



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:32 am GMT

PDB ID : 5CU5  
Title : Crystal structure of ERAP2 without catalytic Zn(II) atom  
Authors : Saridakis, E.; Mathioudakis, N.; Giastas, P.; Mavridis, I.M.; Stratikos, E.  
Deposited on : 2015-07-24  
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

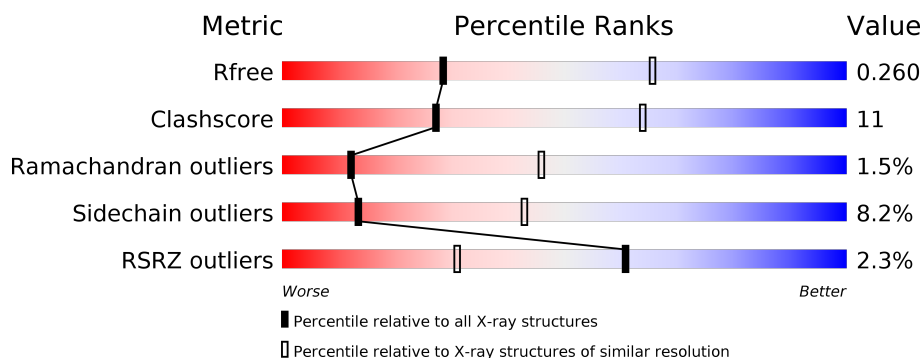
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.02 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))
$R_{free}$	100719	1924 (3.04-3.00)
Clashscore	112137	2279 (3.04-3.00)
Ramachandran outliers	110173	2207 (3.04-3.00)
Sidechain outliers	110143	2210 (3.04-3.00)
RSRZ outliers	101464	1948 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	967	
1	B	967	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14562 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	1	0
			7089	4576	1176	1309	28			
1	B	862	Total	C	N	O	S	0	0	0
			7009	4523	1164	1295	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	conflict	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	2	VAL	PHE	conflict	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



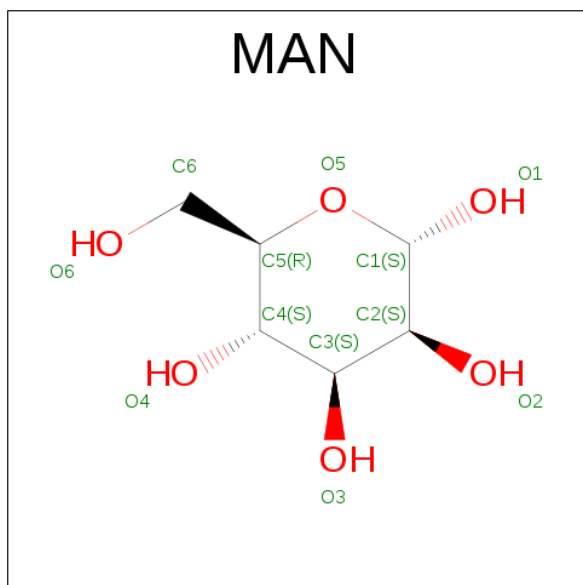
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

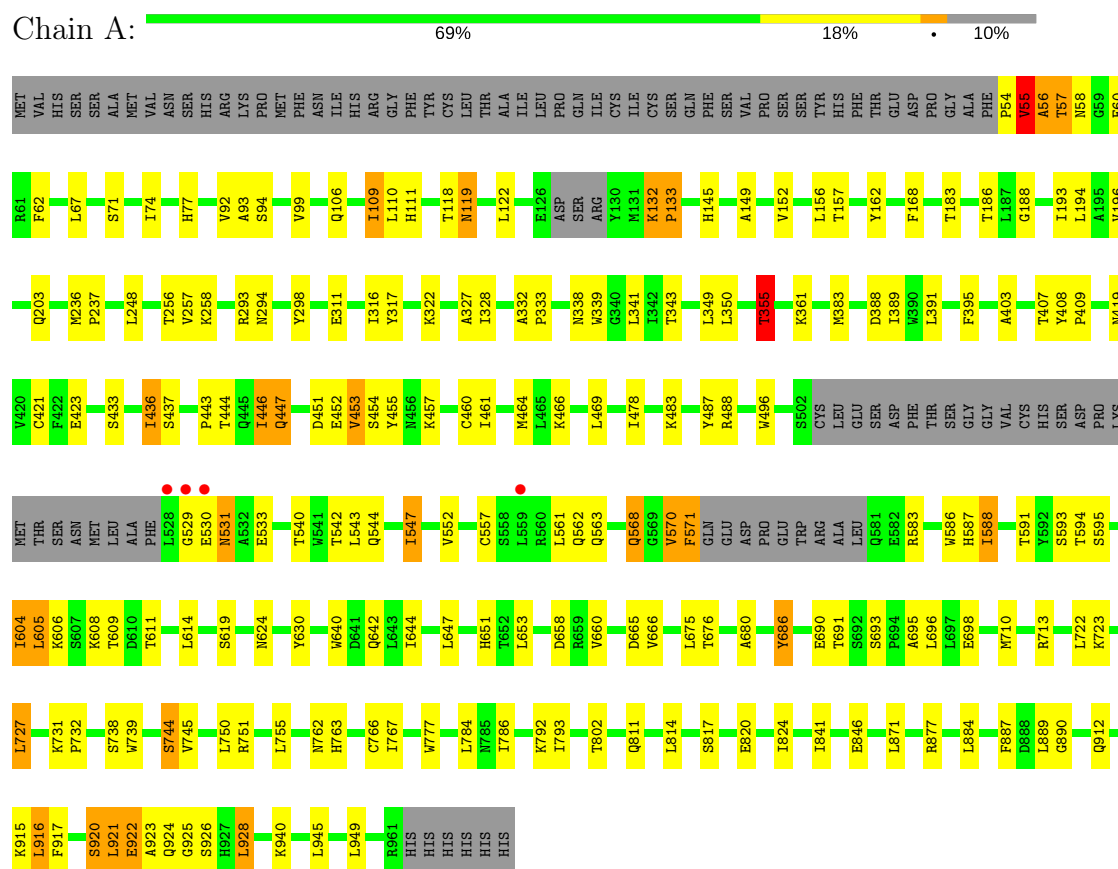
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	84	Total	O	0	0
			84	84		

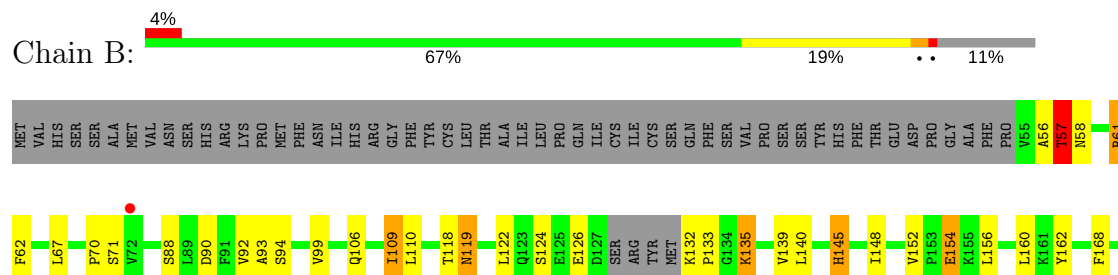
### 3 Residue-property plots [i](#)

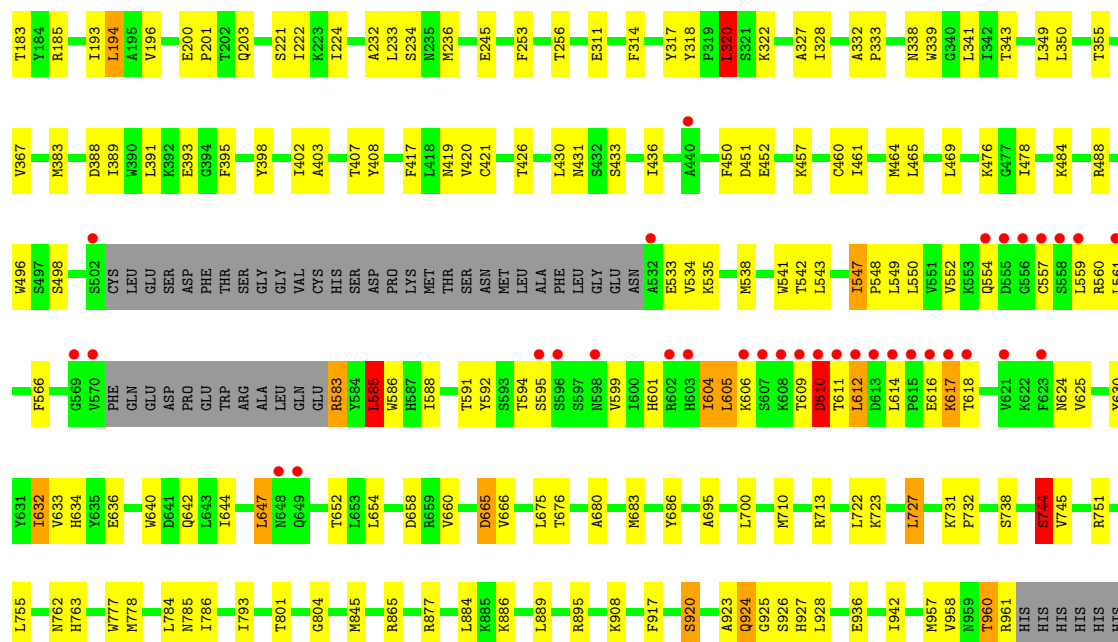
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Endoplasmic reticulum aminopeptidase 2



#### • Molecule 1: Endoplasmic reticulum aminopeptidase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.65Å 135.17Å 126.49Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	48.56 – 3.02 58.32 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.56-3.02) 100.0 (58.32-3.02)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.210 , 0.263 0.210 , 0.260	Depositor DCC
$R_{free}$ test set	2495 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.8	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: NAG, MAN

