LEU:HD23	1.96	0.48
1:B:317:MET:CE	1:B:321:MET:HG2	2.44	0.48
1:C:514:GLY:O	1:C:518:ARG:HG2	2.14	0.48
1:A:394:THR:O	1:A:398:MET:HG2	2.14	0.48
1:A:417:GLU:HG2	1:A:971:ARG:NH2	2.28	0.48
1:C:62:VAL:HA	1:C:90:ILE:HD11	1.94	0.48
1:C:650:ARG:HG3	1:C:650:ARG:HH11	1.79	0.48
1:C:918:ARG:HB3	1:C:920:LEU:HG	1.95	0.48
1:A:438:ILE:O	1:A:442:LEU:HG	2.13	0.48
1:A:470:PHE:CZ	1:A:474:ILE:HG13	2.48	0.48
1:B:626:MET:HE3	1:B:626:MET:HA	1.96	0.48
1:B:843:VAL:O	1:B:847:VAL:HG13	2.13	0.48
1:C:414:GLU:O	1:C:418:ARG:HB2	2.13	0.48
1:C:705:LEU:HD12	1:C:846:ILE:HG23	1.94	0.48
1:B:658:PHE:HD1	1:B:659:LYS:N	2.05	0.48
1:C:527:TYR:CD1	1:C:970:LEU:HD13	2.48	0.48
1:B:108:GLN:CB	1:C:112:GLN:NE2	2.76	0.48
1:B:978:LEU:O	1:B:982:LEU:HD22	2.13	0.48
1:A:360:GLN:HG2	1:A:513:PHE:HD1	1.79	0.48
1:B:27:ILE:HD11	1:B:380:PHE:CD2	2.49	0.48
1:B:330:THR:N	1:B:331:PRO:HD2	2.28	0.48
1:A:449:LEU:HB2	1:A:478:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:HZ	1:A:932:THR:HA	1.78	0.48
1:B:138:MET:HA	1:B:327:TYR:HD1	1.79	0.48
1:B:184:MET:SD	1:B:270:LEU:HD23	2.53	0.48
1:B:555:MET:CE	1:B:913:LEU:HD22	2.41	0.48
1:A:62:VAL:HG21	1:A:82:SER:OG	2.14	0.47
1:A:150:THR:HG22	1:A:153:ASP:OD2	2.13	0.47
1:A:168:ARG:HB3	1:B:75:LEU:HD22	1.94	0.47
1:B:437:GLN:NE2	1:B:947:PHE:HE1	2.11	0.47
1:B:601:LYS:HD2	1:B:601:LYS:N	2.29	0.47
1:B:676:ASN:C	1:B:861:LEU:HD12	2.39	0.47
1:C:880:LEU:O	1:C:901:MET:HE1	2.15	0.47
1:A:402:ILE:O	1:A:406:VAL:HG22	2.15	0.47
1:B:102:ILE:O	1:B:106:GLN:HG3	2.14	0.47
1:B:738:LEU:CD2	1:B:802:ALA:HB1	2.44	0.47
1:C:187:TRP:HA	1:C:773:GLN:O	2.14	0.47
1:C:1009:MET:O	1:C:1013:THR:HG23	2.13	0.47
1:A:14:VAL:CG2	1:B:885:LEU:HB3	2.44	0.47
1:A:578:THR:HG21	1:A:587:THR:HA	1.96	0.47
1:A:692:HIS:CE1	1:A:812:SER:HB2	2.50	0.47
1:B:402:ILE:O	1:B:406:VAL:HG23	2.14	0.47
1:B:456:MET:HB3	1:B:456:MET:HE3	1.62	0.47
1:B:727:LYS:HE2	1:B:809:GLU:OE1	2.14	0.47
1:C:58:GLN:O	1:C:63:GLN:HG3	2.13	0.47
1:C:242:THR:OG1	1:C:245:GLN:HG3	2.14	0.47
1:C:683:PHE:CD2	1:C:818:TYR:HB2	2.49	0.47
1:C:951:LEU:HB2	1:C:961:ALA:HB1	1.96	0.47
1:A:604:SER:CB	1:A:642:ASN:HD21	2.28	0.47
1:A:985:VAL:O	1:A:989:ILE:HG22	2.14	0.47
1:B:757:TYR:CE1	1:B:769:ARG:HB3	2.50	0.47
1:B:943:LEU:C	1:B:969:ARG:HD2	2.40	0.47
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.96	0.47
1:A:158:ILE:O	1:A:162:ILE:HB	2.14	0.47
1:A:572:LEU:HB3	1:A:629:ILE:HB	1.96	0.47
1:B:20:MET:HE2	1:B:20:MET:HB3	1.65	0.47
1:B:879:SER:O	1:B:883:VAL:HG13	2.14	0.47
1:B:900:VAL:HG23	1:B:941:ALA:CB	2.45	0.47
1:C:96:GLN:NE2	1:C:462:SER:HB3	2.30	0.47
1:C:376:LEU:HD12	1:C:376:LEU:HA	1.76	0.47
1:C:398:MET:HG2	1:C:473:THR:HG21	1.96	0.47
1:C:479:ALA:O	1:C:483:ILE:HG12	2.15	0.47
1:C:847:VAL:HG21	1:C:856:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:876:TYR:OH	1:C:927:GLN:HG2	2.15	0.47
1:C:880:LEU:O	1:C:883:VAL:HG22	2.13	0.47
1:A:155:SER:O	1:A:158:ILE:HG22	2.14	0.47
1:B:10:ILE:O	1:B:14:VAL:HG23	2.15	0.47
1:B:437:GLN:CD	1:B:947:PHE:HE1	2.23	0.47
1:B:652:GLN:HA	1:B:655:PHE:CD2	2.50	0.47
1:C:358:PHE:CZ	1:C:516:PHE:HZ	2.33	0.47
1:C:404:LEU:HD21	1:C:936:LEU:HD21	1.96	0.47
1:C:534:ILE:CG2	1:C:541:TYR:HD2	2.26	0.47
1:C:878:LEU:O	1:C:882:VAL:HG23	2.15	0.47
1:C:987:LEU:HD13	1:C:1001:ILE:HG23	1.97	0.47
1:A:599:LEU:HD23	1:A:599:LEU:HA	1.77	0.47
1:B:340:VAL:HG23	1:B:399:VAL:CG1	2.45	0.47
1:C:141:GLY:HA2	1:C:288:GLY:HA2	1.97	0.47
1:B:414:GLU:OE2	1:B:972:PRO:HD3	2.15	0.47
1:B:544:ILE:HG23	1:B:1019:TRP:CH2	2.49	0.47
1:A:388:PHE:HD2	1:A:469:GLN:CD	2.23	0.47
1:A:406:VAL:O	1:A:410:ILE:HG13	2.14	0.47
1:A:456:MET:HG3	1:A:471:SER:HB2	1.97	0.47
1:B:189:ASP:CG	1:B:192:LYS:HG3	2.40	0.47
1:B:891:TYR:OH	1:B:942:ILE:HD13	2.15	0.47
1:B:901:MET:O	1:B:904:VAL:HG12	2.15	0.47
1:C:716:ARG:HD2	1:C:716:ARG:O	2.14	0.47
1:C:986:PRO:HA	1:C:989:ILE:HG13	1.97	0.47
1:A:135:ASN:HD22	1:A:673:GLU:HA	1.79	0.46
