



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 09:44 PM GMT

PDB ID : 3B8C  
Title : Crystal Structure of a Plasma Membrane Proton Pump  
Authors : Pedersen, B.P.; Buch-Pedersen, M.J.; Morth, J.P.; Palmgren, M.G.; Nissen, P.  
Deposited on : 2007-11-01  
Resolution : 3.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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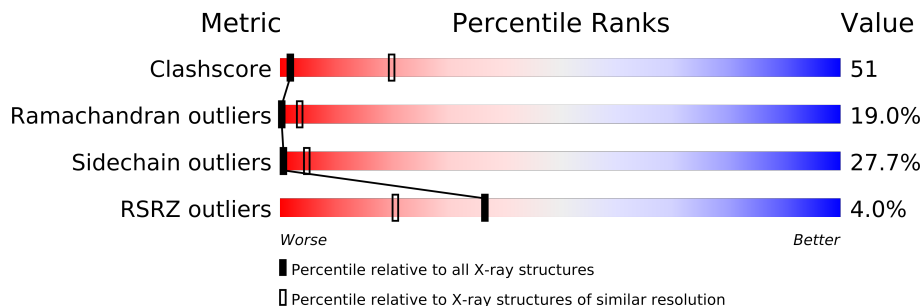
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.60 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))
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	885	
1	B	885	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	1002	-	X
2	MG	B	1004	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12896 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATPase 2, plasma membrane-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6416	4132	1082	1169	33			
1	B	833	Total	C	N	O	S	0	0	0
			6416	4132	1082	1169	33			

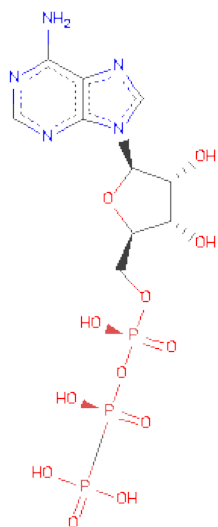
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	876	MET	-	EXPRESSION TAG	UNP P19456
A	877	ARG	-	EXPRESSION TAG	UNP P19456
A	878	GLY	-	EXPRESSION TAG	UNP P19456
A	879	SER	-	EXPRESSION TAG	UNP P19456
A	880	HIS	-	EXPRESSION TAG	UNP P19456
A	881	HIS	-	EXPRESSION TAG	UNP P19456
A	882	HIS	-	EXPRESSION TAG	UNP P19456
A	883	HIS	-	EXPRESSION TAG	UNP P19456
A	884	HIS	-	EXPRESSION TAG	UNP P19456
A	885	HIS	-	EXPRESSION TAG	UNP P19456
B	876	MET	-	EXPRESSION TAG	UNP P19456
B	877	ARG	-	EXPRESSION TAG	UNP P19456
B	878	GLY	-	EXPRESSION TAG	UNP P19456
B	879	SER	-	EXPRESSION TAG	UNP P19456
B	880	HIS	-	EXPRESSION TAG	UNP P19456
B	881	HIS	-	EXPRESSION TAG	UNP P19456
B	882	HIS	-	EXPRESSION TAG	UNP P19456
B	883	HIS	-	EXPRESSION TAG	UNP P19456
B	884	HIS	-	EXPRESSION TAG	UNP P19456
B	885	HIS	-	EXPRESSION TAG	UNP P19456

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

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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONICACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



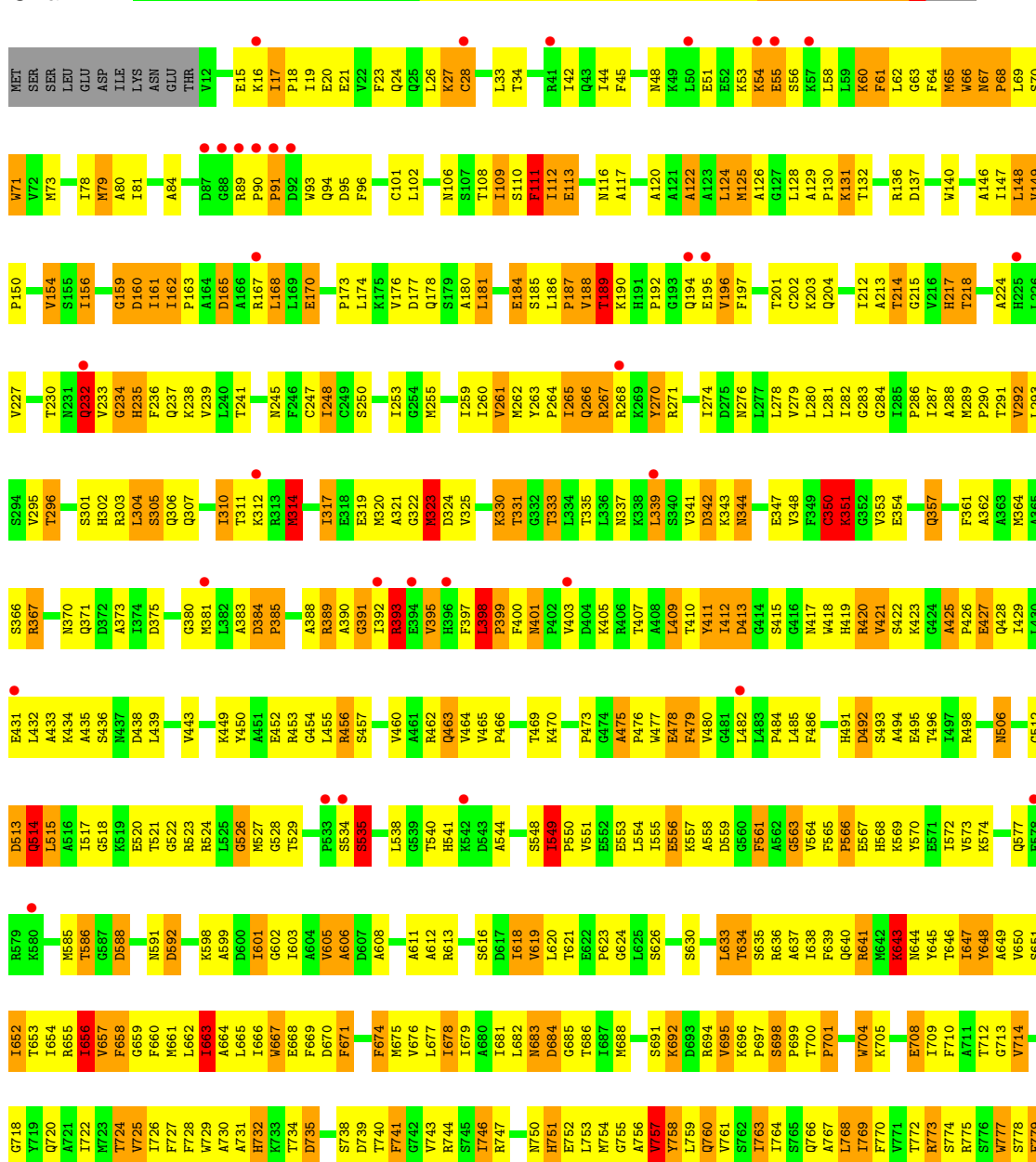
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: ATPase 2, plasma membrane-type

Chain A:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.29Å 144.42Å 312.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60 30.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-3.60) 89.9 (30.00-3.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.350 , 0.366 0.340 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	111.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 21.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	3 of 49496 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	12896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.45	0/6542	0.78	2/8865 (0.0%)
1	B	0.43	0/6542	0.77	2/8865 (0.0%)
All	All	0.44	0/13084	0.78	4/17730 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	691	SER	N-CA-C	-5.83	95.25	111.00
1	A	691	SER	N-CA-C	-5.73	95.53	111.00
1	B	563	GLY	N-CA-C	-5.16	100.20	113.10
1	A	563	GLY	N-CA-C	-5.15	100.22	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6416	0	0	333	0
1	B	6416	0	0	332	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	31	0	13	5	0
3	B	31	0	13	4	0
All	All	12896	0	26	665	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 51.