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	0/7266	0.75	4/9844 (0.0%)
1	B	0.45	0/7179	0.77	9/9726 (0.1%)
All	All	0.46	0/14445	0.76	13/19570 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	320	LEU	CB-CG-CD2	10.64	129.08	111.00
1	B	647	LEU	CA-CB-CG	8.09	133.90	115.30
1	B	665	ASP	CB-CG-OD2	7.33	124.90	118.30
1	B	665	ASP	CB-CG-OD1	-6.45	112.49	118.30
1	B	585	LEU	CA-CB-CG	6.18	129.51	115.30
1	B	647	LEU	CB-CG-CD1	6.17	121.48	111.00
1	A	488	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	585	LEU	CB-CG-CD2	5.53	120.41	111.00
1	B	583	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	665	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	767	ILE	CG1-CB-CG2	-5.26	99.84	111.40
1	B	57	THR	CB-CA-C	5.12	125.42	111.60
1	A	453	VAL	CA-CB-CG1	5.06	118.49	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	530	GLU	Peptide
1	A	531	ASN	Peptide
1	A	56	ALA	Peptide
1	A	921	LEU	Peptide
1	A	922	GLU	Peptide

## 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	7089	0	7041	137	1
1	B	7009	0	6979	183	1
2	A	154	0	139	11	0
2	B	84	0	75	1	0
3	A	11	0	10	0	0
3	B	22	0	19	2	0
4	A	109	0	0	12	0
4	B	84	0	0	38	0
All	All	14562	0	14263	324	1

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 11.

All (324) 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:224:ILE:CD1	1:B:232:ALA:HB1	1.38	1.49
1:B:224:ILE:CD1	1:B:232:ALA:CB	1.96	1.41
1:B:224:ILE:HD12	1:B:232:ALA:CB	1.53	1.37
1:B:610:ASP:O	1:B:611:THR:HG22	1.09	1.22
1:B:611:THR:OG1	1:B:612:LEU:CB	1.91	1.18
1:A:690:GLU:HB3	1:A:696:LEU:HD21	1.19	1.16
1:B:801:THR:HG23	4:B:1101:HOH:O	1.42	1.14
1:B:611:THR:OG1	1:B:612:LEU:HB3	1.41	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:PRO:HG3	1:B:588:ILE:HD11	1.25	1.13
1:B:224:ILE:HD11	1:B:232:ALA:CB	1.73	1.12
1:B:561:LEU:HG	1:B:611:THR:HG21	1.24	1.11