1:A:145:THR:HG22	1:A:320:GLY:O	2.14	0.46
1:B:259:GLN:HE21	1:B:261:ARG:NH2	2.13	0.46
1:B:631:LEU:HD21	1:B:644:VAL:HG23	1.97	0.46
1:C:592:ASP:O	1:C:596:GLU:HG3	2.15	0.46
1:B:214:ILE:CD1	1:C:746:ASN:HB3	2.45	0.46
1:B:361:ASN:HB3	1:B:364:ALA:HB2	1.96	0.46
1:B:516:PHE:HA	1:B:519:MET:HB3	1.98	0.46
1:B:563:PHE:CG	1:B:564:LEU:HD12	2.51	0.46
1:B:604:SER:HB2	1:B:642:ASN:ND2	2.31	0.46
1:C:39:ALA:HB2	1:C:673:GLU:HG3	1.97	0.46
1:B:360:GLN:HG3	1:B:509:LYS:NZ	2.29	0.46
1:B:455:PRO:HB3	1:B:875:LEU:HB3	1.97	0.46
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.77	0.46
1:C:193:LEU:HD22	1:C:198:LEU:O	2.15	0.46
1:C:540:PRO:HA	1:C:543:LEU:HD13	1.97	0.46
1:A:10:ILE:HD12	1:B:894:TRP:CZ2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:HD23	1:A:200:PRO:HB3	1.98	0.46
1:C:575:GLN:HG2	1:C:666:PHE:HE2	1.80	0.46
1:A:78:ILE:HD11	1:A:820:GLY:H	1.79	0.46
1:B:188:LEU:HD21	1:B:203:VAL:HG11	1.98	0.46
1:C:617:PHE:CZ	1:C:626:MET:HE1	2.51	0.46
1:B:187:TRP:HA	1:B:773:GLN:O	2.15	0.46
1:C:102:ILE:O	1:C:106:GLN:HG3	2.14	0.46
1:B:406:VAL:HG12	1:B:410:ILE:HD11	1.98	0.46
1:B:470:PHE:O	1:B:473:THR:HG22	2.16	0.46
1:B:982:LEU:O	1:B:986:PRO:HD3	2.15	0.46
1:A:4:PHE:CE1	1:A:8:ARG:HD2	2.47	0.46
1:A:1014:VAL:O	1:A:1014:VAL:HG22	2.16	0.46
1:B:527:TYR:CZ	1:B:970:LEU:HD13	2.51	0.46
1:B:592:ASP:O	1:B:595:ARG:HG2	2.16	0.46
1:B:836:SER:O	1:B:840:MET:HG3	2.16	0.46
1:B:951:LEU:HD11	1:B:968:MET:CE	2.46	0.46
1:C:64:VAL:HG11	1:C:117:LEU:HB2	1.98	0.46
1:C:685:GLN:HE21	1:C:818:TYR:HD1	1.64	0.46
1:A:355:MET:HE1	1:A:368:PRO:CD	2.42	0.46
1:A:749:VAL:HG22	1:A:753:TRP:CZ3	2.51	0.46
1:B:203:VAL:O	1:B:207:ILE:HG13	2.16	0.46
1:B:749:VAL:HG13	1:B:753:TRP:CZ3	2.51	0.46
1:B:757:TYR:HE1	1:B:769:ARG:HB3	1.81	0.46
1:B:966:CYS:SG	1:B:1021:PRO:HB3	2.56	0.46
1:C:694:VAL:HA	1:C:697:GLN:HG2	1.98	0.46
1:C:27:ILE:HD11	1:C:380:PHE:CD2	2.51	0.45
1:C:383:LEU:HD22	1:C:388:PHE:HB2	1.98	0.45
1:A:984:VAL:HG12	1:A:1006:ILE:HD13	1.99	0.45
1:B:214:ILE:HD11	1:C:746:ASN:HB3	1.98	0.45
1:B:467:TYR:CE1	1:B:924:VAL:HG12	2.51	0.45
1:B:726:TYR:CZ	1:B:806:GLY:HA3	2.51	0.45
1:B:939:LYS:HB2	1:B:939:LYS:HE3	1.74	0.45
1:B:1003:THR:HA	1:B:1006:ILE:CG2	2.46	0.45
1:C:564:LEU:HD22	1:C:925:PHE:CE2	2.51	0.45
1:A:455:PRO:HB3	1:A:878:LEU:HD11	1.98	0.45
1:B:12:ALA:HA	1:B:15:ILE:HG22	1.97	0.45
1:B:459:PHE:HB2	1:B:464:GLY:HA2	1.99	0.45
1:B:570:GLY:C	1:B:631:LEU:HD13	2.42	0.45
1:C:463:THR:HG22	1:C:924:VAL:HG11	1.99	0.45
1:A:410:ILE:CG2	1:A:975:MET:HE3	2.47	0.45
1:B:243:ALA:HB1	1:B:268:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ILE:O	1:B:340:VAL:HG12	2.17	0.45
1:B:396:PHE:HZ	1:B:998:GLN:HE21	1.64	0.45
1:B:428:ARG:HE	1:B:428:ARG:HB3	1.50	0.45
1:C:270:LEU:HD12	1:C:270:LEU:H	1.81	0.45
1:A:213:GLN:CG	1:A:239:ARG:HG2	2.47	0.45
1:B:457:ALA:HB2	1:B:471:SER:OG	2.17	0.45
1:B:515:TRP:CZ3	1:B:519:MET:HB2	2.51	0.45
1:C:501:GLU:H	1:C:501:GLU:CD	2.24	0.45
1:C:947:PHE:O	1:C:951:LEU:HG	2.16	0.45
1:A:146:ASP:HB3	1:A:148:SER:H	1.81	0.45
1:B:847:VAL:HG21	1:B:856:TYR:CE2	2.51	0.45
1:B:958:ILE:HG21	1:B:1029:THR:HG23	1.99	0.45
1:C:918:ARG:HE	1:C:1003:THR:HG21	1.82	0.45
1:A:382:VAL:HG11	1:A:476:SER:OG	2.16	0.45
1:A:626:MET:HE3	1:A:628:PHE:CZ	2.50	0.45
1:B:139:VAL:HA	1:B:289:ILE:O	2.16	0.45
1:B:143:VAL:HG21	1:B:281:PHE:HB3	1.98	0.45
1:B:428:ARG:NH2	1:B:432:ARG:HH11	2.15	0.45
1:C:527:TYR:HE1	1:C:966:CYS:HB3	1.81	0.45
1:C:726:TYR:OH	1:C:782:PRO:HB3	2.16	0.45
1:A:350:LEU:N	1:A:350:LEU:HD23	2.32	0.45
1:A:520:PHE:CZ	1:A:971:ARG:HA	2.51	0.45
1:A:780:MET:CE	1:C:228:GLN:HB2	2.47	0.45
1:B:8:ARG:HG2	1:C:892:GLU:CG	2.47	0.45
1:B:702:PHE:CZ	1:B:843:VAL:HG13	2.52	0.45
1:B:726:TYR:CZ	1:B:782:PRO:HB3	2.52	0.45
1:B:891:TYR:HB3	1:B:896:ILE:HB	1.99	0.45
1:B:943:LEU:HB3	1:B:969:ARG:HD2	1.99	0.45
1:C:543:LEU:N	1:C:543:LEU:HD12	2.31	0.45
1:C:699:ARG:NH1	1:C:717:PRO:HB3	2.32	0.45