All (665) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:ASN:O	1:A:69:LEU:N	2.07	0.88
1:B:67:ASN:O	1:B:69:LEU:N	2.11	0.82
1:A:803:VAL:O	1:A:805:ALA:N	2.17	0.78
1:A:813:ARG:NH1	1:A:814:GLY:O	2.19	0.76
1:B:813:ARG:NH1	1:B:814:GLY:O	2.20	0.75
1:B:803:VAL:O	1:B:805:ALA:N	2.19	0.75
1:A:779:PHE:CB	1:A:783:PRO:CD	2.66	0.74
1:B:779:PHE:CB	1:B:783:PRO:CD	2.67	0.73
1:A:288:ALA:O	1:A:291:THR:N	2.22	0.72
1:A:129:ALA:O	1:A:131:LYS:N	2.21	0.72
1:B:400:PHE:CD1	1:B:401:ASN:N	2.58	0.72
1:A:556:GLU:O	1:A:558:ALA:N	2.23	0.71
1:B:129:ALA:O	1:B:131:LYS:N	2.22	0.71
1:B:556:GLU:O	1:B:558:ALA:N	2.23	0.71
1:B:397:PHE:C	1:B:399:PRO:CD	2.60	0.70
1:B:286:PRO:O	1:B:288:ALA:N	2.24	0.69
1:A:400:PHE:CD1	1:A:401:ASN:N	2.60	0.69
1:B:288:ALA:O	1:B:291:THR:N	2.25	0.69
1:B:491:HIS:CG	1:B:492:ASP:N	2.61	0.68
1:A:491:HIS:CG	1:A:492:ASP:N	2.61	0.68
1:A:286:PRO:O	1:A:288:ALA:N	2.27	0.68
1:A:397:PHE:C	1:A:399:PRO:CD	2.61	0.68
1:B:634:THR:CG2	1:B:635:SER:N	2.57	0.68
1:A:831:TYR:CD2	1:A:832:PHE:CD1	2.83	0.67
1:A:634:THR:CG2	1:A:635:SER:N	2.57	0.67
1:A:655:ARG:O	1:A:657:VAL:N	2.29	0.66
1:A:831:TYR:C	1:A:831:TYR:CD2	2.69	0.66
1:A:288:ALA:O	1:A:292:VAL:N	2.30	0.65
1:A:704:TRP:N	1:A:704:TRP:CE3	2.64	0.65
1:A:456:ARG:CG	1:A:456:ARG:NH1	2.59	0.64
1:B:704:TRP:N	1:B:704:TRP:CE3	2.66	0.64
1:B:288:ALA:O	1:B:292:VAL:N	2.30	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:758:TYR:CD1	1:A:758:TYR:O	2.51	0.64
1:B:831:TYR:CD2	1:B:832:PHE:CD1	2.85	0.64
1:B:565:PHE:CD1	1:B:568:HIS:CE1	2.86	0.64
1:B:655:ARG:O	1:B:657:VAL:N	2.31	0.64
1:B:658:PHE:CD2	1:B:671:PHE:CE2	2.85	0.63
1:B:831:TYR:CD2	1:B:831:TYR:C	2.71	0.63
1:B:769:ILE:O	1:B:769:ILE:CG2	2.45	0.63
1:A:53:LYS:O	1:A:55:GLU:N	2.31	0.63
1:A:344:ASN:N	1:A:344:ASN:OD1	2.32	0.63
1:A:692:LYS:CG	1:A:770:PHE:CZ	2.82	0.63
1:B:478:GLU:O	1:B:479:PHE:O	2.16	0.63
1:A:752:GLU:OE1	1:A:810:ALA:O	2.16	0.63
1:A:769:ILE:CG2	1:A:769:ILE:O	2.46	0.62
1:B:184:GLU:O	1:B:186:LEU:N	2.32	0.62
1:A:58:LEU:C	1:A:60:LYS:N	2.51	0.62
1:B:344:ASN:N	1:B:344:ASN:OD1	2.32	0.62
1:A:727:PHE:CZ	1:A:819:TRP:CH2	2.87	0.62
1:A:478:GLU:O	1:A:479:PHE:O	2.17	0.62
1:B:53:LYS:O	1:B:55:GLU:N	2.32	0.62
1:A:658:PHE:CD2	1:A:671:PHE:CE2	2.87	0.62
1:B:727:PHE:CZ	1:B:819:TRP:CH2	2.88	0.62
1:B:526:GLY:O	1:B:528:GLY:N	2.33	0.62
1:A:674:PHE:CD2	1:A:674:PHE:O	2.53	0.62
1:B:418:TRP:CD1	1:B:465:VAL:CG1	2.83	0.62
1:B:752:GLU:OE1	1:B:810:ALA:O	2.17	0.62
1:B:764:ILE:CG1	1:B:791:PHE:CD2	2.83	0.62
1:B:58:LEU:C	1:B:60:LYS:N	2.50	0.61
1:A:526:GLY:O	1:A:528:GLY:N	2.33	0.61
1:B:400:PHE:CE1	3:B:1003:ACP:C2	2.83	0.61
1:A:283:GLY:O	1:A:656:ILE:CG2	2.49	0.61
1:A:184:GLU:O	1:A:186:LEU:N	2.33	0.61
1:B:692:LYS:CG	1:B:770:PHE:CZ	2.83	0.61
1:B:456:ARG:CG	1:B:456:ARG:NH1	2.63	0.61
1:B:683:ASN:C	1:B:683:ASN:ND2	2.54	0.61
1:B:842:ARG:O	1:B:844:ILE:N	2.33	0.61
1:B:754:MET:O	1:B:756:ALA:N	2.33	0.61
1:A:683:ASN:ND2	1:A:683:ASN:C	2.53	0.61
1:B:758:TYR:CD1	1:B:758:TYR:O	2.53	0.61
1:A:565:PHE:CD1	1:A:568:HIS:CE1	2.89	0.61
1:A:791:PHE:O	1:A:792:LEU:CD2	2.49	0.61
1:A:337:ASN:O	1:A:337:ASN:CG	2.38	0.61
1:B:337:ASN:CG	1:B:337:ASN:O	2.38	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:431:GLU:O	1:A:433:ALA:N	2.34	0.60
1:A:764:ILE:CG1	1:A:791:PHE:CD2	2.84	0.60
1:A:161:ILE:O	1:A:162:ILE:O	2.18	0.60
1:A:418:TRP:CD1	1:A:465:VAL:CG1	2.84	0.60
1:B:108:THR:O	1:B:110:SER:N	2.35	0.60
1:B:431:GLU:O	1:B:433:ALA:N	2.35	0.59
1:B:757:VAL:C	1:B:759:LEU:N	2.54	0.59
1:A:671:PHE:N	1:A:751:HIS:NE2	2.49	0.59
1:A:823:ILE:O	1:A:827:SER:N	2.36	0.59
1:A:161:ILE:O	1:A:162:ILE:C	2.38	0.59
1:B:364:MET:SD	1:B:420:ARG:O	2.61	0.59
1:A:400:PHE:CE1	3:A:1001:ACP:C2	2.85	0.59
1:B:347:GLU:OE2	1:B:347:GLU:N	2.36	0.58
1:A:657:VAL:O	1:A:661:MET:CG	2.51	0.58
1:B:791:PHE:O	1:B:792:LEU:CD2	2.51	0.58
1:A:364:MET:SD	1:A:420:ARG:O	2.61	0.58
1:B:657:VAL:O	1:B:661:MET:CG	2.51	0.58
1:B:342:ASP:OD2	1:B:342:ASP:N	2.36	0.58
1:A:108:THR:O	1:A:110:SER:N	2.37	0.58
1:A:754:MET:O	1:A:756:ALA:N	2.36	0.58
1:A:262:MET:CE	1:A:266:GLN:NE2	2.66	0.58
1:B:384:ASP:OD1	1:B:384:ASP:N	2.37	0.58
1:B:310:ILE:CG2	1:B:311:THR:N	2.66	0.58
1:B:108:THR:CG2	1:B:109:ILE:N	2.66	0.58
1:A:704:TRP:CD2	1:A:704:TRP:N	2.71	0.57
1:A:342:ASP:OD2	1:A:342:ASP:N	2.37	0.57
1:A:777:TRP:C	1:A:777:TRP:CD1	2.77	0.57
1:A:292:VAL:CG2	1:A:293:LEU:N	2.67	0.57
1:A:146:ALA:O	1:A:148:LEU:N	2.37	0.57
1:B:398:LEU:N	1:B:399:PRO:CD	2.68	0.57
1:A:813:ARG:CG	1:A:814:GLY:N	2.68	0.57
1:A:757:VAL:C	1:A:759:LEU:N	2.55	0.57
1:B:777:TRP:C	1:B:777:TRP:CD1	2.78	0.57
1:A:292:VAL:CG2	1:A:645:TYR:CE2	2.88	0.57
1:B:704:TRP:CD2	1:B:704:TRP:N	2.73	0.57
1:A:310:ILE:CG2	1:A:311:THR:N	2.68	0.57
1:B:813:ARG:CG	1:B:814:GLY:N	2.69	0.56
1:B:674:PHE:O	1:B:674:PHE:CD2	2.57	0.56
1:A:671:PHE:O	1:A:751:HIS:CE1	2.58	0.56
1:A:670:ASP:C	1:A:751:HIS:NE2	2.58	0.56
1:B:262:MET:CE	1:B:266:GLN:NE2	2.69	0.56
1:B:684:ASP:O	1:B:686:THR:N	2.38	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:283:GLY:O	1:B:656:ILE:CG2	2.53	0.56
1:B:292:VAL:CG2	1:B:293:LEU:N	2.66	0.56
1:B:751:HIS:C	1:B:753:LEU:N	2.59	0.56
1:A:684:ASP:O	1:A:686:THR:N	2.39	0.56
1:A:384:ASP:OD1	1:A:384:ASP:N	2.39	0.56
1:B:565:PHE:O	1:B:568:HIS:CD2	2.59	0.56
1:A:108:THR:CG2	1:A:109:ILE:N	2.66	0.56
1:B:361:PHE:CD2	1:B:362:ALA:N	2.73	0.56
1:B:161:ILE:O	1:B:162:ILE:C	2.43	0.56
1:B:569:LYS:NZ	1:B:592:ASP:OD1	2.39	0.56
1:B:450:TYR:O	1:B:455:LEU:N	2.39	0.56
1:A:398:LEU:N	1:A:399:PRO:CD	2.69	0.55
1:A:842:ARG:O	1:A:844:ILE:N	2.40	0.55
1:A:347:GLU:N	1:A:347:GLU:OE2	2.39	0.55
1:A:636:ARG:NH1	1:A:698:SER:CA	2.70	0.55
1:B:146:ALA:O	1:B:148:LEU:N	2.39	0.55
1:B:671:PHE:N	1:B:751:HIS:NE2	2.53	0.55
1:B:565:PHE:O	1:B:568:HIS:CG	2.60	0.55
1:A:569:LYS:NZ	1:A:592:ASP:OD1	2.39	0.55
1:B:339:LEU:CA	1:B:486:PHE:O	2.55	0.55
1:B:375:ASP:OD1	3:B:1003:ACP:N6	2.40	0.55
1:B:823:ILE:O	1:B:827:SER:N	2.39	0.55
1:A:333:THR:C	1:A:335:THR:N	2.60	0.55
1:B:790:ALA:O	1:B:791:PHE:CD1	2.59	0.55
1:B:714:VAL:O	1:B:718:GLY:N	2.40	0.55
1:A:188:VAL:O	1:A:189:THR:O	2.25	0.55
1:A:492:ASP:OD2	1:A:492:ASP:N	2.40	0.54
1:A:670:ASP:CA	1:A:751:HIS:CD2	2.90	0.54
1:B:663:ILE:CG2	1:B:664:ALA:N	2.70	0.54
1:B:671:PHE:O	1:B:751:HIS:CE1	2.60	0.54
1:B:842:ARG:C	1:B:844:ILE:N	2.60	0.54
1:A:837:PHE:O	1:A:840:ALA:N	2.40	0.54
1:A:779:PHE:CD2	1:A:783:PRO:CD	2.90	0.54
1:B:495:GLU:O	1:B:498:ARG:CB	2.56	0.54
1:B:341:VAL:CG1	1:B:484:PRO:O	2.55	0.54
1:B:764:ILE:CD1	1:B:791:PHE:O	2.55	0.54
1:A:754:MET:C	1:A:756:ALA:N	2.61	0.54
1:B:670:ASP:C	1:B:751:HIS:NE2	2.61	0.54
1:B:754:MET:C	1:B:756:ALA:N	2.60	0.54
1:A:388:ALA:C	1:A:389:ARG:CZ	2.76	0.54
1:B:321:ALA:C	1:B:700:THR:OG1	2.46	0.54
1:A:751:HIS:C	1:A:753:LEU:N	2.60	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:333:THR:C	1:B:335:THR:N	2.61	0.54
1:A:361:PHE:CD2	1:A:362:ALA:N	2.75	0.54
1:A:659:GLY:N	1:A:671:PHE:CE2	2.75	0.54
1:A:565:PHE:O	1:A:568:HIS:CG	2.61	0.54
1:A:676:VAL:O	1:A:679:ILE:CG2	2.56	0.54
1:B:659:GLY:N	1:B:671:PHE:CE2	2.76	0.53
1:A:764:ILE:CD1	1:A:791:PHE:O	2.56	0.53
1:B:837:PHE:O	1:B:840:ALA:N	2.41	0.53
1:A:64:PHE:O	1:A:66:TRP:N	2.41	0.53
1:A:321:ALA:C	1:A:700:THR:OG1	2.47	0.53
1:B:636:ARG:NH1	1:B:698:SER:CA	2.71	0.53
1:A:450:TYR:O	1:A:455:LEU:N	2.42	0.53
1:B:506:ASN:N	1:B:506:ASN:ND2	2.56	0.53
1:B:676:VAL:O	1:B:679:ILE:CG2	2.56	0.53
1:B:384:ASP:O	1:B:385:PRO:O	2.27	0.53
1:A:785:ALA:O	1:A:787:LEU:N	2.40	0.53
1:A:663:ILE:CG2	1:A:664:ALA:N	2.70	0.53
1:B:759:LEU:O	1:B:760:GLN:NE2	2.41	0.53
1:A:389:ARG:NE	1:A:389:ARG:CA	2.72	0.53
1:B:64:PHE:O	1:B:66:TRP:N	2.42	0.53
1:B:292:VAL:CG2	1:B:645:TYR:CE2	2.91	0.53
1:A:692:LYS:CE	1:A:770:PHE:CE2	2.92	0.53
1:A:405:LYS:O	1:A:423:LYS:O	2.26	0.53
1:A:42:ILE:O	1:A:45:PHE:CD2	2.61	0.53
1:A:796:LEU:O	1:A:799:THR:N	2.41	0.53
1:A:759:LEU:O	1:A:760:GLN:NE2	2.42	0.53
1:B:779:PHE:CD2	1:B:783:PRO:CD	2.92	0.53
1:B:655:ARG:CB	1:B:658:PHE:CE1	2.91	0.53
1:B:692:LYS:CE	1:B:770:PHE:CE2	2.91	0.53
1:A:565:PHE:O	1:A:568:HIS:CD2	2.61	0.53
1:A:341:VAL:CG1	1:A:484:PRO:O	2.57	0.53
1:A:65:MET:O	1:A:111:PHE:CZ	2.62	0.53
1:B:456:ARG:NH1	1:B:513:ASP:OD1	2.40	0.53
1:B:492:ASP:N	1:B:492:ASP:OD2	2.42	0.53
1:B:661:MET:O	1:B:663:ILE:N	2.41	0.53
1:B:569:LYS:O	1:B:570:TYR:C	2.46	0.53
1:A:790:ALA:O	1:A:791:PHE:CD1	2.61	0.52
1:B:486:PHE:CZ	1:B:524:ARG:NH1	2.78	0.52
1:A:339:LEU:CA	1:A:486:PHE:O	2.57	0.52
1:A:411:TYR:N	1:A:411:TYR:CD2	2.78	0.52
1:B:389:ARG:NE	1:B:389:ARG:CA	2.72	0.52
1:A:656:ILE:CG2	1:A:658:PHE:CZ	2.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:732:HIS:C	1:A:734:THR:N	2.63	0.52
1:A:506:ASN:ND2	1:A:506:ASN:N	2.56	0.52
1:B:411:TYR:CD2	1:B:411:TYR:N	2.77	0.52
1:A:842:ARG:C	1:A:844:ILE:N	2.62	0.52
1:B:405:LYS:O	1:B:423:LYS:O	2.27	0.52
1:B:388:ALA:C	1:B:389:ARG:CZ	2.78	0.52
1:B:670:ASP:CA	1:B:751:HIS:CD2	2.93	0.52
1:A:820:ALA:O	1:A:823:ILE:N	2.43	0.52
1:A:714:VAL:O	1:A:718:GLY:N	2.43	0.52
1:B:188:VAL:O	1:B:189:THR:O	2.28	0.52
1:B:456:ARG:N	1:B:485:LEU:O	2.42	0.52
1:B:774:SER:O	1:B:839:PHE:CZ	2.63	0.52
1:A:661:MET:O	1:A:663:ILE:N	2.43	0.52
1:B:775:ARG:C	1:B:777:TRP:N	2.63	0.52
1:A:384:ASP:O	1:A:385:PRO:O	2.28	0.52
1:B:732:HIS:C	1:B:734:THR:N	2.63	0.52
1:A:655:ARG:CB	1:A:658:PHE:CE1	2.93	0.51
1:A:569:LYS:O	1:A:570:TYR:C	2.47	0.51
1:A:361:PHE:CE1	1:A:422:SER:O	2.62	0.51
1:A:839:PHE:N	1:A:839:PHE:CD1	2.78	0.51
1:B:65:MET:O	1:B:111:PHE:CZ	2.63	0.51
1:B:42:ILE:O	1:B:45:PHE:CD2	2.63	0.51