1:A:690:GLU:HB3	1:A:696:LEU:CD2	1.82	1.09
1:B:610:ASP:O	1:B:611:THR:CG2	2.00	1.09
1:B:224:ILE:HD11	1:B:232:ALA:HB3	1.30	1.05
1:A:619:SER:O	1:A:642:GLN:NE2	1.90	1.04
1:A:619:SER:O	1:A:642:GLN:CD	2.01	0.99
1:B:548:PRO:CG	1:B:588:ILE:HD11	1.94	0.98
1:B:314:PHE:HB2	4:B:1109:HOH:O	1.61	0.98
1:B:561:LEU:CG	1:B:611:THR:HG21	1.93	0.97
1:B:224:ILE:HD12	1:B:232:ALA:HB1	1.04	0.96
1:A:570:VAL:HG12	1:A:571:PHE:H	1.32	0.95
1:B:801:THR:O	4:B:1101:HOH:O	1.86	0.92
1:A:294:ASN:H	2:A:1011:NAG:H82	1.35	0.91
1:B:611:THR:OG1	1:B:612:LEU:HB2	1.68	0.91
1:A:690:GLU:CB	1:A:696:LEU:HD21	1.99	0.91
1:B:548:PRO:CG	1:B:588:ILE:CD1	2.49	0.91
1:B:957:MET:O	4:B:1102:HOH:O	1.88	0.90
1:A:606:LYS:HA	4:A:1101:HOH:O	1.72	0.89
1:A:690:GLU:O	1:A:696:LEU:HD11	1.74	0.88
1:B:957:MET:SD	4:B:1105:HOH:O	2.31	0.88
1:B:804:GLY:N	4:B:1101:HOH:O	2.06	0.88
1:B:541:TRP:CZ2	1:B:588:ILE:HG12	2.10	0.85
1:B:636:GLU:HB3	4:B:1119:HOH:O	1.75	0.85
1:B:421:CYS:HG	1:B:460:CYS:HG	0.88	0.84
1:A:605:LEU:HD23	4:A:1101:HOH:O	1.77	0.84
1:A:54:PRO:C	1:A:55:VAL:HG12	1.98	0.83
1:B:804:GLY:CA	4:B:1101:HOH:O	2.28	0.82
1:B:224:ILE:HD12	1:B:232:ALA:HB2	1.61	0.82
1:B:611:THR:HA	1:B:612:LEU:HB2	1.61	0.80
1:B:611:THR:CA	1:B:612:LEU:HB2	2.11	0.79
1:A:55:VAL:HG21	1:A:62:PHE:HB2	1.64	0.79
1:B:612:LEU:O	4:B:1103:HOH:O	2.00	0.78
1:B:465:LEU:HD11	1:B:538:MET:HE1	1.66	0.78
1:B:609:THR:OG1	4:B:1104:HOH:O	2.01	0.78
1:B:224:ILE:HD13	1:B:232:ALA:HB1	1.62	0.77
1:A:454:SER:HB2	4:A:1104:HOH:O	1.84	0.76
1:B:633:VAL:HG12	4:B:1110:HOH:O	1.86	0.75
1:A:56:ALA:HB1	1:A:57:THR:HA	1.68	0.75
1:A:587:HIS:HA	4:A:1101:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:TRP:HB3	1:B:588:ILE:HG13	1.67	0.75
1:A:619:SER:O	1:A:642:GLN:OE1	2.05	0.73
1:B:960:THR:OG1	4:B:1105:HOH:O	2.07	0.73
1:B:465:LEU:HD11	1:B:538:MET:CE	2.19	0.72
1:B:559:LEU:O	1:B:611:THR:HG23	1.88	0.72
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.71	0.72
1:B:957:MET:HA	4:B:1105:HOH:O	1.88	0.72
1:B:561:LEU:HD12	1:B:611:THR:HB	1.70	0.72