1:A:417:GLU:HG2	1:A:971:ARG:HH22	1.82	0.45
1:A:443:VAL:O	1:A:446:ALA:HB3	2.17	0.45
1:A:715:VAL:HA	1:A:827:LEU:O	2.17	0.45
1:A:726:TYR:OH	1:A:806:GLY:HA3	2.17	0.45
1:B:108:GLN:OE1	1:C:112:GLN:CD	2.60	0.45
1:C:326:PRO:HB3	1:C:610:PHE:HB2	1.99	0.45
1:C:594:MET:O	1:C:598:LEU:HD12	2.17	0.45
1:C:879:SER:O	1:C:883:VAL:HG13	2.17	0.45
1:A:680:PHE:HB2	1:A:858:TRP:HZ3	1.81	0.45
1:A:948:ALA:HB1	1:A:1024:TYR:HE1	1.81	0.45
1:B:24:GLY:O	1:B:28:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:HD3	1:B:863:TYR:CD2	2.52	0.45
1:B:159:VAL:HA	1:B:163:GLN:HB2	1.98	0.45
1:B:969:ARG:C	1:B:972:PRO:HD2	2.42	0.45
1:B:977:SER:O	1:B:981:ILE:HD13	2.16	0.45
1:C:68:GLN:HG3	1:C:114:ALA:HB2	1.98	0.45
1:C:984:VAL:HG11	1:C:1005:VAL:CG1	2.46	0.45
1:A:568:ASP:OD1	1:A:568:ASP:C	2.60	0.44
1:A:668:PRO:HB2	1:A:672:LEU:HD23	1.98	0.44
1:B:360:GLN:OE1	1:B:360:GLN:HA	2.16	0.44
1:B:671:VAL:HG13	1:B:674:LEU:HB2	1.99	0.44
1:B:791:ARG:HG3	1:B:792:ASN:H	1.82	0.44
1:B:1015:LEU:O	1:B:1019:TRP:HD1	1.99	0.44
1:C:375:VAL:HB	1:C:405:LEU:HD13	1.99	0.44
1:C:945:VAL:HG23	1:C:1020:VAL:HG12	1.99	0.44
1:C:1015:LEU:O	1:C:1019:TRP:CD1	2.70	0.44
1:C:1025:VAL:O	1:C:1029:THR:HG23	2.16	0.44
1:A:14:VAL:HG23	1:B:885:LEU:HB3	1.99	0.44
1:A:35:TYR:CZ	1:A:564:LEU:HD13	2.52	0.44
1:A:555:MET:HB3	1:A:912:LEU:HD13	1.99	0.44
1:A:900:VAL:O	1:A:903:VAL:HG12	2.17	0.44
1:B:184:MET:CE	1:B:268:VAL:HG13	2.48	0.44
1:B:488:LEU:O	1:B:492:LEU:HG	2.17	0.44
1:B:578:THR:HG21	1:B:587:THR:HA	1.98	0.44
1:B:585:GLU:OE2	1:B:585:GLU:O	2.35	0.44
1:C:30:LEU:HD13	1:C:390:ILE:HG13	1.98	0.44
1:C:210:GLN:NE2	1:C:249:ILE:HG23	2.32	0.44
1:C:262:LEU:HA	1:C:262:LEU:HD12	1.77	0.44
1:B:95:GLU:OE1	1:B:95:GLU:HA	2.16	0.44
1:C:76:ARG:HE	1:C:95:GLU:CD	2.25	0.44
1:A:439:GLN:O	1:A:443:VAL:HG12	2.17	0.44
1:A:548:ILE:HD13	1:A:548:ILE:HA	1.74	0.44
1:A:924:VAL:HA	1:A:927:GLN:OE1	2.17	0.44
1:B:146:ASP:CG	1:B:320:GLY:HA3	2.42	0.44
1:B:535:LEU:O	1:B:538:ARG:HG3	2.16	0.44
1:B:599:LEU:O	1:B:599:LEU:HD13	2.18	0.44
1:C:188:LEU:HD21	1:C:203:VAL:HG21	1.99	0.44
1:C:310:ILE:O	1:C:314:GLU:HG3	2.17	0.44
1:C:669:PRO:HG3	1:C:861:LEU:HD21	1.99	0.44
1:C:880:LEU:HD21	1:C:904:VAL:HG21	1.98	0.44
1:A:47:VAL:HB	1:A:127:ILE:HG23	2.00	0.44
1:A:61:VAL:HA	1:A:118:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:C	1:A:165:PRO:HD2	2.43	0.44
1:A:231:ASN:ND2	1:B:622:GLN:HB2	2.32	0.44
1:A:764:ARG:HG2	1:B:689:GLY:HA3	1.99	0.44
1:A:891:TYR:HD2	1:A:896:ILE:HB	1.82	0.44
1:A:899:SER:HA	1:A:1023:PHE:HB3	2.00	0.44
1:C:757:TYR:HB2	1:C:771:TYR:CZ	2.52	0.44
1:A:139:VAL:O	1:A:326:PRO:HD2	2.17	0.44
1:A:189:ASP:O	1:A:193:LEU:HB2	2.18	0.44
1:A:216:SER:HB2	1:A:234:ILE:O	2.17	0.44
1:A:418:ARG:O	1:A:422:GLU:HB2	2.18	0.44
1:B:393:LEU:HD11	1:B:466:ILE:HD12	2.00	0.44
1:B:703:LEU:HD21	1:B:717:PRO:CD	2.46	0.44
1:C:699:ARG:HG3	1:C:700:ASN:N	2.32	0.44
1:C:868:SER:OG	1:C:924:VAL:HG12	2.17	0.44
1:A:972:PRO:C	1:A:975:MET:HB2	2.41	0.44
1:B:416:VAL:HG11	1:B:497:LEU:CD1	2.48	0.44
1:B:554:TRP:O	1:B:558:ARG:HB2	2.18	0.44
1:C:31:PRO:HG2	1:C:389:SER:HB3	1.99	0.44
1:C:518:ARG:O	1:C:522:SER:HB3	2.18	0.44
1:A:545:TYR:CD1	1:A:1023:PHE:HZ	2.36	0.44
1:B:446:ALA:HA	1:B:478:MET:HE1	1.99	0.44
1:C:20:MET:HE3	1:C:20:MET:HB3	1.82	0.44
1:C:185:ARG:HD3	1:C:771:TYR:HB2	1.99	0.44
1:C:527:TYR:HD2	1:C:1018:PHE:CE1	2.36	0.44
1:C:726:TYR:CZ	1:C:782:PRO:HB3	2.52	0.44
1:A:262:LEU:HD12	1:A:265:VAL:HG23	2.00	0.44
1:A:348:ILE:H	1:A:348:ILE:HG13	1.64	0.44
1:B:47:VAL:HG12	1:B:88:MET:CE	2.46	0.44
1:B:958:ILE:HG22	1:B:1025:VAL:HG12	2.00	0.44
1:C:308:GLN:O	1:C:311:ALA:HB3	2.17	0.44
1:A:314:GLU:HA	1:A:317:MET:CE	2.47	0.43
1:A:851:PRO:O	1:A:854:VAL:HG12	2.16	0.43
1:A:918:ARG:HD2	1:A:1003:THR:OG1	2.18	0.43
1:B:108:GLN:CG	1:C:112:GLN:NE2	2.81	0.43
1:B:539:ALA:N	1:B:540:PRO:HD2	2.33	0.43
1:B:632:LYS:HD2	1:B:632:LYS:HA	1.86	0.43
1:C:365:THR:O	1:C:368:PRO:HD2	2.19	0.43