1:B:773:ARG:CG	1:B:843:TYR:OH	2.58	0.51
1:B:495:GLU:O	1:B:498:ARG:N	2.43	0.51
1:B:452:GLU:C	1:B:454:GLY:N	2.64	0.51
1:A:520:GLU:C	1:A:522:GLY:N	2.64	0.51
1:A:314:MET:O	1:A:317:ILE:CG1	2.59	0.51
1:A:720:GLN:NE2	1:A:758:TYR:CB	2.74	0.51
1:B:796:LEU:O	1:B:799:THR:N	2.43	0.51
1:B:361:PHE:CE1	1:B:422:SER:O	2.64	0.51
1:B:820:ALA:O	1:B:823:ILE:N	2.43	0.51
1:B:520:GLU:C	1:B:522:GLY:N	2.63	0.51
1:B:785:ALA:O	1:B:787:LEU:N	2.43	0.51
1:B:751:HIS:ND1	1:B:752:GLU:N	2.59	0.51
1:A:636:ARG:CZ	1:A:698:SER:O	2.59	0.51
1:A:486:PHE:CZ	1:A:524:ARG:NH1	2.79	0.51
1:A:803:VAL:C	1:A:805:ALA:N	2.64	0.51
1:A:495:GLU:O	1:A:498:ARG:CB	2.59	0.51
1:B:839:PHE:N	1:B:839:PHE:CD1	2.79	0.51
1:B:161:ILE:O	1:B:162:ILE:O	2.28	0.51
1:B:656:ILE:O	1:B:656:ILE:CG1	2.57	0.51
1:A:775:ARG:C	1:A:777:TRP:N	2.64	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:708:GLU:OE1	1:B:708:GLU:C	2.50	0.51
1:A:778:SER:C	1:A:780:VAL:N	2.64	0.50
1:A:492:ASP:O	1:A:495:GLU:N	2.44	0.50
1:A:495:GLU:O	1:A:498:ARG:N	2.44	0.50
1:A:456:ARG:NH1	1:A:513:ASP:OD1	2.44	0.50
1:A:751:HIS:ND1	1:A:752:GLU:N	2.60	0.50
1:A:841:ILE:O	1:A:844:ILE:O	2.29	0.50
1:A:660:PHE:O	1:A:660:PHE:CD2	2.65	0.50
1:A:759:LEU:O	1:A:760:GLN:CG	2.60	0.50
1:A:333:THR:O	1:A:335:THR:N	2.44	0.50
1:A:774:SER:O	1:A:839:PHE:CZ	2.65	0.50
1:A:643:LYS:NZ	1:A:704:TRP:CZ3	2.80	0.50
1:B:724:THR:O	1:B:726:ILE:N	2.45	0.50
1:B:108:THR:C	1:B:110:SER:N	2.64	0.50
1:A:452:GLU:C	1:A:454:GLY:N	2.64	0.50
1:B:652:ILE:CG2	1:B:653:THR:N	2.75	0.50
1:A:647:ILE:N	1:A:647:ILE:CD1	2.74	0.50
1:B:778:SER:C	1:B:780:VAL:N	2.64	0.50
1:A:456:ARG:N	1:A:485:LEU:O	2.44	0.50
1:A:778:SER:O	1:A:780:VAL:N	2.45	0.50
1:A:701:PRO:O	1:A:704:TRP:CH2	2.65	0.50
1:B:726:ILE:O	1:B:730:ALA:CB	2.60	0.50
1:A:364:MET:SD	1:A:411:TYR:CE2	3.04	0.50
1:A:450:TYR:O	1:A:454:GLY:N	2.45	0.50
1:A:322:GLY:O	1:A:324:ASP:N	2.45	0.50
1:B:235:HIS:O	1:B:235:HIS:CD2	2.65	0.50
1:A:235:HIS:CD2	1:A:235:HIS:O	2.64	0.49
1:A:491:HIS:CE1	1:B:455:LEU:CD1	2.96	0.49
1:A:388:ALA:O	1:A:389:ARG:NH2	2.45	0.49
1:A:68:PRO:CA	1:A:71:TRP:CB	2.90	0.49
1:B:803:VAL:C	1:B:805:ALA:N	2.65	0.49
1:A:808:GLU:O	1:A:811:LYS:O	2.29	0.49
1:B:561:PHE:CZ	1:B:572:ILE:CG2	2.95	0.49
1:B:795:GLN:NE2	1:B:795:GLN:CA	2.73	0.49
1:B:701:PRO:O	1:B:704:TRP:CH2	2.65	0.49
1:A:708:GLU:C	1:A:708:GLU:OE1	2.50	0.49
1:B:235:HIS:CD2	1:B:239:VAL:CG1	2.95	0.49
1:A:237:GLN:C	1:A:239:VAL:N	2.65	0.49
1:B:314:MET:O	1:B:317:ILE:CG1	2.60	0.49
1:A:512:GLY:CA	1:A:563:GLY:O	2.60	0.49
1:A:148:LEU:O	1:A:149:VAL:O	2.30	0.49
1:A:654:ILE:CG2	1:A:654:ILE:O	2.59	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:322:GLY:O	1:B:324:ASP:N	2.45	0.49
1:A:108:THR:C	1:A:110:SER:N	2.66	0.49
1:B:636:ARG:CZ	1:B:698:SER:O	2.61	0.49
1:A:375:ASP:OD1	3:A:1001:ACP:N6	2.46	0.49
1:A:724:THR:O	1:A:727:PHE:N	2.44	0.49
1:A:720:GLN:NE2	1:A:758:TYR:C	2.66	0.49
1:B:724:THR:O	1:B:727:PHE:N	2.45	0.49
1:B:364:MET:SD	1:B:411:TYR:CE2	3.06	0.49
1:B:512:GLY:CA	1:B:563:GLY:O	2.61	0.49
1:A:773:ARG:CG	1:A:843:TYR:OH	2.61	0.49
1:A:561:PHE:CZ	1:A:572:ILE:CG2	2.95	0.49
1:A:740:THR:O	1:A:741:PHE:C	2.51	0.49
1:B:554:LEU:O	1:B:555:ILE:C	2.51	0.49
1:B:841:ILE:O	1:B:844:ILE:O	2.31	0.49
1:A:724:THR:O	1:A:726:ILE:N	2.46	0.48
1:A:146:ALA:C	1:A:148:LEU:N	2.65	0.48
1:B:778:SER:O	1:B:780:VAL:N	2.46	0.48
1:B:647:ILE:CD1	1:B:647:ILE:N	2.75	0.48
1:B:782:ARG:O	1:B:783:PRO:C	2.50	0.48
1:B:276:ASN:ND2	1:B:670:ASP:N	2.60	0.48
1:B:388:ALA:O	1:B:389:ARG:NH2	2.46	0.48
1:B:654:ILE:O	1:B:654:ILE:CG2	2.61	0.48
1:B:570:TYR:CE1	1:B:574:LYS:NZ	2.81	0.48
1:B:148:LEU:O	1:B:149:VAL:O	2.32	0.48
1:B:19:ILE:O	1:B:21:GLU:N	2.47	0.48
1:B:808:GLU:O	1:B:811:LYS:O	2.32	0.48
1:B:274:ILE:O	1:B:278:LEU:N	2.46	0.48
1:A:113:GLU:O	1:A:117:ALA:CB	2.62	0.48
1:A:795:GLN:NE2	1:A:795:GLN:CA	2.76	0.48
1:A:426:PRO:O	1:A:428:GLN:N	2.47	0.48
1:A:276:ASN:ND2	1:A:670:ASP:N	2.61	0.48
1:B:568:HIS:N	1:B:568:HIS:CD2	2.81	0.48
1:A:17:ILE:CG1	1:A:18:PRO:CD	2.91	0.48
1:B:270:TYR:CD2	1:B:271:ARG:N	2.81	0.48
1:B:641:ARG:NH2	1:B:694:ARG:N	2.61	0.48
1:B:214:THR:OG1	1:B:217:HIS:CG	2.67	0.48
1:B:462:ARG:CG	1:B:463:GLN:N	2.77	0.48
1:B:333:THR:O	1:B:335:THR:N	2.46	0.48
1:B:732:HIS:CD2	1:B:735:ASP:OD1	2.67	0.48
1:B:425:ALA:CB	1:B:426:PRO:CD	2.91	0.48
1:B:237:GLN:C	1:B:239:VAL:N	2.67	0.48
1:A:270:TYR:CD2	1:A:271:ARG:N	2.81	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:400:PHE:CE1	3:B:1003:ACP:H2	2.48	0.48
1:A:656:ILE:CG1	1:A:656:ILE:O	2.60	0.48
1:A:726:ILE:O	1:A:730:ALA:CB	2.61	0.48
1:B:643:LYS:NZ	1:B:704:TRP:CZ3	2.82	0.48
1:A:235:HIS:CD2	1:A:239:VAL:CG1	2.96	0.48
1:A:19:ILE:O	1:A:21:GLU:N	2.46	0.48
1:B:68:PRO:CA	1:B:71:TRP:CB	2.91	0.48
1:A:90:PRO:O	1:A:91:PRO:O	2.32	0.48
1:A:292:VAL:CG2	1:A:645:TYR:OH	2.62	0.47
1:A:568:HIS:CD2	1:A:568:HIS:N	2.82	0.47
1:B:422:SER:O	1:B:423:LYS:CD	2.63	0.47
1:B:644:ASN:CB	1:B:694:ARG:NH1	2.77	0.47
1:B:450:TYR:O	1:B:454:GLY:N	2.46	0.47
1:A:570:TYR:CE1	1:A:574:LYS:NZ	2.83	0.47
1:B:660:PHE:CD2	1:B:660:PHE:O	2.66	0.47
1:A:782:ARG:O	1:A:783:PRO:C	2.49	0.47
1:B:261:VAL:CG2	1:B:261:VAL:O	2.63	0.47
1:A:802:ALA:O	1:A:803:VAL:CG1	2.63	0.47
1:A:400:PHE:CG	1:A:401:ASN:N	2.83	0.47
1:A:517:ILE:CD1	1:A:518:GLY:N	2.78	0.47
1:B:670:ASP:O	1:B:671:PHE:C	2.52	0.47
1:A:462:ARG:CG	1:A:463:GLN:N	2.77	0.47
1:A:409:LEU:N	1:A:421:VAL:CG1	2.78	0.47
1:B:837:PHE:O	1:B:838:LYS:C	2.53	0.47
1:B:529:THR:O	1:B:535:SER:CB	2.62	0.47
1:A:160:ASP:N	1:A:160:ASP:OD1	2.48	0.47
1:A:261:VAL:O	1:A:261:VAL:CG2	2.63	0.47
1:B:160:ASP:N	1:B:160:ASP:OD1	2.48	0.47
1:B:740:THR:O	1:B:741:PHE:C	2.52	0.47
1:A:747:ARG:O	1:A:750:ASN:N	2.48	0.47
1:A:428:GLN:O	1:A:428:GLN:OE1	2.33	0.47
1:A:641:ARG:NH2	1:A:694:ARG:N	2.61	0.47
1:B:90:PRO:O	1:B:91:PRO:O	2.33	0.47
1:A:289:MET:N	1:A:290:PRO:CD	2.78	0.47
1:A:659:GLY:CA	1:A:671:PHE:CE2	2.98	0.47
1:B:708:GLU:OE1	1:B:709:ILE:N	2.48	0.47
1:A:425:ALA:CB	1:A:426:PRO:CD	2.93	0.47
1:B:17:ILE:CG1	1:B:18:PRO:CD	2.93	0.47
1:A:660:PHE:C	1:A:660:PHE:CD2	2.88	0.47
1:A:274:ILE:O	1:A:278:LEU:N	2.48	0.47
1:B:400:PHE:CG	1:B:401:ASN:N	2.83	0.47
1:A:186:LEU:O	1:A:187:PRO:O	2.33	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:517:ILE:CD1	1:B:518:GLY:N	2.77	0.47
1:A:464:VAL:CG1	1:A:477:TRP:CZ2	2.99	0.47
1:A:419:HIS:CD2	1:A:464:VAL:CG2	2.98	0.47
1:A:235:HIS:C	1:A:236:PHE:CD2	2.89	0.47
1:A:78:ILE:C	1:A:80:ALA:N	2.68	0.47
1:A:598:LYS:O	1:A:599:ALA:C	2.52	0.47
1:A:831:TYR:O	1:A:831:TYR:CD2	2.68	0.46
1:A:670:ASP:O	1:A:671:PHE:C	2.53	0.46
1:A:337:ASN:OD1	1:A:373:ALA:CB	2.63	0.46
1:B:110:SER:O	1:B:112:ILE:N	2.47	0.46
1:B:409:LEU:N	1:B:421:VAL:CG1	2.78	0.46
1:B:426:PRO:O	1:B:428:GLN:N	2.48	0.46
1:A:529:THR:O	1:A:535:SER:CB	2.63	0.46
1:B:598:LYS:O	1:B:599:ALA:C	2.54	0.46
1:A:279:VAL:CG2	1:A:280:LEU:N	2.78	0.46
1:B:146:ALA:C	1:B:148:LEU:N	2.67	0.46
1:A:554:LEU:O	1:A:555:ILE:C	2.52	0.46
1:B:668:GLU:O	1:B:669:PHE:C	2.53	0.46
1:B:464:VAL:CG1	1:B:477:TRP:NE1	2.79	0.46
1:A:825:LEU:O	1:A:829:VAL:CG1	2.63	0.46
1:B:330:LYS:NZ	1:B:331:THR:OG1	2.48	0.46
1:B:419:HIS:CD2	1:B:464:VAL:CG2	2.98	0.46
1:A:668:GLU:O	1:A:669:PHE:C	2.54	0.46
1:B:276:ASN:O	1:B:279:VAL:CG2	2.63	0.46
1:B:337:ASN:OD1	1:B:373:ALA:CB	2.63	0.46
1:A:708:GLU:OE1	1:A:709:ILE:N	2.49	0.46
1:B:350:CYS:O	1:B:351:LYS:CB	2.64	0.46
1:B:113:GLU:O	1:B:117:ALA:CB	2.64	0.46
1:B:276:ASN:ND2	1:B:669:PHE:CA	2.79	0.46
1:B:659:GLY:CA	1:B:671:PHE:CE2	2.99	0.46
1:B:769:ILE:O	1:B:770:PHE:CD1	2.68	0.46
1:B:464:VAL:CG1	1:B:477:TRP:CZ2	2.99	0.46
1:B:720:GLN:NE2	1:B:758:TYR:C	2.68	0.46
1:A:799:THR:C	1:A:801:ILE:N	2.69	0.46
1:A:276:ASN:O	1:A:279:VAL:CG2	2.63	0.46
1:B:656:ILE:CG2	1:B:658:PHE:CZ	2.99	0.46
1:B:78:ILE:C	1:B:80:ALA:N	2.68	0.46
1:B:831:TYR:CD2	1:B:831:TYR:O	2.69	0.46
1:B:279:VAL:CG2	1:B:280:LEU:N	2.78	0.46
1:B:759:LEU:O	1:B:760:GLN:CG	2.63	0.46
1:B:263:TYR:N	1:B:264:PRO:CD	2.79	0.46
1:B:289:MET:N	1:B:290:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:750:ASN:O	1:A:753:LEU:CB	2.64	0.46
1:B:720:GLN:NE2	1:B:758:TYR:CB	2.79	0.46
1:B:802:ALA:O	1:B:803:VAL:CG1	2.64	0.46
1:A:19:ILE:C	1:A:21:GLU:N	2.69	0.46
1:A:725:VAL:CG1	1:A:725:VAL:O	2.64	0.46
1:B:420:ARG:O	1:B:421:VAL:CG1	2.64	0.45
1:A:698:SER:OG	1:A:699:PRO:CD	2.64	0.45
1:A:237:GLN:O	1:A:239:VAL:N	2.49	0.45
1:A:79:MET:SD	1:A:79:MET:N	2.89	0.45
1:A:214:THR:OG1	1:A:217:HIS:CG	2.69	0.45
1:B:450:TYR:CD1	1:B:450:TYR:N	2.84	0.45
1:A:132:THR:OG1	1:A:163:PRO:CG	2.64	0.45
1:A:605:VAL:O	1:A:608:ALA:CB	2.64	0.45
1:B:464:VAL:CA	1:B:477:TRP:NE1	2.79	0.45
1:B:515:LEU:O	1:B:515:LEU:CD1	2.64	0.45
1:B:492:ASP:O	1:B:495:GLU:N	2.49	0.45
1:A:643:LYS:CE	1:A:701:PRO:O	2.64	0.45
1:A:464:VAL:CG1	1:A:477:TRP:NE1	2.80	0.45
1:A:420:ARG:O	1:A:421:VAL:CG1	2.64	0.45
1:B:235:HIS:C	1:B:236:PHE:CD2	2.90	0.45
1:B:660:PHE:CD2	1:B:660:PHE:C	2.89	0.45
1:A:263:TYR:N	1:A:264:PRO:CD	2.80	0.45
1:A:390:ALA:O	1:A:391:GLY:C	2.55	0.45
1:B:109:ILE:O	1:B:109:ILE:CG2	2.64	0.45
1:A:109:ILE:O	1:A:109:ILE:CG2	2.64	0.45
1:A:513:ASP:O	1:A:514:GLN:C	2.55	0.45
1:B:751:HIS:O	1:B:753:LEU:N	2.50	0.45
1:B:464:VAL:CG2	1:B:465:VAL:N	2.80	0.45
1:B:237:GLN:O	1:B:239:VAL:N	2.50	0.45
1:B:19:ILE:C	1:B:21:GLU:N	2.69	0.45
1:B:750:ASN:O	1:B:753:LEU:CB	2.64	0.45
1:B:763:ILE:CG2	1:B:791:PHE:CE2	3.00	0.45
1:B:698:SER:OG	1:B:699:PRO:CD	2.64	0.45
1:A:350:CYS:O	1:A:351:LYS:CB	2.64	0.45
1:A:670:ASP:CA	1:A:751:HIS:NE2	2.80	0.45
1:B:655:ARG:CG	1:B:658:PHE:CD1	3.00	0.45