1:A:690:GLU:HG3	1:A:696:LEU:HG	1.72	0.71
1:A:388:ASP:HB3	1:A:391:LEU:HD12	1.72	0.71
1:B:611:THR:CB	1:B:612:LEU:HB2	2.19	0.71
1:B:549:LEU:HD13	1:B:632:ILE:HD12	1.72	0.71
1:A:586:TRP:O	4:A:1101:HOH:O	2.07	0.70
1:A:921:LEU:O	1:A:926:SER:N	2.24	0.70
3:B:1001:MAN:O3	3:B:1002:MAN:H5	1.92	0.70
1:A:403:ALA:O	1:A:407:THR:HG23	1.93	0.69
1:A:570:VAL:HG12	1:A:571:PHE:N	2.08	0.68
1:B:548:PRO:HG3	1:B:588:ILE:CD1	2.08	0.68
1:A:55:VAL:HG11	1:A:62:PHE:N	2.08	0.67
1:B:804:GLY:HA3	4:B:1101:HOH:O	1.90	0.66
1:A:55:VAL:HG11	1:A:62:PHE:H	1.61	0.66
1:B:548:PRO:CG	1:B:588:ILE:HD13	2.24	0.66
1:A:563:GLN:NE2	1:A:605:LEU:HD21	2.12	0.65
1:A:466:LYS:NZ	2:A:1006:NAG:H81	2.12	0.65
1:A:436:ILE:HD11	1:A:542:THR:HB	1.78	0.65
1:A:257:VAL:HG11	1:A:487:TYR:CE1	2.32	0.64
1:B:58:ASN:O	4:B:1106:HOH:O	2.15	0.64
1:B:56:ALA:HB3	1:B:61:ARG:HA	1.79	0.64
1:B:548:PRO:HG2	1:B:588:ILE:HD13	1.78	0.64
1:A:443:PRO:HA	1:A:446:ILE:CD1	2.28	0.64
1:B:224:ILE:HG12	1:B:253:PHE:HE2	1.63	0.62
1:A:690:GLU:HB3	1:A:696:LEU:HD23	1.79	0.62
1:A:436:ILE:HD12	1:A:437:SER:N	2.14	0.62
1:B:62:PHE:HB3	4:B:1130:HOH:O	1.98	0.62
1:A:571:PHE:N	1:A:571:PHE:CD1	2.66	0.62
1:B:561:LEU:CB	1:B:611:THR:HG21	2.30	0.61
1:B:586:TRP:CB	1:B:588:ILE:HG13	2.30	0.61
1:A:690:GLU:CB	1:A:696:LEU:CD2	2.66	0.61
1:A:409:PRO:HB3	4:A:1105:HOH:O	2.00	0.60
1:B:958:VAL:C	4:B:1102:HOH:O	2.40	0.60
1:B:610:ASP:C	1:B:611:THR:HG22	2.11	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PRO:C	1:A:55:VAL:CG1	2.67	0.59
1:A:186:THR:HG22	1:A:188:GLY:H	1.67	0.59
1:B:124:SER:OG	1:B:132:LYS:HG2	2.02	0.59
1:B:586:TRP:HB2	1:B:588:ILE:CD1	2.32	0.59
1:B:548:PRO:HG2	1:B:588:ILE:CD1	2.30	0.59
1:B:550:LEU:HD23	4:B:1110:HOH:O	2.02	0.59
1:A:338:ASN:HB2	1:A:341:LEU:O	2.02	0.58
1:A:55:VAL:HG23	1:A:56:ALA:N	2.18	0.58
1:B:407:THR:HG23	1:B:408:TYR:CD2	2.38	0.57
1:B:407:THR:HG23	1:B:408:TYR:HD2	1.69	0.57
1:B:957:MET:CE	4:B:1105:HOH:O	2.52	0.57
1:B:461:ILE:O	1:B:465:LEU:HD13	2.04	0.57
1:B:338:ASN:HB2	1:B:341:LEU:O	2.04	0.57