1:C:531:VAL:HG12	1:C:963:ILE:HG12	1.99	0.43
1:C:953:GLU:OE1	1:C:953:GLU:N	2.46	0.43
1:A:480:LEU:HD12	1:A:480:LEU:HA	1.80	0.43
1:A:763:ASP:OD1	1:A:763:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD21	1:A:297:ALA:O	2.18	0.43
1:A:696:LEU:CA	1:A:824:MET:HE1	2.35	0.43
2:B:1101:CLM:H3	2:B:1101:CLM:H11	1.45	0.43
1:C:149:MET:HE2	1:C:149:MET:HB3	1.90	0.43
1:C:580:PRO:HG3	1:C:721:SER:HB3	1.99	0.43
1:C:598:LEU:HD22	1:C:606:VAL:HG21	2.00	0.43
1:A:393:LEU:HG	1:A:466:ILE:HG23	2.00	0.43
1:B:157:TYR:CD2	1:B:321:MET:HE1	2.54	0.43
1:B:449:LEU:HA	1:B:452:VAL:HG12	2.00	0.43
1:B:598:LEU:HA	1:B:602:GLU:HB2	2.00	0.43
1:C:409:ALA:O	1:C:413:VAL:HG22	2.18	0.43
1:C:412:VAL:HG22	1:C:438:ILE:HD11	1.99	0.43
1:C:530:GLY:O	1:C:534:ILE:HG13	2.18	0.43
1:C:732:ASP:HA	1:C:735:ALA:HB3	2.01	0.43
1:C:967:ARG:NH2	1:C:968:MET:HE1	2.33	0.43
1:A:11:PHE:CD2	1:B:889:ALA:HB1	2.53	0.43
1:A:14:VAL:HG21	1:B:885:LEU:O	2.18	0.43
1:B:158:ILE:HD13	1:B:289:ILE:CD1	2.47	0.43
1:B:372:VAL:N	1:B:373:PRO:HD2	2.34	0.43
1:B:486:LEU:C	1:B:487:ILE:HD12	2.43	0.43
1:C:47:VAL:H	1:C:88:MET:HE3	1.84	0.43
1:C:184:MET:HE1	1:C:270:LEU:HG	2.00	0.43
1:C:317:MET:SD	1:C:321:MET:HG2	2.58	0.43
1:C:360:GLN:HG2	1:C:513:PHE:CD1	2.53	0.43
1:A:61:VAL:HG13	1:A:118:LEU:HD22	2.01	0.43
1:A:188:LEU:HD11	1:A:772:LEU:HD11	2.01	0.43
1:A:884:PHE:HE2	1:A:898:PHE:CE1	2.36	0.43
1:B:142:VAL:O	1:B:142:VAL:HG23	2.17	0.43
1:B:877:ALA:O	1:B:880:LEU:HB3	2.19	0.43
1:B:947:PHE:CE2	1:B:969:ARG:NH1	2.86	0.43
1:C:343:THR:HG21	1:C:987:LEU:HD23	2.00	0.43
1:C:816:GLU:HB2	1:C:823:ALA:O	2.18	0.43
1:A:978:LEU:O	1:A:982:LEU:HD23	2.19	0.43
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.53	0.43
1:C:54:ALA:N	1:C:84:SER:HA	2.33	0.43
1:C:543:LEU:HD12	1:C:543:LEU:H	1.84	0.43
1:C:575:GLN:HG2	1:C:666:PHE:CE2	2.54	0.43
1:C:633:PRO:O	1:C:637:ARG:HG2	2.18	0.43
1:C:867:LEU:HD12	1:C:867:LEU:HA	1.80	0.43
1:C:967:ARG:CZ	1:C:968:MET:HE1	2.48	0.43
1:B:108:GLN:CD	1:C:112:GLN:HE21	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:THR:HG22	1:B:153:ASP:CG	2.43	0.43
1:C:69:MET:HE3	1:C:107:VAL:HG13	2.01	0.43
1:C:214:ILE:HA	1:C:214:ILE:HD13	1.73	0.43
1:C:685:GLN:NE2	1:C:818:TYR:HD1	2.17	0.43
1:C:731:ASP:OD2	1:C:734:LYS:HG3	2.18	0.43
1:C:1015:LEU:O	1:C:1019:TRP:HD1	2.01	0.43
1:A:282:ASN:OD1	1:A:599:LEU:HD11	2.19	0.43
1:B:184:MET:HE2	1:B:268:VAL:HG13	2.01	0.43
1:C:34:GLN:HB2	1:C:333:VAL:HG22	2.01	0.43
1:C:362:PHE:HE1	1:C:366:LEU:HD22	1.83	0.43
1:C:417:GLU:HG3	1:C:418:ARG:N	2.33	0.43
1:A:456:MET:HB3	1:A:875:LEU:HD13	2.01	0.43
1:A:680:PHE:HB2	1:A:858:TRP:CZ3	2.54	0.43
1:B:425:LEU:HD22	1:B:429:GLU:CB	2.49	0.43
1:C:192:LYS:O	1:C:196:TYR:HD1	2.02	0.43
1:C:580:PRO:HB2	1:C:723:GLU:HB3	2.00	0.43
1:C:641:GLU:HG3	1:C:650:ARG:NH1	2.34	0.43
1:C:722:ASP:HA	1:C:813:PRO:HD3	2.00	0.43
1:A:592:ASP:O	1:A:596:GLU:HG3	2.18	0.42
1:A:739:GLY:O	1:A:792:ASN:HB2	2.18	0.42
1:A:908:VAL:HA	1:A:930:LEU:HD11	2.01	0.42
1:B:38:ILE:HD13	1:B:466:ILE:CD1	2.49	0.42
1:B:416:VAL:HG11	1:B:497:LEU:HD12	2.00	0.42
1:B:457:ALA:HA	1:B:468:ARG:HB2	2.00	0.42
1:A:188:LEU:CD1	1:A:772:LEU:HD11	2.48	0.42
1:A:200:PRO:HG2	1:A:748:THR:HG23	2.01	0.42
1:A:780:MET:HE2	1:C:225:VAL:N	2.25	0.42
1:A:994:GLY:O	1:A:998:GLN:HG3	2.19	0.42
1:A:1025:VAL:O	1:A:1029:THR:HG23	2.19	0.42
1:B:985:VAL:HG22	1:B:986:PRO:HD3	2.00	0.42
1:C:575:GLN:CG	1:C:666:PHE:HE2	2.32	0.42
1:C:720:MET:HB2	1:C:813:PRO:CG	2.50	0.42
1:C:739:GLY:C	1:C:792:ASN:HB2	2.45	0.42
1:A:1022:LEU:HD12	1:A:1022:LEU:O	2.19	0.42
1:B:185:ARG:HD2	1:B:185:ARG:HA	1.57	0.42
1:C:251:LEU:HD13	1:C:261:ARG:C	2.44	0.42
1:C:416:VAL:HG22	1:C:430:ALA:O	2.19	0.42
1:B:58:GLN:HA	1:B:62:VAL:HB	2.01	0.42
1:C:57:VAL:HB	1:C:82:SER:HB3	2.02	0.42
1:C:377:LEU:HD23	1:C:377:LEU:HA	1.84	0.42
1:C:599:LEU:HA	1:C:599:LEU:HD23	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1023:PHE:O	1:C:1027:VAL:HG23	2.20	0.42