1:A:534:SER:O	1:A:535:SER:O	2.34	0.45
1:B:132:THR:OG1	1:B:163:PRO:CG	2.65	0.45
1:B:265:ILE:C	1:B:267:ARG:N	2.70	0.45
1:A:671:PHE:O	1:A:751:HIS:NE2	2.50	0.45
1:B:667:TRP:CZ3	1:B:724:THR:OG1	2.69	0.45
1:A:683:ASN:ND2	1:A:683:ASN:O	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:725:VAL:O	1:B:725:VAL:CG1	2.65	0.45
1:A:618:ILE:CG2	1:A:619:VAL:N	2.79	0.45
1:A:656:ILE:CA	1:A:658:PHE:CE2	2.99	0.45
1:A:276:ASN:ND2	1:A:669:PHE:CA	2.80	0.45
1:A:652:ILE:CG2	1:A:653:THR:N	2.80	0.45
1:A:195:GLU:O	1:A:197:PHE:N	2.50	0.45
1:A:464:VAL:CG2	1:A:465:VAL:N	2.81	0.44
1:B:825:LEU:C	1:B:827:SER:N	2.71	0.44
1:B:400:PHE:CD1	3:B:1003:ACP:H2	2.52	0.44
1:A:751:HIS:O	1:A:753:LEU:N	2.50	0.44
1:A:464:VAL:CA	1:A:477:TRP:NE1	2.80	0.44
1:B:768:LEU:CD1	1:B:768:LEU:N	2.80	0.44
1:B:412:ILE:CG1	1:B:413:ASP:N	2.80	0.44
1:A:663:ILE:C	1:A:665:LEU:N	2.68	0.44
1:B:727:PHE:O	1:B:728:PHE:CD1	2.70	0.44
1:B:747:ARG:O	1:B:750:ASN:N	2.50	0.44
1:B:683:ASN:O	1:B:683:ASN:ND2	2.51	0.44
1:A:419:HIS:CE1	1:A:464:VAL:CG1	3.01	0.44
1:A:837:PHE:O	1:A:840:ALA:CB	2.65	0.44
1:A:549:ILE:CG2	1:A:550:PRO:N	2.80	0.44
1:A:93:TRP:O	1:A:95:ASP:N	2.51	0.44
1:B:232:GLN:O	1:B:234:GLY:N	2.50	0.44
1:B:671:PHE:O	1:B:751:HIS:NE2	2.51	0.44
1:A:106:ASN:O	1:A:110:SER:CB	2.66	0.44
1:B:534:SER:O	1:B:535:SER:O	2.36	0.44
1:A:292:VAL:CG2	1:A:645:TYR:CZ	3.01	0.44
1:B:108:THR:O	1:B:112:ILE:CB	2.66	0.44
1:A:422:SER:O	1:A:423:LYS:CD	2.65	0.44
1:A:732:HIS:CD2	1:A:735:ASP:OD1	2.70	0.44
1:A:709:ILE:O	1:A:710:PHE:C	2.54	0.44
1:B:618:ILE:CG2	1:B:619:VAL:N	2.79	0.44
1:A:667:TRP:CZ3	1:A:724:THR:OG1	2.71	0.44
1:A:124:LEU:O	1:A:126:ALA:N	2.51	0.44
1:B:27:LYS:O	1:B:28:CYS:C	2.55	0.44
1:B:513:ASP:O	1:B:514:GLN:C	2.56	0.44
1:A:835:ASP:O	1:A:839:PHE:CD1	2.70	0.44
1:B:585:MET:CG	1:B:586:THR:N	2.81	0.44
1:A:232:GLN:O	1:A:234:GLY:N	2.51	0.44
1:B:292:VAL:CG2	1:B:645:TYR:OH	2.66	0.44
1:A:304:LEU:O	1:A:306:GLN:N	2.51	0.44
1:B:390:ALA:O	1:B:391:GLY:C	2.55	0.44
1:B:605:VAL:O	1:B:608:ALA:CB	2.66	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:768:LEU:CD1	1:A:768:LEU:N	2.81	0.44
1:A:709:ILE:O	1:A:712:THR:N	2.51	0.44
1:B:317:ILE:CD1	1:B:317:ILE:N	2.81	0.44
1:B:428:GLN:O	1:B:428:GLN:OE1	2.36	0.44
1:A:330:LYS:NZ	1:A:331:THR:OG1	2.51	0.44
1:A:667:TRP:NE1	1:A:669:PHE:O	2.51	0.43
1:A:837:PHE:O	1:A:838:LYS:C	2.57	0.43
1:A:26:LEU:O	1:A:27:LYS:C	2.56	0.43
1:A:395:VAL:CG2	1:A:410:THR:O	2.67	0.43
1:A:785:ALA:C	1:A:787:LEU:N	2.71	0.43
1:B:799:THR:C	1:B:801:ILE:N	2.71	0.43
1:A:515:LEU:O	1:A:515:LEU:CD1	2.66	0.43
1:A:462:ARG:NH1	1:A:463:GLN:NE2	2.67	0.43
1:A:727:PHE:O	1:A:728:PHE:CD1	2.72	0.43
1:A:108:THR:O	1:A:112:ILE:CB	2.67	0.43
1:B:26:LEU:O	1:B:27:LYS:C	2.56	0.43
1:B:630:SER:O	1:B:633:LEU:N	2.52	0.43
1:B:195:GLU:O	1:B:197:PHE:N	2.50	0.43
1:A:803:VAL:CB	1:A:816:GLY:CA	2.96	0.43
1:B:254:GLY:O	1:B:258:GLU:N	2.51	0.43
1:B:79:MET:SD	1:B:79:MET:N	2.92	0.43
1:B:93:TRP:O	1:B:95:ASP:N	2.52	0.43
1:A:655:ARG:CG	1:A:658:PHE:CD1	3.02	0.43
1:B:709:ILE:O	1:B:712:THR:N	2.52	0.43
1:A:165:ASP:OD1	1:A:212:ILE:O	2.35	0.43
1:B:663:ILE:C	1:B:665:LEU:N	2.69	0.43
1:B:670:ASP:CA	1:B:751:HIS:NE2	2.82	0.43
1:A:769:ILE:O	1:A:770:PHE:CD1	2.72	0.43
1:B:186:LEU:O	1:B:187:PRO:O	2.37	0.43
1:B:106:ASN:O	1:B:110:SER:CB	2.66	0.43
1:A:110:SER:O	1:A:112:ILE:N	2.52	0.43
1:B:674:PHE:O	1:B:678:ILE:CG1	2.66	0.43
1:B:684:ASP:C	1:B:686:THR:N	2.72	0.43
1:A:651:SER:OG	1:A:712:THR:CB	2.66	0.43
1:A:60:LYS:O	1:A:63:GLY:N	2.52	0.43
1:B:825:LEU:O	1:B:829:VAL:CG1	2.67	0.43
1:A:641:ARG:NH2	1:A:694:ARG:CG	2.82	0.43
1:A:265:ILE:C	1:A:267:ARG:N	2.72	0.43
1:B:643:LYS:CE	1:B:701:PRO:O	2.67	0.43
1:A:763:ILE:CG2	1:A:791:PHE:CE2	3.01	0.43
1:B:785:ALA:C	1:B:787:LEU:N	2.73	0.43
1:B:549:ILE:CG2	1:B:550:PRO:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:620:LEU:CD1	1:A:620:LEU:N	2.82	0.43
1:B:419:HIS:ND1	1:B:419:HIS:O	2.52	0.42
1:A:684:ASP:C	1:A:686:THR:N	2.73	0.42
1:B:89:ARG:C	1:B:91:PRO:CD	2.87	0.42
1:A:27:LYS:O	1:A:28:CYS:C	2.57	0.42
1:A:588:ASP:N	1:A:588:ASP:OD1	2.52	0.42
1:A:450:TYR:CD1	1:A:450:TYR:N	2.86	0.42
1:A:284:GLY:O	1:A:653:THR:CG2	2.67	0.42
1:B:409:LEU:CD1	1:B:410:THR:N	2.82	0.42
1:A:347:GLU:O	1:A:347:GLU:CG	2.67	0.42
1:B:553:GLU:O	1:B:554:LEU:C	2.57	0.42
1:A:89:ARG:C	1:A:91:PRO:CD	2.88	0.42
1:B:816:GLY:C	1:B:817:TRP:CD1	2.93	0.42
1:B:61:PHE:C	1:B:63:GLY:N	2.72	0.42
1:B:709:ILE:O	1:B:710:PHE:C	2.58	0.42
1:A:120:ALA:C	1:A:122:ALA:N	2.73	0.42
1:A:825:LEU:C	1:A:827:SER:N	2.73	0.42
1:A:412:ILE:CG1	1:A:413:ASP:N	2.80	0.42
1:A:56:SER:C	1:A:58:LEU:N	2.72	0.42
1:A:431:GLU:C	1:A:433:ALA:N	2.73	0.42
1:A:419:HIS:O	1:A:419:HIS:ND1	2.52	0.42
1:B:160:ASP:O	1:B:161:ILE:C	2.58	0.42
1:A:624:GLY:C	1:A:626:SER:N	2.73	0.42
1:B:588:ASP:OD1	1:B:588:ASP:N	2.53	0.42
1:A:492:ASP:O	1:A:494:ALA:N	2.52	0.42
1:B:832:PHE:N	1:B:833:PRO:CD	2.82	0.42
1:A:61:PHE:C	1:A:63:GLY:N	2.72	0.42
1:B:464:VAL:O	1:B:465:VAL:C	2.58	0.42
1:A:779:PHE:O	1:A:783:PRO:CD	2.68	0.42
1:A:400:PHE:CD1	3:A:1001:ACP:C2	3.02	0.42
1:B:462:ARG:NH1	1:B:463:GLN:NE2	2.68	0.42
1:B:165:ASP:OD1	1:B:212:ILE:O	2.38	0.42
1:B:124:LEU:O	1:B:126:ALA:N	2.53	0.42
1:B:323:MET:CE	1:B:326:LEU:N	2.83	0.42
1:B:667:TRP:CD1	1:B:668:GLU:O	2.73	0.42
1:A:409:LEU:CD1	1:A:410:THR:N	2.83	0.42
1:B:235:HIS:C	1:B:235:HIS:CD2	2.93	0.42
1:B:644:ASN:ND2	1:B:694:ARG:NH2	2.68	0.42
1:A:320:MET:SD	1:A:618:ILE:CD1	3.08	0.42
1:A:650:VAL:O	1:A:653:THR:N	2.52	0.42
1:B:392:ILE:O	1:B:393:ARG:CB	2.68	0.42
1:A:585:MET:CG	1:A:586:THR:N	2.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:803:VAL:CB	1:B:816:GLY:CA	2.98	0.42
1:A:514:GLN:O	1:A:517:ILE:CD1	2.68	0.41
1:B:60:LYS:O	1:B:63:GLY:N	2.53	0.41
1:B:431:GLU:C	1:B:433:ALA:N	2.74	0.41
1:A:235:HIS:C	1:A:235:HIS:CD2	2.93	0.41
1:A:816:GLY:O	1:A:817:TRP:CB	2.68	0.41
1:B:419:HIS:CE1	1:B:464:VAL:CG1	3.02	0.41
1:A:367:ARG:NH2	1:A:370:ASN:CB	2.83	0.41
1:A:304:LEU:O	1:A:307:GLN:N	2.54	0.41
1:B:248:ILE:O	1:B:250:SER:N	2.54	0.41
1:B:438:ASP:CG	1:B:439:LEU:N	2.74	0.41
1:A:159:GLY:O	1:A:611:ALA:N	2.53	0.41
1:A:304:LEU:CD2	1:A:634:THR:CG2	2.97	0.41
1:A:279:VAL:O	1:A:280:LEU:C	2.58	0.41
1:B:462:ARG:CB	1:B:478:GLU:N	2.84	0.41
1:B:837:PHE:O	1:B:840:ALA:CB	2.68	0.41
1:B:491:HIS:CD2	1:B:492:ASP:N	2.88	0.41
1:A:398:LEU:O	1:A:399:PRO:C	2.59	0.41
1:A:635:SER:C	1:A:637:ALA:N	2.74	0.41
1:B:812:ILE:CG2	1:B:812:ILE:O	2.69	0.41
1:B:304:LEU:O	1:B:306:GLN:N	2.53	0.41
1:B:120:ALA:C	1:B:122:ALA:N	2.74	0.41
1:A:400:PHE:CD1	3:A:1001:ACP:H2	2.55	0.41
1:A:60:LYS:CE	1:A:63:GLY:O	2.68	0.41
1:A:606:ALA:C	1:A:608:ALA:N	2.73	0.41
1:A:630:SER:O	1:A:633:LEU:N	2.53	0.41
1:B:816:GLY:O	1:B:817:TRP:CB	2.68	0.41
1:B:565:PHE:O	1:B:566:PRO:C	2.58	0.41
1:B:656:ILE:CA	1:B:658:PHE:CE2	3.03	0.41
1:A:766:GLN:CG	1:A:767:ALA:N	2.84	0.41
1:B:838:LYS:C	1:B:840:ALA:N	2.74	0.41
1:B:204:GLN:N	1:B:204:GLN:NE2	2.69	0.41
1:B:345:LEU:O	1:B:345:LEU:CG	2.68	0.41
1:A:248:ILE:O	1:A:250:SER:N	2.52	0.41
1:B:292:VAL:CG2	1:B:645:TYR:CZ	3.03	0.41
1:B:446:ILE:O	1:B:450:TYR:CD1	2.74	0.41
1:A:462:ARG:CB	1:A:478:GLU:N	2.84	0.41
1:B:110:SER:C	1:B:112:ILE:N	2.74	0.41
1:B:347:GLU:CG	1:B:347:GLU:O	2.69	0.41
1:B:641:ARG:NH2	1:B:694:ARG:CG	2.84	0.41
1:A:644:ASN:CB	1:A:694:ARG:NH1	2.84	0.41
1:B:159:GLY:O	1:B:611:ALA:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:392:ILE:O	1:A:393:ARG:CB	2.69	0.41
1:A:319:GLU:O	1:A:323:MET:N	2.54	0.41
1:A:612:ALA:O	1:A:613:ARG:C	2.59	0.41
1:A:438:ASP:CG	1:A:439:LEU:N	2.74	0.41
1:B:719:TYR:O	1:B:722:ILE:N	2.54	0.41
1:B:804:TYR:CD2	1:B:804:TYR:C	2.95	0.41
1:B:398:LEU:O	1:B:399:PRO:C	2.59	0.41
1:A:674:PHE:O	1:A:678:ILE:CG1	2.68	0.41
1:B:647:ILE:CD1	1:B:705:LYS:CG	2.99	0.41
1:A:807:TRP:CD1	1:A:807:TRP:N	2.89	0.41
1:A:241:THR:O	1:A:245:ASN:N	2.54	0.41
1:A:565:PHE:O	1:A:566:PRO:C	2.59	0.40
1:B:599:ALA:O	1:B:600:ASP:C	2.60	0.40
1:A:295:VAL:CG2	1:A:296:THR:N	2.84	0.40
1:B:601:ILE:N	1:B:601:ILE:CD1	2.84	0.40
1:A:661:MET:O	1:A:665:LEU:CB	2.70	0.40
1:B:395:VAL:CG2	1:B:410:THR:O	2.69	0.40
1:B:434:LYS:O	1:B:436:SER:N	2.54	0.40
1:A:781:GLU:O	1:A:781:GLU:CD	2.59	0.40
1:A:804:TYR:CD2	1:A:804:TYR:C	2.95	0.40
3:A:1001:ACP:H8	3:A:1001:ACP:H2'	1.92	0.40
1:B:279:VAL:O	1:B:280:LEU:C	2.58	0.40
1:B:257:ILE:O	1:B:261:VAL:CG2	2.69	0.40
1:B:90:PRO:N	1:B:91:PRO:CD	2.85	0.40
1:A:648:TYR:CD2	1:A:649:ALA:N	2.90	0.40
1:A:434:LYS:O	1:A:436:SER:N	2.53	0.40
1:B:492:ASP:O	1:B:494:ALA:N	2.54	0.40
1:B:658:PHE:CD2	1:B:659:GLY:N	2.90	0.40
1:A:148:LEU:O	1:A:149:VAL:C	2.59	0.40
1:B:592:ASP:O	1:B:593:ALA:C	2.59	0.40
1:B:650:VAL:O	1:B:653:THR:N	2.55	0.40
1:A:180:ALA:O	1:A:181:LEU:C	2.60	0.40
1:A:475:ALA:CB	1:A:476:PRO:CD	3.00	0.40
1:B:475:ALA:CB	1:B:476:PRO:CD	2.99	0.40
1:A:816:GLY:C	1:A:817:TRP:CD1	2.95	0.40
1:A:317:ILE:CG2	1:A:635:SER:OG	2.69	0.40
1:B:514:GLN:O	1:B:517:ILE:CD1	2.70	0.40
1:A:464:VAL:O	1:A:465:VAL:C	2.59	0.40
1:B:106:ASN:C	1:B:108:THR:N	2.75	0.40
1:A:407:THR:O	1:A:421:VAL:CB	2.69	0.40
1:B:835:ASP:O	1:B:839:PHE:CD1	2.75	0.40
1:B:122:ALA:O	1:B:123:ALA:C	2.60	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:648:TYR:CD2	1:B:649:ALA:N	2.90	0.40
1:B:781:GLU:O	1:B:781:GLU:CD	2.60	0.40
1:A:812:ILE:O	1:A:812:ILE:CG2	2.69	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	831/885 (94%)	454 (55%)	215 (26%)	162 (20%)	0	3
1	B	831/885 (94%)	455 (55%)	222 (27%)	154 (18%)	0	4
All	All	1662/1770 (94%)	909 (55%)	437 (26%)	316 (19%)	0	3