1:A:294:ASN:CG	2:A:1011:NAG:N2	2.58	0.57
1:B:222:ILE:HD12	1:B:234:SER:OG	2.05	0.56
1:A:119:ASN:OD1	2:A:1012:NAG:N2	2.38	0.56
1:A:332:ALA:HB3	1:A:333:PRO:HD3	1.88	0.56
1:A:588:ILE:HG23	1:A:605:LEU:HD22	1.87	0.56
1:B:660:VAL:HG12	1:B:695:ALA:HA	1.88	0.56
1:B:632:ILE:HG22	1:B:665:ASP:OD1	2.06	0.56
1:B:961:ARG:N	4:B:1102:HOH:O	1.96	0.55
1:A:568:GLN:HG2	1:A:940:LYS:HD2	1.88	0.55
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.88	0.55
1:A:444:THR:HA	1:A:447:GLN:CD	2.27	0.55
1:A:660:VAL:HG12	1:A:695:ALA:HA	1.89	0.55
1:B:57:THR:HG22	1:B:58:ASN:HA	1.89	0.55
1:B:152:VAL:HG21	1:B:156:LEU:CD1	2.36	0.55
1:B:640:TRP:O	1:B:644:ILE:HD12	2.06	0.55
1:A:552:VAL:HG12	1:A:561:LEU:CD2	2.36	0.55
1:B:436:ILE:HD11	1:B:457:LYS:HG2	1.89	0.55
1:B:586:TRP:HB2	1:B:588:ILE:HD11	1.89	0.55
1:A:640:TRP:O	1:A:644:ILE:HD12	2.06	0.55
1:B:431:ASN:OD1	2:B:1007:NAG:O5	2.21	0.54
1:A:294:ASN:N	2:A:1011:NAG:H82	2.16	0.54
1:A:407:THR:HG1	1:A:408:TYR:HD2	1.52	0.54
1:A:594:THR:CG2	1:A:614:LEU:HD11	2.36	0.54
1:B:960:THR:N	4:B:1102:HOH:O	2.41	0.54
1:B:185:ARG:HD3	4:B:1128:HOH:O	2.07	0.54
1:B:332:ALA:HB3	1:B:333:PRO:HD3	1.88	0.54
1:B:194:LEU:HD12	1:B:196:VAL:HG22	1.90	0.54
1:A:55:VAL:HG23	1:A:56:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:CD	1:B:109:ILE:CG2	2.85	0.53
1:B:611:THR:CA	1:B:612:LEU:CB	2.85	0.53
2:A:1011:NAG:H2	4:A:1103:HOH:O	2.08	0.53
1:B:140:LEU:HD22	4:B:1106:HOH:O	2.08	0.53
1:B:388:ASP:HB3	1:B:391:LEU:HD13	1.91	0.53
1:B:594:THR:CG2	1:B:618:THR:HG21	2.39	0.53
1:B:70:PRO:HD3	1:B:109:ILE:HG21	1.91	0.53
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.89	0.53
1:B:70:PRO:CD	1:B:109:ILE:HG21	2.39	0.53
1:B:566:PHE:HB2	1:B:632:ILE:HD11	1.91	0.53
1:A:690:GLU:CG	1:A:696:LEU:HG	2.38	0.53
1:B:561:LEU:HB2	1:B:611:THR:CG2	2.39	0.53
1:B:961:ARG:HB2	4:B:1148:HOH:O	2.07	0.53
1:B:388:ASP:HB3	1:B:391:LEU:CD1	2.39	0.52
1:A:820:GLU:O	1:A:824:ILE:HG13	2.09	0.52
1:B:140:LEU:CD2	4:B:1106:HOH:O	2.58	0.52
1:B:676:THR:HA	4:B:1124:HOH:O	2.10	0.52