1:A:951:LEU:HD23	1:A:964:GLU:HB3	2.01	0.42
1:B:671:VAL:O	1:B:674:LEU:HB2	2.19	0.42
1:B:680:PHE:HA	1:B:862:SER:OG	2.19	0.42
1:C:188:LEU:O	1:C:775:ARG:HG2	2.19	0.42
1:C:463:THR:HG21	1:C:868:SER:CB	2.47	0.42
1:C:669:PRO:HD3	1:C:678:THR:N	2.34	0.42
1:A:519:MET:SD	1:A:519:MET:C	3.03	0.42
1:B:446:ALA:HB2	1:B:482:VAL:HG21	2.00	0.42
1:B:726:TYR:OH	1:B:782:PRO:HB3	2.19	0.42
1:B:924:VAL:O	1:B:928:VAL:HG13	2.19	0.42
1:C:42:ALA:HB3	1:C:132:ALA:HB3	2.01	0.42
1:A:134:LYS:HD2	1:A:675:GLY:HA2	2.00	0.42
1:A:135:ASN:HD22	1:A:672:LEU:C	2.27	0.42
1:B:196:TYR:HB3	1:B:252:LYS:HE2	2.02	0.42
1:B:280:GLN:HE21	1:B:588:GLN:NE2	2.13	0.42
1:B:574:ALA:HA	1:B:665:ALA:HA	2.02	0.42
1:B:655:PHE:CE2	1:B:665:ALA:HB2	2.55	0.42
1:C:906:LEU:HA	1:C:906:LEU:HD23	1.81	0.42
1:A:360:GLN:HE22	1:A:517:ASN:CG	2.27	0.42
1:A:368:PRO:HB3	1:A:409:ALA:HB1	2.02	0.42
1:A:402:ILE:HA	1:A:405:LEU:HB2	2.01	0.42
1:B:250:LEU:HD12	1:B:251:LEU:N	2.35	0.42
1:B:555:MET:HE1	1:B:913:LEU:HA	2.01	0.42
1:C:488:LEU:HG	1:C:492:LEU:CD2	2.50	0.42
1:C:545:TYR:CE1	1:C:549:VAL:HG21	2.55	0.42
1:C:859:THR:O	1:C:862:SER:HB2	2.20	0.42
1:C:1017:ILE:H	1:C:1017:ILE:HG12	1.71	0.42
1:A:360:GLN:HG2	1:A:513:PHE:CD1	2.54	0.42
1:A:437:GLN:HG2	1:A:947:PHE:CE1	2.54	0.42
1:A:535:LEU:CD2	1:A:1025:VAL:HG11	2.49	0.42
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.81	0.42
1:B:38:ILE:HD13	1:B:466:ILE:HD11	2.01	0.42
1:B:40:PRO:HG3	1:B:76:ARG:HH12	1.85	0.42
1:B:1010:VAL:O	1:B:1014:VAL:HG13	2.19	0.42
1:C:252:LYS:HB3	1:C:260:VAL:HG21	2.02	0.42
1:C:343:THR:HG23	1:C:986:PRO:HB2	2.01	0.42
1:C:455:PRO:HG2	1:C:879:SER:HA	2.02	0.42
1:C:559:ILE:HD11	1:C:912:LEU:HB3	2.01	0.42
1:A:185:ARG:HB3	1:A:187:TRP:CZ2	2.54	0.42
1:A:559:ILE:HD13	1:A:912:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:887:LEU:HA	1:B:887:LEU:HD23	1.69	0.42
1:B:1024:TYR:C	1:B:1024:TYR:CD2	2.98	0.42
1:C:507:GLU:HA	1:C:517:ASN:HD22	1.84	0.42
1:A:352:PHE:CD1	1:A:353:LEU:HD23	2.55	0.41
1:A:388:PHE:HD2	1:A:469:GLN:OE1	2.03	0.41
1:A:534:ILE:HG22	1:A:541:TYR:CZ	2.55	0.41
1:A:891:TYR:N	1:A:891:TYR:CD1	2.88	0.41
1:B:355:MET:HE1	1:B:413:VAL:HG11	2.02	0.41
1:B:442:LEU:O	1:B:445:ILE:HG13	2.20	0.41
1:B:742:LEU:HA	1:B:742:LEU:HD23	1.77	0.41
1:C:146:ASP:OD2	1:C:148:SER:HB3	2.20	0.41
1:C:175:PHE:CD1	1:C:175:PHE:N	2.86	0.41
1:A:4:PHE:CD1	1:A:4:PHE:C	2.98	0.41
1:B:199:THR:HB	1:B:200:PRO:HD2	2.01	0.41
1:C:904:VAL:HG12	1:C:905:PRO:HD3	2.02	0.41
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.89	0.41
1:A:165:PRO:HG3	1:A:313:LEU:HD11	2.01	0.41
1:A:750:SER:HA	1:C:215:SER:O	2.21	0.41
1:B:34:GLN:HG2	1:B:35:TYR:CD1	2.55	0.41
1:B:456:MET:CE	1:B:928:VAL:HG12	2.49	0.41
1:A:251:LEU:HD21	1:A:265:VAL:HG21	2.02	0.41
1:A:425:LEU:CB	1:A:430:ALA:HB2	2.50	0.41
1:A:910:GLY:HA3	1:A:1007:GLY:O	2.20	0.41
1:A:933:THR:O	1:A:937:SER:HB3	2.20	0.41
1:B:298:ASN:O	1:B:302:THR:HG23	2.21	0.41
1:B:872:ALA:N	1:B:873:PRO:HD2	2.35	0.41
1:C:181:GLN:OE1	1:C:768:LYS:HG2	2.20	0.41
1:C:969:ARG:C	1:C:972:PRO:HD2	2.45	0.41
1:A:695:LEU:HG	1:A:824:MET:CE	2.51	0.41
1:A:773:GLN:HG2	1:A:774:GLY:H	1.86	0.41
1:A:1024:TYR:CD2	1:A:1024:TYR:C	2.97	0.41
1:B:393:LEU:HD13	1:B:466:ILE:HG23	2.01	0.41
1:B:605:SER:HA	1:B:642:ASN:HB3	2.02	0.41
1:B:900:VAL:HG23	1:B:941:ALA:HB3	2.03	0.41
1:C:203:VAL:HG13	1:C:262:LEU:CD1	2.44	0.41
1:C:393:LEU:HD11	1:C:466:ILE:HD13	2.01	0.41
1:C:520:PHE:CE2	1:C:971:ARG:HA	2.55	0.41
1:C:542:LEU:HD23	1:C:1022:LEU:HD21	2.02	0.41
1:A:695:LEU:HG	1:A:824:MET:HE3	2.03	0.41
1:B:11:PHE:O	1:B:15:ILE:HG22	2.21	0.41
1:B:64:VAL:HG11	1:B:118:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:PHE:CD2	1:B:136:PHE:N	2.87	0.41
1:B:405:LEU:HD21	1:B:477:ALA:HB1	2.02	0.41
1:B:584:ALA:HB2	1:B:622:GLN:HE21	1.84	0.41
1:C:831:ALA:HB3	1:C:834:LEU:CD1	2.51	0.41