All (316) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	23	PHE
1	A	28	CYS
1	A	48	ASN
1	A	54	LYS
1	A	60	LYS
1	A	65	MET
1	A	84	ALA
1	A	91	PRO
1	A	94	GLN
1	A	130	PRO
1	A	136	ARG
1	A	137	ASP
1	A	168	LEU
1	A	185	SER
1	A	187	PRO
1	A	189	THR

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Mol	Chain	Res	Type
1	A	232	GLN
1	A	235	HIS
1	A	265	ILE
1	A	270	TYR
1	A	305	SER
1	A	323	MET
1	A	351	LYS
1	A	354	GLU
1	A	385	PRO
1	A	415	SER
1	A	425	ALA
1	A	432	LEU
1	A	466	PRO
1	A	473	PRO
1	A	479	PHE
1	A	527	MET
1	A	535	SER
1	A	557	LYS
1	A	619	VAL
1	A	623	PRO
1	A	643	LYS
1	A	656	ILE
1	A	666	ILE
1	A	695	VAL
1	A	698	SER
1	A	701	PRO
1	A	743	VAL
1	A	761	VAL
1	A	773	ARG
1	A	803	VAL
1	A	804	TYR
1	A	812	ILE
1	B	17	ILE
1	B	23	PHE
1	B	28	CYS
1	B	48	ASN
1	B	54	LYS
1	B	60	LYS
1	B	65	MET
1	B	84	ALA
1	B	91	PRO
1	B	94	GLN