1:A:328:ILE:CD1	1:A:343:THR:HG22	2.39	0.52
1:B:552:VAL:HG12	1:B:561:LEU:CD2	2.40	0.52
1:B:328:ILE:CD1	1:B:343:THR:HG22	2.39	0.52
1:A:328:ILE:HD11	1:A:343:THR:HG22	1.92	0.52
1:A:436:ILE:HD11	1:A:542:THR:CB	2.40	0.52
1:A:647:LEU:HD22	1:A:686:TYR:CE2	2.45	0.52
1:A:183:THR:HG22	1:A:193:ILE:HD13	1.91	0.51
1:A:447:GLN:HG3	1:A:890:GLY:O	2.09	0.51
1:B:152:VAL:HG21	1:B:156:LEU:HD12	1.92	0.51
1:B:224:ILE:HG13	1:B:224:ILE:O	2.10	0.51
1:A:118:THR:O	1:A:119:ASN:HB2	2.11	0.51
1:B:328:ILE:HD11	1:B:343:THR:HG22	1.92	0.51
1:A:666:VAL:HG11	1:A:680:ALA:HA	1.93	0.51
1:B:586:TRP:HB3	1:B:588:ILE:CG1	2.40	0.51
1:B:548:PRO:CB	1:B:588:ILE:CD1	2.88	0.51
1:B:183:THR:HG22	1:B:193:ILE:HD13	1.92	0.51
1:B:327:ALA:HB2	1:B:349:LEU:HD23	1.93	0.51
1:B:393:GLU:OE1	4:B:1108:HOH:O	2.19	0.50
1:B:561:LEU:CB	1:B:611:THR:CG2	2.89	0.50
2:A:1011:NAG:H61	4:A:1162:HOH:O	2.11	0.50
1:A:55:VAL:CG2	1:A:62:PHE:HB2	2.38	0.50
1:A:327:ALA:HB2	1:A:349:LEU:HD23	1.93	0.50
1:B:778:MET:HE2	1:B:804:GLY:HA2	1.93	0.50
1:A:738:SER:O	1:A:751:ARG:CD	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:TRP:CZ2	1:A:766:CYS:SG	3.05	0.50
1:B:160:LEU:HA	4:B:1114:HOH:O	2.11	0.50
1:A:152:VAL:HG21	1:A:156:LEU:CD1	2.41	0.50
1:A:457:LYS:HG2	1:A:461:ILE:HD13	1.94	0.49
1:A:739:TRP:HZ2	1:A:766:CYS:SG	2.34	0.49
1:B:430:LEU:HD23	1:B:936:GLU:HB2	1.93	0.49
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.94	0.49
1:A:466:LYS:HZ2	2:A:1006:NAG:H81	1.77	0.49
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.94	0.49
1:B:541:TRP:HZ2	1:B:588:ILE:HG12	1.69	0.49
1:A:55:VAL:CG2	1:A:56:ALA:N	2.74	0.49
1:B:224:ILE:CD1	1:B:232:ALA:HB3	1.95	0.49
1:B:666:VAL:HG11	1:B:680:ALA:HA	1.94	0.49
1:B:738:SER:O	1:B:751:ARG:CD	2.61	0.49
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.94	0.49
1:A:604:ILE:O	1:A:605:LEU:CB	2.60	0.49
1:A:257:VAL:HG12	1:A:258:LYS:N	2.28	0.48
1:B:132:LYS:HD2	1:B:135:LYS:HD3	1.95	0.48
1:A:443:PRO:HA	1:A:446:ILE:HD11	1.93	0.48
1:A:912:GLN:HE21	1:A:916:LEU:HD13	1.78	0.48