1:A:15:ILE:HA	1:A:18:VAL:HG12	2.02	0.41
1:A:251:LEU:HD12	1:A:251:LEU:N	2.35	0.41
1:B:124:ARG:HG2	1:C:120:GLN:OE1	2.20	0.41
1:B:228:GLN:HG3	1:B:229:GLN:N	2.36	0.41
1:B:352:PHE:HA	1:B:365:THR:CG2	2.51	0.41
1:B:789:TYR:CE2	1:B:799:PRO:HG3	2.56	0.41
1:B:948:ALA:HB2	1:B:965:ALA:HB3	2.02	0.41
1:C:2:SER:O	1:C:6:ILE:HG13	2.21	0.41
1:A:713:GLN:HG2	1:A:830:PRO:O	2.20	0.41
1:A:866:ARG:HD2	1:A:866:ARG:HA	1.77	0.41
1:A:917:MET:HE3	1:A:917:MET:HB2	1.82	0.41
1:B:337:ILE:HG13	1:B:338:HIS:H	1.86	0.41
1:C:605:SER:OG	1:C:647:LEU:HD13	2.21	0.41
1:C:969:ARG:HD3	1:C:969:ARG:HA	1.79	0.41
1:A:158:ILE:HD11	1:A:289:ILE:HG22	2.02	0.41
1:A:466:ILE:HG23	1:A:466:ILE:HD12	1.85	0.41
1:A:468:ARG:HA	1:A:471:SER:HB3	2.03	0.41
1:A:575:GLN:O	1:A:663:VAL:HA	2.21	0.41
1:A:702:PHE:CD1	1:A:702:PHE:C	2.98	0.41
1:A:965:ALA:HA	1:A:968:MET:HB2	2.02	0.41
1:A:1015:LEU:O	1:A:1019:TRP:HD1	2.04	0.41
1:B:23:GLY:HA3	1:B:377:LEU:O	2.21	0.41
1:B:141:GLY:O	1:B:323:VAL:HA	2.20	0.41
1:B:240:LEU:HD23	1:B:240:LEU:N	2.35	0.41
1:B:472:ILE:HA	1:B:475:VAL:HG12	2.03	0.41
1:B:555:MET:HB3	1:B:555:MET:HE3	1.75	0.41
1:B:680:PHE:CE2	1:B:843:VAL:HG21	2.56	0.41
1:B:952:HIS:NE2	1:B:958:ILE:HG13	2.35	0.41
1:C:13:TRP:HH2	1:C:370:ILE:HG12	1.86	0.41
1:C:410:ILE:HD12	1:C:976:THR:HA	2.02	0.41
1:C:740:VAL:HG11	1:C:790:VAL:HG13	2.03	0.41
1:B:142:VAL:HG22	1:B:158:ILE:HD11	2.02	0.41
1:B:545:TYR:HA	1:B:548:ILE:HD12	2.02	0.41
1:B:909:ILE:HA	1:B:912:LEU:HD13	2.02	0.41
1:B:943:LEU:CB	1:B:969:ARG:HD2	2.50	0.41
1:B:1015:LEU:HD12	1:B:1015:LEU:HA	1.88	0.41
1:C:188:LEU:HD21	1:C:203:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LYS:HB3	1:C:260:VAL:CG2	2.51	0.41
1:A:246:PHE:O	1:A:249:ILE:HG13	2.20	0.40
1:A:457:ALA:HB2	1:A:471:SER:OG	2.22	0.40
1:C:418:ARG:NH1	1:C:968:MET:HG3	2.36	0.40
1:C:695:LEU:HD21	1:C:824:MET:HG3	2.01	0.40
1:C:789:TYR:CE2	1:C:799:PRO:HG3	2.56	0.40
1:C:922:ASN:HA	1:C:926:PHE:CD1	2.56	0.40
1:B:186:ILE:HD12	1:B:207:ILE:HD13	2.02	0.40
1:B:306:ILE:HD13	1:B:306:ILE:HG21	1.80	0.40
1:B:864:GLU:O	1:B:868:SER:HB3	2.20	0.40
1:C:716:ARG:CD	1:C:827:LEU:HB2	2.51	0.40
1:A:159:VAL:CG1	1:A:181:GLN:HB3	2.50	0.40
1:A:701:LYS:O	1:A:704:MET:HG3	2.21	0.40
1:B:2:SER:HB3	1:B:435:MET:HG3	2.02	0.40
1:B:108:GLN:CB	1:C:112:GLN:HE22	2.17	0.40
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.75	0.40
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.94	0.40
1:C:893:SER:HG	1:C:896:ILE:HD12	1.86	0.40
1:A:4:PHE:C	1:A:4:PHE:HD1	2.29	0.40
1:A:4:PHE:HD1	1:A:4:PHE:O	2.05	0.40
1:A:214:ILE:HG23	1:B:750:SER:OG	2.22	0.40
1:A:402:ILE:HG22	1:A:406:VAL:HG13	2.03	0.40
1:A:564:LEU:HD12	1:A:671:VAL:HG22	2.02	0.40
1:A:753:TRP:CE2	1:A:785:LEU:HD22	2.57	0.40
1:A:884:PHE:HD2	1:A:901:MET:HE1	1.86	0.40
1:B:594:MET:H	1:B:594:MET:HG3	1.45	0.40
1:B:910:GLY:N	1:B:1011:THR:HG21	2.35	0.40
1:C:113:LEU:O	1:C:116:PRO:HD2	2.21	0.40
1:C:352:PHE:HD2	1:C:353:LEU:HD23	1.86	0.40
1:A:427:PRO:HG3	1:A:499:PRO:HD3	2.03	0.40
1:B:397:GLY:O	1:B:474:ILE:HG22	2.22	0.40
1:B:699:ARG:HD2	1:B:717:PRO:HB3	2.03	0.40
1:C:189:ASP:OD1	1:C:192:LYS:HG3	2.21	0.40
1:C:216:SER:O	1:C:234:ILE:HB	2.22	0.40
1:C:544:ILE:HG23	1:C:1019:TRP:CH2	2.57	0.40
1:C:894:TRP:HB3	1:C:898:PHE:HE2	1.87	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	1020/1054 (97%)	939 (92%)	81 (8%)	0	100	100
1	B	1028/1054 (98%)	946 (92%)	82 (8%)	0	100	100
1	C	1028/1054 (98%)	957 (93%)	70 (7%)	1 (0%)	48	77
All	All	3076/3162 (97%)	2842 (92%)	233 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	659	LYS

### 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	836/862 (97%)	789 (94%)	47 (6%)	19	50
1	B	841/862 (98%)	811 (96%)	30 (4%)	31	65
1	C	841/862 (98%)	806 (96%)	35 (4%)	26	60
All	All	2518/2586 (97%)	2406 (96%)	112 (4%)	25	59

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	14	VAL

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Mol	Chain	Res	Type