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Mol	Chain	Res	Type
1	B	130	PRO
1	B	136	ARG
1	B	137	ASP
1	B	168	LEU
1	B	185	SER
1	B	187	PRO
1	B	189	THR
1	B	232	GLN
1	B	235	HIS
1	B	265	ILE
1	B	270	TYR
1	B	305	SER
1	B	323	MET
1	B	351	LYS
1	B	354	GLU
1	B	385	PRO
1	B	415	SER
1	B	425	ALA
1	B	432	LEU
1	B	466	PRO
1	B	473	PRO
1	B	479	PHE
1	B	527	MET
1	B	535	SER
1	B	557	LYS
1	B	618	ILE
1	B	619	VAL
1	B	623	PRO
1	B	643	LYS
1	B	656	ILE
1	B	666	ILE
1	B	695	VAL
1	B	698	SER
1	B	701	PRO
1	B	743	VAL
1	B	773	ARG
1	B	803	VAL
1	B	804	TYR
1	B	812	ILE
1	B	843	TYR
1	A	20	GLU
1	A	27	LYS

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Mol	Chain	Res	Type
1	A	34	THR
1	A	68	PRO
1	A	109	ILE
1	A	111	PHE
1	A	125	MET
1	A	147	ILE
1	A	148	LEU
1	A	173	PRO
1	A	177	ASP
1	A	196	VAL
1	A	213	ALA
1	A	227	VAL
1	A	233	VAL
1	A	234	GLY
1	A	267	ARG
1	A	287	ILE
1	A	314	MET
1	A	330	LYS
1	A	350	CYS
1	A	366	SER
1	A	383	ALA
1	A	391	GLY
1	A	393	ARG
1	A	403	VAL
1	A	413	ASP
1	A	427	GLU
1	A	435	ALA
1	A	493	SER
1	A	618	ILE
1	A	671	PHE
1	A	697	PRO
1	A	713	GLY
1	A	725	VAL
1	A	779	PHE
1	A	786	LEU
1	A	806	ASN
1	A	813	ARG
1	A	843	TYR
1	B	20	GLU
1	B	27	LYS
1	B	34	THR
1	B	68	PRO

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Mol	Chain	Res	Type
1	B	109	ILE
1	B	111	PHE
1	B	125	MET
1	B	148	LEU
1	B	173	PRO
1	B	177	ASP
1	B	196	VAL
1	B	213	ALA
1	B	227	VAL
1	B	233	VAL
1	B	234	GLY
1	B	267	ARG
1	B	287	ILE
1	B	314	MET
1	B	330	LYS
1	B	350	CYS
1	B	366	SER
1	B	383	ALA
1	B	391	GLY
1	B	393	ARG
1	B	403	VAL
1	B	413	ASP
1	B	427	GLU
1	B	435	ALA
1	B	493	SER
1	B	544	ALA
1	B	671	PHE
1	B	697	PRO
1	B	713	GLY
1	B	725	VAL
1	B	761	VAL
1	B	779	PHE
1	B	786	LEU
1	B	806	ASN
1	B	813	ARG
1	A	16	LYS
1	A	51	GLU
1	A	67	ASN
1	A	131	LYS
1	A	170	GLU
1	A	203	LYS
1	A	218	THR