1:B:457:LYS:NZ	4:B:1117:HOH:O	2.46	0.48
1:B:484:LYS:O	1:B:488:ARG:NH1	2.47	0.48
1:B:561:LEU:HB2	1:B:611:THR:HG22	1.95	0.48
1:B:604:ILE:O	1:B:605:LEU:CB	2.61	0.48
1:B:561:LEU:CG	1:B:611:THR:CG2	2.81	0.47
1:B:464:MET:CE	1:B:630:TYR:H	2.27	0.47
1:B:311:GLU:HG2	1:B:317:TYR:HA	1.96	0.47
1:A:690:GLU:O	1:A:696:LEU:HD21	2.14	0.47
1:A:727:LEU:HD21	1:A:763:HIS:HB2	1.97	0.47
1:A:570:VAL:CG1	1:A:571:PHE:H	2.13	0.47
1:A:647:LEU:HD23	1:A:651:HIS:HB2	1.96	0.47
1:B:109:ILE:HD13	1:B:148:ILE:O	2.14	0.47
1:B:70:PRO:HD2	1:B:109:ILE:CG2	2.44	0.47
1:A:54:PRO:O	1:A:55:VAL:HG12	2.15	0.47
1:B:430:LEU:HD23	1:B:936:GLU:CB	2.44	0.47
1:A:93:ALA:HB3	1:A:168:PHE:CE1	2.50	0.47
1:B:236:MET:HG2	1:B:256:THR:HG22	1.97	0.47
1:A:464:MET:CE	1:A:630:TYR:H	2.28	0.47
1:B:561:LEU:HD12	1:B:611:THR:CB	2.41	0.47
1:B:640:TRP:CD1	1:B:675:LEU:HD21	2.50	0.47
1:B:126:GLU:HB2	1:B:160:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:LEU:N	1:B:611:THR:CG2	2.78	0.46
1:B:957:MET:HE3	4:B:1105:HOH:O	2.13	0.46
1:B:801:THR:C	4:B:1101:HOH:O	2.44	0.46
1:B:450:PHE:O	1:B:895:ARG:NH2	2.46	0.46
1:B:70:PRO:HD2	1:B:109:ILE:HG22	1.98	0.46
1:B:549:LEU:CD1	1:B:632:ILE:HD12	2.44	0.46
1:A:841:ILE:HD12	1:A:871:LEU:HD21	1.97	0.46
1:A:640:TRP:CD1	1:A:675:LEU:HD11	2.51	0.46
1:A:604:ILE:N	1:A:604:ILE:HD12	2.31	0.46
1:A:723:LYS:O	1:A:727:LEU:HD12	2.16	0.46
1:B:93:ALA:HB3	1:B:168:PHE:CE1	2.51	0.46
1:B:591:THR:O	1:B:624:ASN:N	2.49	0.46
1:B:549:LEU:HD21	4:B:1150:HOH:O	2.15	0.46
1:A:731:LYS:N	1:A:732:PRO:HD2	2.30	0.46
1:A:421:CYS:CB	1:A:460:CYS:HG	2.25	0.45
1:A:496:TRP:CZ2	1:A:542:THR:HG21	2.50	0.45
1:B:604:ILE:HD12	1:B:604:ILE:N	2.31	0.45
1:B:727:LEU:HD21	1:B:763:HIS:HB2	1.97	0.45
1:A:56:ALA:CB	1:A:57:THR:HA	2.42	0.45
1:A:917:PHE:O	1:A:921:LEU:HD13	2.16	0.45
1:B:465:LEU:HD11	1:B:538:MET:SD	2.56	0.45
1:B:88:SER:HG	1:B:90:ASP:CG	2.19	0.45
1:A:236:MET:HG2	1:A:256:THR:HG22	1.97	0.45
1:A:744:SER:OG	1:A:745:VAL:N	2.50	0.45
1:B:57:THR:CB	1:B:58:ASN:HA	2.47	0.45