1	A	47	VAL
1	A	75	LEU
1	A	91	THR
1	A	109	ASN
1	A	118	LEU
1	A	130	THR
1	A	142	VAL
1	A	205	SER
1	A	225	VAL
1	A	230	LEU
1	A	233	THR
1	A	309	THR
1	A	344	LEU
1	A	350	LEU
1	A	351	VAL
1	A	353	LEU
1	A	354	VAL
1	A	377	LEU
1	A	417	GLU
1	A	435	MET
1	A	450	SER
1	A	452	VAL
1	A	484	VAL
1	A	523	THR
1	A	542	LEU
1	A	546	VAL
1	A	572	LEU
1	A	605	SER
1	A	623	SER
1	A	671	VAL
1	A	736	SER
1	A	796	GLU
1	A	800	PHE
1	A	801	ASN
1	A	805	THR
1	A	814	LYS
1	A	821	VAL
1	A	893	SER
1	A	900	VAL
1	A	918	ARG
1	A	933	THR
1	A	937	SER

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Mol	Chain	Res	Type
1	A	939	LYS
1	A	951	LEU
1	A	1030	LEU
1	B	63	GLN
1	B	102	ILE
1	B	120	GLN
1	B	161	ASN
1	B	183	SER
1	B	214	ILE
1	B	340	VAL
1	B	407	ASP
1	B	426	SER
1	B	450	SER
1	B	534	ILE
1	B	542	LEU
1	B	558	ARG
1	B	561	THR
1	B	589	VAL
1	B	599	LEU
1	B	605	SER
1	B	673	GLU
1	B	674	LEU
1	B	740	VAL
1	B	810	TYR
1	B	856	TYR
1	B	866	ARG
1	B	880	LEU
1	B	886	CYS
1	B	895	SER
1	B	927	GLN
1	B	987	LEU
1	B	990	SER
1	B	1030	LEU
1	C	150	THR
1	C	180	SER
1	C	195	SER
1	C	204	SER
1	C	215	SER
1	C	225	VAL
1	C	226	LYS
1	C	238	THR
1	C	253	VAL

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Mol	Chain	Res	Type
1	C	273	GLN
1	C	280	GLN
1	C	295	THR
1	C	376	LEU
1	C	426	SER
1	C	434	SER
1	C	492	LEU
1	C	523	THR
1	C	558	ARG
1	C	605	SER
1	C	611	THR
1	C	624	SER
1	C	626	MET
1	C	749	VAL
1	C	770	VAL
1	C	812	SER
1	C	814	LYS
1	C	857	SER
1	C	881	LEU
1	C	893	SER
1	C	895	SER
1	C	916	SER
1	C	953	GLU
1	C	960	GLU
1	C	995	SER
1	C	1005	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	74	ASN
1	A	135	ASN
1	A	163	GLN
1	A	176	GLN
1	A	197	GLN
1	A	218	GLN
1	A	308	GLN
1	A	360	GLN
1	A	517	ASN
1	A	642	ASN
1	A	692	HIS

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Mol	Chain	Res	Type
1	A	819	ASN
1	A	999	HIS
1	B	34	GLN
1	B	254	ASN
1	B	273	GLN
1	B	517	ASN
1	B	575	GLN
1	B	577	GLN
1	B	622	GLN
1	B	642	ASN
1	B	819	ASN
1	B	922	ASN
1	C	34	GLN
1	C	74	ASN
1	C	280	GLN
1	C	508	HIS
1	C	569	GLN
1	C	577	GLN
1	C	676	ASN
1	C	697	GLN
1	C	773	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
2	CLM	B	1101	-	19,20,20	0.99	1 (5%)	23,27,27	3.20	11 (47%)

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
2	CLM	B	1101	-	-	12/20/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	CLM	C5-C3	3.00	1.57	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	CLM	C3-N2-C2	6.79	135.07	123.07
2	B	1101	CLM	C5-C3-N2	6.27	121.93	110.05
2	B	1101	CLM	C2-C1-CL1	5.93	121.30	109.61
2	B	1101	CLM	C10-C9-N9	-4.76	115.79	119.38
2	B	1101	CLM	C2-C1-CL2	4.30	118.08	109.61
2	B	1101	CLM	O5-C5-C3	4.09	118.92	107.99
2	B	1101	CLM	CL2-C1-CL1	3.56	119.06	110.30
2	B	1101	CLM	C8-C9-N9	3.41	121.94	119.38
2	B	1101	CLM	C4-C3-N2	-3.22	104.15	109.27
2	B	1101	CLM	C11-C6-C5	-2.16	117.51	120.73
2	B	1101	CLM	C7-C6-C5	2.05	123.78	120.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	CLM	C5-C3-C4-O4
2	B	1101	CLM	N2-C3-C5-O5

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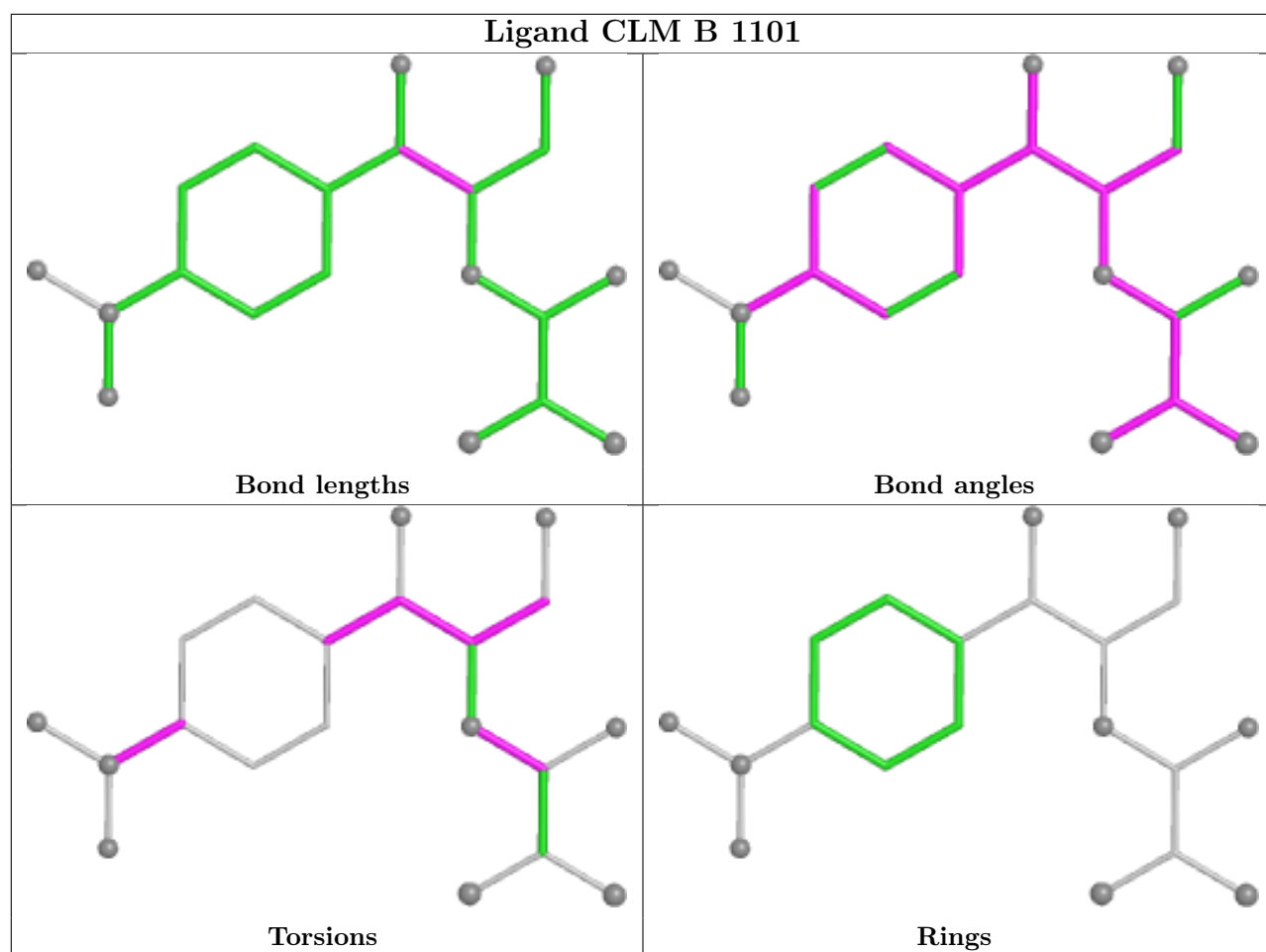
Mol	Chain	Res	Type	Atoms
2	B	1101	CLM	N2-C3-C5-C6
2	B	1101	CLM	C4-C3-C5-O5
2	B	1101	CLM	C4-C3-C5-C6
2	B	1101	CLM	C10-C9-N9-O9B
2	B	1101	CLM	C3-C5-C6-C7
2	B	1101	CLM	C3-C5-C6-C11
2	B	1101	CLM	O2-C2-N2-C3
2	B	1101	CLM	C1-C2-N2-C3
2	B	1101	CLM	N2-C3-C4-O4
2	B	1101	CLM	C8-C9-N9-O9B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	CLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	1024/1054 (97%)	0.37	64 (6%)	26	20	66, 110, 159, 201	0
1	B	1030/1054 (97%)	0.62	90 (8%)	16	13	79, 141, 189, 221	0
1	C	1030/1054 (97%)	0.29	45 (4%)	39	30	73, 118, 162, 211	0
All	All	3084/3162 (97%)	0.43	199 (6%)	25	20	66, 123, 176, 221	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	668	PRO	8.2
1	B	667	ALA	6.6
1	B	333	VAL	5.8
1	B	670	SER	5.8
1	B	669	PRO	5.3