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Mol	Chain	Res	Type
1	A	224	ALA
1	A	268	ARG
1	A	333	THR
1	A	514	GLN
1	A	544	ALA
1	A	588	ASP
1	A	606	ALA
1	A	674	PHE
1	A	678	ILE
1	A	744	ARG
1	B	16	LYS
1	B	51	GLU
1	B	67	ASN
1	B	147	ILE
1	B	203	LYS
1	B	218	THR
1	B	224	ALA
1	B	268	ARG
1	B	333	THR
1	B	514	GLN
1	B	588	ASP
1	B	606	ALA
1	B	674	PHE
1	B	735	ASP
1	B	744	ARG
1	B	755	GLY
1	A	33	LEU
1	A	122	ALA
1	A	140	TRP
1	A	149	VAL
1	A	162	ILE
1	A	165	ASP
1	A	601	ILE
1	A	722	ILE
1	A	731	ALA
1	A	735	ASP
1	A	746	ILE
1	A	755	GLY
1	A	760	GLN
1	B	33	LEU
1	B	122	ALA
1	B	131	LYS

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Mol	Chain	Res	Type
1	B	149	VAL
1	B	165	ASP
1	B	170	GLU
1	B	192	PRO
1	B	381	MET
1	B	548	SER
1	B	601	ILE
1	B	678	ILE
1	B	688	MET
1	B	722	ILE
1	B	731	ALA
1	B	746	ILE
1	B	815	ILE
1	A	159	GLY
1	A	192	PRO
1	A	238	LYS
1	A	281	LEU
1	A	282	ILE
1	A	381	MET
1	A	398	LEU
1	A	409	LEU
1	A	470	LYS
1	A	548	SER
1	A	688	MET
1	A	692	LYS
1	A	738	SER
1	A	741	PHE
1	A	785	ALA
1	A	815	ILE
1	B	140	TRP
1	B	238	LYS
1	B	281	LEU
1	B	282	ILE
1	B	398	LEU
1	B	409	LEU
1	B	470	LYS
1	B	662	LEU
1	B	738	SER
1	B	741	PHE
1	B	760	GLN
1	B	785	ALA
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	188	VAL
1	A	357	GLN
1	A	399	PRO
1	A	566	PRO
1	A	662	LEU
1	A	663	ILE
1	A	685	GLY
1	A	739	ASP
1	A	751	HIS
1	A	782	ARG
1	B	159	GLY
1	B	162	ILE
1	B	188	VAL
1	B	399	PRO
1	B	566	PRO
1	B	663	ILE
1	B	685	GLY
1	B	751	HIS
1	B	782	ARG
1	A	150	PRO
1	A	215	GLY
1	A	380	GLY
1	A	602	GLY
1	B	150	PRO
1	B	215	GLY
1	B	380	GLY
1	B	475	ALA
1	B	602	GLY
1	A	475	ALA
1	B	526	GLY
1	A	260	ILE
1	A	292	VAL
1	A	526	GLY
1	A	757	VAL
1	B	156	ILE
1	A	154	VAL
1	A	156	ILE
1	A	549	ILE
1	B	154	VAL
1	B	260	ILE
1	B	757	VAL
1	A	81	ILE

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Mol	Chain	Res	Type
1	A	161	ILE
1	A	259	ILE
1	A	310	ILE
1	B	81	ILE
1	B	549	ILE

### 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	685/731 (94%)	496 (72%)	189 (28%)	0	5
1	B	685/731 (94%)	494 (72%)	191 (28%)	0	5
All	All	1370/1462 (94%)	990 (72%)	380 (28%)	0	5

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	24	GLN
1	A	44	ILE
1	A	54	LYS
1	A	55	GLU
1	A	61	PHE
1	A	62	LEU
1	A	66	TRP
1	A	70	SER
1	A	71	TRP
1	A	73	MET
1	A	79	MET
1	A	96	PHE
1	A	101	CYS
1	A	102	LEU
1	A	111	PHE
1	A	112	ILE
1	A	113	GLU
1	A	116	ASN
1	A	125	MET

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Mol	Chain	Res	Type
1	A	128	LEU
1	A	154	VAL
1	A	156	ILE
1	A	160	ASP
1	A	167	ARG
1	A	168	LEU
1	A	170	GLU
1	A	174	LEU
1	A	176	VAL
1	A	178	GLN
1	A	181	LEU
1	A	184	GLU
1	A	189	THR
1	A	190	LYS
1	A	194	GLN
1	A	196	VAL
1	A	201	THR
1	A	202	CYS
1	A	204	GLN
1	A	214	THR
1	A	217	HIS
1	A	218	THR
1	A	230	THR
1	A	232	GLN
1	A	247	CYS
1	A	248	ILE
1	A	253	ILE
1	A	255	MET
1	A	261	VAL
1	A	266	GLN
1	A	296	THR
1	A	301	SER
1	A	302	HIS
1	A	303	ARG
1	A	304	LEU
1	A	305	SER
1	A	312	LYS
1	A	314	MET
1	A	317	ILE
1	A	323	MET
1	A	325	VAL
1	A	331	THR

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Mol	Chain	Res	Type
1	A	339	LEU
1	A	342	ASP
1	A	343	LYS
1	A	344	ASN
1	A	348	VAL
1	A	350	CYS
1	A	351	LYS
1	A	353	VAL
1	A	357	GLN
1	A	367	ARG
1	A	371	GLN
1	A	384	ASP
1	A	389	ARG
1	A	393	ARG
1	A	395	VAL
1	A	398	LEU
1	A	401	ASN
1	A	411	TYR
1	A	412	ILE
1	A	417	ASN
1	A	420	ARG
1	A	421	VAL
1	A	427	GLU
1	A	429	ILE
1	A	443	VAL
1	A	449	LYS
1	A	453	ARG
1	A	456	ARG
1	A	457	SER
1	A	460	VAL
1	A	463	GLN
1	A	469	THR
1	A	478	GLU
1	A	480	VAL
1	A	482	LEU
1	A	492	ASP
1	A	496	THR
1	A	506	ASN
1	A	513	ASP
1	A	514	GLN
1	A	515	LEU
1	A	521	THR

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Mol	Chain	Res	Type
1	A	523	ARG
1	A	535	SER
1	A	538	LEU
1	A	540	THR
1	A	541	HIS
1	A	549	ILE
1	A	551	VAL
1	A	553	GLU
1	A	556	GLU
1	A	559	ASP
1	A	561	PHE
1	A	564	VAL
1	A	567	GLU
1	A	573	VAL
1	A	577	GLN
1	A	586	THR
1	A	591	ASN
1	A	592	ASP
1	A	601	ILE
1	A	603	ILE
1	A	605	VAL
1	A	616	SER
1	A	621	THR
1	A	633	LEU
1	A	634	THR
1	A	638	ILE
1	A	639	PHE
1	A	640	GLN
1	A	641	ARG
1	A	643	LYS
1	A	646	THR
1	A	647	ILE
1	A	648	TYR
1	A	652	ILE
1	A	656	ILE
1	A	657	VAL
1	A	658	PHE
1	A	663	ILE
1	A	667	TRP
1	A	675	MET
1	A	677	LEU
1	A	681	ILE

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Mol	Chain	Res	Type
1	A	682	LEU
1	A	683	ASN
1	A	684	ASP
1	A	695	VAL
1	A	696	LYS
1	A	704	TRP
1	A	705	LYS
1	A	708	GLU
1	A	714	VAL
1	A	724	THR
1	A	729	TRP
1	A	732	HIS
1	A	746	ILE
1	A	757	VAL
1	A	758	TYR
1	A	763	ILE
1	A	768	LEU
1	A	769	ILE
1	A	772	THR
1	A	777	TRP
1	A	781	GLU
1	A	786	LEU
1	A	788	MET
1	A	791	PHE
1	A	793	ILE
1	A	795	GLN
1	A	796	LEU
1	A	803	VAL
1	A	804	TYR
1	A	806	ASN
1	A	807	TRP
1	A	819	TRP
1	A	823	ILE
1	A	825	LEU
1	A	827	SER
1	A	831	TYR
1	A	834	LEU
1	A	835	ASP
1	A	836	VAL
1	A	837	PHE
1	A	838	LYS
1	A	839	PHE

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Mol	Chain	Res	Type
1	A	844	ILE
1	B	15	GLU
1	B	24	GLN
1	B	44	ILE
1	B	54	LYS
1	B	55	GLU
1	B	61	PHE
1	B	62	LEU
1	B	66	TRP
1	B	70	SER
1	B	71	TRP
1	B	73	MET
1	B	79	MET
1	B	96	PHE
1	B	101	CYS
1	B	102	LEU
1	B	111	PHE
1	B	112	ILE
1	B	113	GLU
1	B	116	ASN
1	B	125	MET
1	B	128	LEU
1	B	154	VAL
1	B	156	ILE
1	B	160	ASP
1	B	167	ARG
1	B	168	LEU
1	B	170	GLU
1	B	174	LEU
1	B	176	VAL
1	B	178	GLN
1	B	181	LEU
1	B	184	GLU
1	B	189	THR
1	B	190	LYS
1	B	194	GLN
1	B	196	VAL
1	B	201	THR
1	B	202	CYS
1	B	204	GLN
1	B	214	THR
1	B	217	HIS

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Mol	Chain	Res	Type
1	B	218	THR
1	B	230	THR
1	B	232	GLN
1	B	247	CYS
1	B	248	ILE
1	B	253	ILE
1	B	255	MET
1	B	261	VAL
1	B	266	GLN
1	B	296	THR
1	B	301	SER
1	B	302	HIS
1	B	303	ARG
1	B	304	LEU
1	B	305	SER
1	B	312	LYS
1	B	314	MET
1	B	317	ILE
1	B	323	MET
1	B	325	VAL
1	B	331	THR
1	B	339	LEU
1	B	342	ASP
1	B	343	LYS
1	B	344	ASN
1	B	348	VAL
1	B	350	CYS
1	B	351	LYS
1	B	353	VAL
1	B	357	GLN
1	B	367	ARG
1	B	371	GLN
1	B	384	ASP
1	B	389	ARG
1	B	393	ARG
1	B	395	VAL
1	B	398	LEU
1	B	401	ASN
1	B	411	TYR
1	B	412	ILE
1	B	417	ASN
1	B	420	ARG

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Mol	Chain	Res	Type
1	B	421	VAL
1	B	427	GLU
1	B	429	ILE
1	B	443	VAL
1	B	449	LYS
1	B	453	ARG
1	B	456	ARG
1	B	457	SER
1	B	460	VAL
1	B	463	GLN
1	B	469	THR
1	B	478	GLU
1	B	480	VAL
1	B	482	LEU
1	B	492	ASP
1	B	496	THR
1	B	506	ASN
1	B	513	ASP
1	B	514	GLN
1	B	515	LEU
1	B	521	THR
1	B	523	ARG
1	B	535	SER
1	B	538	LEU
1	B	540	THR
1	B	541	HIS
1	B	549	ILE
1	B	551	VAL
1	B	553	GLU
1	B	556	GLU
1	B	559	ASP
1	B	561	PHE
1	B	564	VAL
1	B	567	GLU
1	B	573	VAL
1	B	577	GLN
1	B	586	THR
1	B	591	ASN
1	B	592	ASP
1	B	601	ILE
1	B	603	ILE
1	B	605	VAL

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Mol	Chain	Res	Type
1	B	616	SER
1	B	621	THR
1	B	633	LEU
1	B	634	THR
1	B	638	ILE
1	B	639	PHE
1	B	640	GLN
1	B	641	ARG
1	B	643	LYS
1	B	646	THR
1	B	647	ILE
1	B	648	TYR
1	B	652	ILE
1	B	656	ILE
1	B	657	VAL
1	B	658	PHE
1	B	663	ILE
1	B	667	TRP
1	B	675	MET
1	B	676	VAL
1	B	677	LEU
1	B	681	ILE
1	B	682	LEU
1	B	683	ASN
1	B	684	ASP
1	B	689	THR
1	B	695	VAL
1	B	696	LYS
1	B	704	TRP
1	B	705	LYS
1	B	708	GLU
1	B	714	VAL
1	B	724	THR
1	B	729	TRP
1	B	732	HIS
1	B	746	ILE
1	B	757	VAL
1	B	758	TYR
1	B	763	ILE
1	B	768	LEU
1	B	769	ILE
1	B	772	THR

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Mol	Chain	Res	Type
1	B	777	TRP
1	B	781	GLU
1	B	786	LEU
1	B	788	MET
1	B	791	PHE
1	B	793	ILE
1	B	795	GLN
1	B	796	LEU
1	B	803	VAL
1	B	804	TYR
1	B	806	ASN
1	B	807	TRP
1	B	819	TRP
1	B	823	ILE
1	B	825	LEU
1	B	827	SER
1	B	831	TYR
1	B	834	LEU
1	B	835	ASP
1	B	836	VAL
1	B	837	PHE
1	B	838	LYS
1	B	839	PHE
1	B	844	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACP	A	1001	-	33,33,33	3.58	13 (39%)	52,52,52	2.80	20 (38%)
3	ACP	B	1003	-	33,33,33	2.76	12 (36%)	52,52,52	3.23	26 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	A	1001	-	-	0/20/38/38	0/1/3/3
3	ACP	B	1003	-	2/2/7/7	0/20/38/38	0/1/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	ACP	PB-C3B	-13.93	1.67	1.79
3	A	1001	ACP	PG-C3B	-9.95	1.71	1.79
3	B	1003	ACP	PB-C3B	-9.80	1.71	1.79
3	B	1003	ACP	PG-C3B	-6.34	1.74	1.79
3	A	1001	ACP	PG-O3G	4.48	1.63	1.54
3	A	1001	ACP	O3'-C3'	-4.25	1.32	1.43
3	A	1001	ACP	PA-O3A	4.06	1.67	1.59
3	B	1003	ACP	C4-N9	-3.87	1.32	1.37
3	B	1003	ACP	PA-O3A	3.83	1.66	1.59
3	B	1003	ACP	PB-O3A	3.51	1.68	1.59
3	A	1001	ACP	C4-N3	3.47	1.40	1.35
3	B	1003	ACP	C3'-C4'	3.22	1.61	1.53
3	A	1001	ACP	PB-O3A	2.97	1.67	1.59
3	A	1001	ACP	C2'-C1'	-2.63	1.49	1.53
3	B	1003	ACP	C8-N9	-2.55	1.32	1.36
3	B	1003	ACP	C2-N3	2.52	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1003	ACP	C2'-C1'	-2.48	1.49	1.53
3	A	1001	ACP	C2-N3	2.40	1.36	1.32
3	B	1003	ACP	PG-O2G	2.40	1.59	1.54
3	B	1003	ACP	O4'-C1'	2.29	1.44	1.41
3	A	1001	ACP	C5-C4	2.19	1.45	1.40
3	A	1001	ACP	PB-O2B	2.04	1.61	1.56
3	A	1001	ACP	C4-N9	-2.03	1.34	1.37
3	B	1003	ACP	C8-N7	2.02	1.38	1.34
3	A	1001	ACP	C8-N9	-2.01	1.33	1.36

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	ACP	C4'-O4'-C1'	-9.42	99.52	109.75
3	B	1003	ACP	O4'-C1'-N9	-8.98	100.08	108.44
3	B	1003	ACP	O4'-C1'-C2'	-6.83	96.30	106.77
3	B	1003	ACP	PA-O3A-PB	6.80	152.16	131.74
3	B	1003	ACP	O1G-PG-C3B	6.26	122.02	110.79
3	A	1001	ACP	C8-N9-C4	6.09	111.55	106.90
3	B	1003	ACP	C8-N9-C4	6.07	111.53	106.90
3	A	1001	ACP	O3'-C3'-C4'	5.75	128.01	111.08
3	B	1003	ACP	C5'-C4'-C3'	5.57	137.52	115.21
3	A	1001	ACP	PA-O3A-PB	5.55	148.43	131.74
3	B	1003	ACP	PB-C3B-PG	-5.28	110.03	117.62
3	B	1003	ACP	O2'-C2'-C3'	-5.09	95.27	111.83
3	A	1001	ACP	O3A-PB-C3B	5.03	122.47	106.62
3	B	1003	ACP	O3A-PB-C3B	4.63	121.22	106.62
3	B	1003	ACP	O4'-C4'-C3'	-4.59	95.86	105.17
3	A	1001	ACP	O4'-C4'-C3'	-4.53	95.99	105.17
3	A	1001	ACP	N3-C4-N9	4.52	133.59	125.43
3	A	1001	ACP	O1G-PG-C3B	4.32	118.54	110.79
3	B	1003	ACP	N6-C6-N1	4.16	127.53	119.36
3	B	1003	ACP	C4'-O4'-C1'	3.80	113.88	109.75
3	B	1003	ACP	O2G-PG-C3B	-3.80	97.19	106.40
3	A	1001	ACP	O3A-PB-O1B	-3.68	103.71	111.51
3	B	1003	ACP	O2B-PB-O3A	-3.65	98.16	107.18
3	A	1001	ACP	O4'-C1'-C2'	-3.50	101.40	106.77
3	B	1003	ACP	O1B-PB-C3B	3.38	117.98	109.49
3	B	1003	ACP	O3G-PG-C3B	3.19	114.13	106.40
3	A	1001	ACP	O3G-PG-O1G	-3.08	104.34	112.56
3	A	1001	ACP	O2B-PB-O3A	-3.04	99.67	107.18
3	A	1001	ACP	C3'-C2'-C1'	3.00	105.60	100.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	ACP	C5-C4-N9	-2.91	102.96	107.16
3	A	1001	ACP	N6-C6-N1	2.86	124.97	119.36
3	A	1001	ACP	N3-C2-N1	2.83	131.07	128.71
3	B	1003	ACP	PA-O5'-C5'	-2.80	101.86	122.03
3	B	1003	ACP	O3'-C3'-C4'	-2.79	102.86	111.08
3	B	1003	ACP	O2B-PB-C3B	-2.72	100.34	106.61
3	A	1001	ACP	O3G-PG-O2G	-2.59	100.14	108.35
3	B	1003	ACP	O5'-PA-O1A	2.50	119.19	109.37
3	B	1003	ACP	O3G-PG-O1G	-2.48	105.95	112.56
3	B	1003	ACP	C3'-C2'-C1'	-2.41	97.14	100.91
3	A	1001	ACP	O4'-C1'-N9	2.32	110.60	108.44
3	A	1001	ACP	O3A-PA-O5'	2.23	113.37	103.41
3	B	1003	ACP	C5-C4-N9	-2.16	104.04	107.16
3	A	1001	ACP	O3'-C3'-C2'	-2.12	104.92	111.83
3	B	1003	ACP	O3G-PG-O2G	-2.08	101.75	108.35
3	B	1003	ACP	O4'-C4'-C5'	2.04	116.64	109.36
3	B	1003	ACP	C5-C6-N6	-2.01	116.16	120.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1003	ACP	C4'
3	B	1003	ACP	C3'

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	833/885 (94%)	0.22	33 (3%)	36 20	69, 163, 264, 365	0
1	B	833/885 (94%)	0.20	34 (4%)	35 20	102, 165, 266, 353	0
All	All	1666/1770 (94%)	0.21	67 (4%)	36 20	69, 164, 266, 365	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	ARG	6.8
1	B	533	PRO	6.2
1	A	195	GLU	5.8
1	B	532	TYR	5.5
1	A	90	PRO	4.6
1	B	534	SER	4.6
1	A	392	ILE	4.5
1	B	226	LEU	4.5
1	A	268	ARG	4.5
1	A	394	GLU	4.2
1	A	50	LEU	3.9
1	B	41	ARG	3.7
1	B	807	TRP	3.7
1	B	171	GLY	3.6
1	A	225	HIS	3.6
1	B	531	MET	3.4
1	A	194	GLN	3.4
1	A	91	PRO	3.3
1	B	225	HIS	3.3
1	B	170	GLU	3.3
1	B	224	ALA	3.2
1	A	533	PRO	3.2
1	A	88	GLY	3.1
1	B	87	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	57	LYS	3.0
1	A	232	GLN	2.9
1	A	28	CYS	2.9
1	B	731	ALA	2.9
1	A	55	GLU	2.7
1	B	169	LEU	2.7
1	B	58	LEU	2.6
1	A	57	LYS	2.5
1	B	523	ARG	2.5
1	B	227	VAL	2.5
1	A	41	ARG	2.4
1	B	144	GLU	2.4
1	A	167	ARG	2.4
1	A	381	MET	2.3
1	A	542	LYS	2.3
1	A	580	LYS	2.3
1	A	54	LYS	2.3
1	B	777	TRP	2.3
1	B	231	ASN	2.3
1	B	92	ASP	2.2
1	A	482	LEU	2.2
1	B	396	HIS	2.2
1	A	92	ASP	2.2
1	A	312	LYS	2.2
1	B	394	GLU	2.2
1	A	534	SER	2.2
1	A	396	HIS	2.2
1	B	195	GLU	2.2
1	B	30	ARG	2.2
1	A	339	LEU	2.1
1	A	403	VAL	2.1
1	B	415	SER	2.1
1	A	16	LYS	2.1
1	B	800	LEU	2.1
1	B	696	LYS	2.1
1	A	578	GLU	2.1
1	A	87	ASP	2.1
1	B	804	TYR	2.1
1	B	18	PRO	2.0
1	B	61	PHE	2.0
1	B	268	ARG	2.0
1	B	542	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	431	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	1004	1/1	0.43	20.82	52,52,52,52	0
2	MG	A	1002	1/1	0.40	6.02	60,60,60,60	0
3	ACP	A	1001	31/31	0.34	1.38	152,152,152,152	0
3	ACP	B	1003	31/31	0.31	0.90	150,150,150,150	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.