1	C	253	VAL	5.2
1	B	502	LYS	5.1
1	B	407	ASP	5.0
1	B	569	GLN	4.9
1	B	677	ALA	4.9
1	B	976	THR	4.8
1	B	408	ASP	4.6
1	B	958	ILE	4.4
1	A	136	PHE	4.3
1	B	571	VAL	4.3
1	C	728	LEU	4.3
1	B	573	PHE	4.3
1	A	292	LYS	4.2
1	A	875	LEU	4.2
1	A	174	ASP	4.1
1	C	815	LEU	4.1
1	A	872	ALA	4.1
1	C	720	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	175	PHE	4.0
1	C	800	PHE	4.0
1	A	744	ASP	3.9
1	B	350	LEU	3.9
1	B	790	VAL	3.8
1	B	899	SER	3.8
1	C	809	GLU	3.8
1	C	730	ILE	3.8
1	A	676	ASN	3.8
1	B	174	ASP	3.7
1	B	671	VAL	3.7
1	A	740	VAL	3.7
1	A	412	VAL	3.6
1	C	521	LEU	3.6
1	A	230	LEU	3.6
1	A	532	ALA	3.5
1	A	656	PHE	3.5
1	B	661	ALA	3.5
1	A	327	TYR	3.4
1	A	466	ILE	3.4
1	B	673	GLU	3.4
1	B	132	ALA	3.3
1	B	134	LYS	3.3
1	B	433	LYS	3.3
1	C	70	ASN	3.3
1	B	424	GLY	3.2
1	A	299	ALA	3.2
1	A	979	ALA	3.2
1	A	628	PHE	3.2
1	A	290	ALA	3.2
1	A	943	LEU	3.1
1	B	503	GLY	3.1
1	A	386	PHE	3.1
1	B	136	PHE	3.1
1	B	327	TYR	3.0
1	A	413	VAL	3.0
1	C	385	ALA	3.0
1	B	500	ILE	3.0
1	A	741	SER	3.0
1	A	385	ALA	3.0
1	A	176	GLN	3.0
1	A	810	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	437	GLN	2.9
1	B	676	ASN	2.9
1	A	745	ILE	2.9
1	B	675	GLY	2.9
1	B	34	GLN	2.8
1	B	176	GLN	2.8
1	C	615	PHE	2.8
1	B	278	ASN	2.8
1	C	834	LEU	2.8
1	A	443	VAL	2.8
1	A	876	TYR	2.8
1	C	658	PHE	2.8
1	C	803	PHE	2.8
1	C	958	ILE	2.8
1	B	903	VAL	2.8
1	A	980	PHE	2.8
1	A	437	GLN	2.7
1	C	1014	VAL	2.7
1	B	666	PHE	2.7
1	B	137	LEU	2.7
1	B	386	PHE	2.7
1	C	250	LEU	2.7
1	B	270	LEU	2.7
1	C	510	GLY	2.7
1	A	7	ASP	2.6
1	C	230	LEU	2.6
1	B	271	GLY	2.6
1	A	861	LEU	2.6
1	B	989	ILE	2.6
1	A	610	PHE	2.6
1	B	406	VAL	2.6
1	C	1	MET	2.5
1	B	962	ALA	2.5
1	C	227	GLY	2.5
1	C	719	GLY	2.5
1	C	524	THR	2.5
1	B	542	LEU	2.5
1	B	936	LEU	2.5
1	A	416	VAL	2.5
1	B	49	TYR	2.5
1	B	300	LEU	2.5
1	A	291	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	423	GLU	2.5
1	A	938	ALA	2.5
1	B	334	SER	2.4
1	C	997	SER	2.4
1	A	178	PHE	2.4
1	A	493	CYS	2.4
1	A	742	LEU	2.4
1	A	951	LEU	2.4
1	B	355	MET	2.4
1	B	425	LEU	2.4
1	A	935	GLY	2.4
1	B	798	VAL	2.4
1	C	442	LEU	2.4
1	A	586	ARG	2.4
1	B	613	THR	2.4
1	A	435	MET	2.4
1	C	126	GLY	2.4
1	C	660	ASP	2.4
1	B	567	GLU	2.4
1	B	454	LEU	2.4
1	B	674	LEU	2.4
1	A	6	ILE	2.4
1	B	249	ILE	2.4
1	B	410	ILE	2.4
1	A	109	ASN	2.3
1	A	869	GLY	2.3
1	B	566	ASP	2.3
1	A	738	LEU	2.3
1	B	35	TYR	2.3
1	B	405	LEU	2.3
1	A	790	VAL	2.3
1	C	1027	VAL	2.3
1	B	290	ALA	2.3
1	C	742	LEU	2.3
1	A	463	THR	2.3
1	B	591	VAL	2.3
1	A	229	GLN	2.3
1	A	448	VAL	2.3
1	B	223	PRO	2.3
1	C	275	TYR	2.3
1	B	513	PHE	2.2
1	B	485	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	601	LYS	2.2
1	C	577	GLN	2.2
1	C	407	ASP	2.2
1	C	508	HIS	2.2
1	B	656	PHE	2.2
1	C	556	PHE	2.2
1	B	970	LEU	2.2
1	B	549	VAL	2.2
1	C	753	TRP	2.2
1	B	815	LEU	2.2
1	A	282	ASN	2.2
1	A	354	VAL	2.2
1	A	411	VAL	2.2
1	C	895	SER	2.2
1	B	248	ASN	2.2
1	C	175	PHE	2.2
1	B	415	ASN	2.1
1	B	329	THR	2.1
1	A	300	LEU	2.1
1	A	615	PHE	2.1
1	B	262	LEU	2.1
1	B	672	LEU	2.1
1	A	462	SER	2.1
1	A	507	GLU	2.1
1	B	27	ILE	2.1
1	B	32	VAL	2.1
1	C	717	PRO	2.1
1	B	980	PHE	2.1
1	C	136	PHE	2.1
1	A	809	GLU	2.1
1	B	28	LEU	2.1
1	C	1019	TRP	2.1
1	B	299	ALA	2.1
1	B	724	PRO	2.1
1	B	570	GLY	2.1
1	B	947	PHE	2.1
1	C	566	ASP	2.1
1	B	789	TYR	2.1
1	A	870	SER	2.0
1	A	499	PRO	2.0
1	A	436	GLY	2.0
1	C	628	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	679	GLY	2.0
1	B	135	ASN	2.0
1	B	586	ARG	2.0
1	A	983	GLY	2.0
1	B	277	ILE	2.0
1	A	735	ALA	2.0
1	C	653	MET	2.0
1	C	590	VAL	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

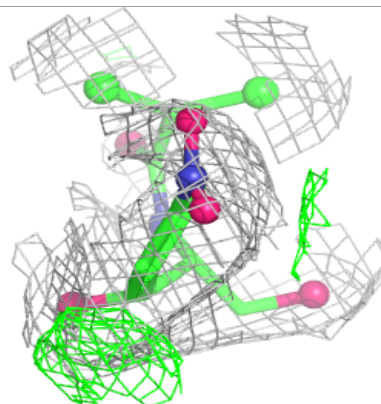
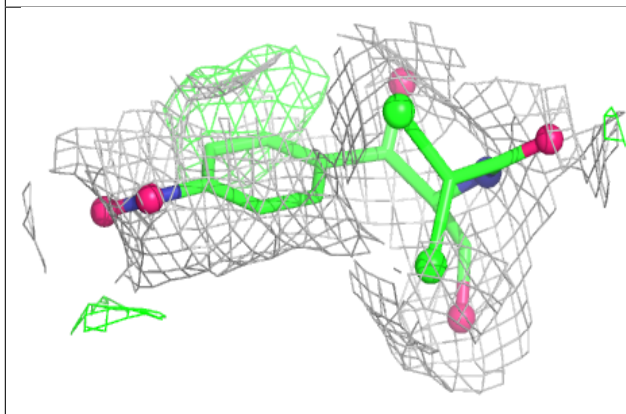
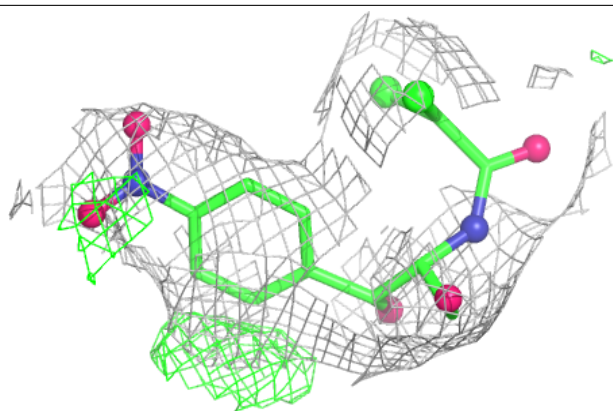
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CLM	B	1101	20/20	0.79	0.14	146,166,180,186	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around CLM B 1101:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.