1:A:257:VAL:HG11	1:A:487:TYR:CD1	2.51	0.45
1:A:846:GLU:OE1	4:A:1102:HOH:O	2.21	0.45
1:A:293:ARG:NH2	3:B:1001:MAN:O2	2.50	0.45
1:A:496:TRP:HZ2	1:A:542:THR:HG21	1.82	0.45
1:B:461:ILE:O	1:B:465:LEU:CD1	2.65	0.45
1:B:723:LYS:O	1:B:727:LEU:HD12	2.17	0.45
1:A:152:VAL:HG21	1:A:156:LEU:HD12	1.98	0.45
1:A:453:VAL:C	1:A:455:TYR:H	2.20	0.45
1:B:118:THR:O	1:B:119:ASN:HB2	2.17	0.45
1:B:731:LYS:N	1:B:732:PRO:HD2	2.30	0.45
1:A:591:THR:O	1:A:624:ASN:N	2.50	0.45
1:B:845:MET:O	1:B:886:LYS:HE3	2.17	0.44
1:A:884:LEU:HD12	1:A:887:PHE:O	2.18	0.44
1:B:744:SER:OG	1:B:745:VAL:N	2.50	0.44
1:B:647:LEU:CD2	1:B:683:MET:CG	2.96	0.44
1:B:960:THR:CB	4:B:1105:HOH:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:THR:OG1	1:A:408:TYR:CD2	2.66	0.44
1:A:298:TYR:CZ	1:A:361:LYS:HD2	2.53	0.44
1:A:183:THR:CG2	1:A:193:ILE:HD13	2.47	0.44
1:A:922:GLU:HA	1:A:926:SER:HB2	2.00	0.44
1:A:57:THR:OG1	1:A:58:ASN:N	2.47	0.43
1:A:710:MET:O	1:A:713:ARG:O	2.37	0.43
1:A:132:LYS:HB2	1:A:133:PRO:CD	2.48	0.43
1:B:594:THR:HG21	1:B:618:THR:HG21	2.00	0.43
1:A:444:THR:O	1:A:447:GLN:HG2	2.18	0.43
1:B:398:TYR:CE1	1:B:402:ILE:HG13	2.54	0.43
1:B:865:ARG:HG2	1:B:865:ARG:HH11	1.83	0.43
1:A:111:HIS:HE1	4:A:1111:HOH:O	2.02	0.43
1:A:540:THR:OG1	1:A:544:GLN:NE2	2.51	0.43
1:A:691:THR:HA	1:A:696:LEU:HD11	1.99	0.43
1:B:403:ALA:O	1:B:407:THR:HG22	2.19	0.43
1:A:355:THR:HG21	1:A:817:SER:CB	2.48	0.43
1:B:710:MET:O	1:B:713:ARG:O	2.36	0.43
1:A:562:GLN:HG3	1:A:609:THR:HG22	2.00	0.43
1:B:183:THR:CG2	1:B:193:ILE:HD13	2.49	0.43
1:B:496:TRP:HZ2	1:B:542:THR:HG21	1.82	0.43
1:B:62:PHE:CZ	1:B:109:ILE:HD11	2.53	0.42
1:B:654:LEU:HA	4:B:1127:HOH:O	2.19	0.42
1:B:865:ARG:HG2	1:B:865:ARG:NH1	2.34	0.42
1:B:908:LYS:HE3	1:B:942:ILE:HG21	2.01	0.42
1:B:417:PHE:O	1:B:420:VAL:HG22	2.18	0.42
1:B:594:THR:HG23	1:B:618:THR:HG21	2.01	0.42
1:B:634:HIS:CE1	1:B:675:LEU:HD11	2.55	0.42
1:A:889:LEU:C	1:A:889:LEU:HD12	2.40	0.42
1:A:608:LYS:NZ	4:A:1106:HOH:O	2.43	0.42
1:A:547:ILE:HD12	1:A:630:TYR:CE2	2.54	0.42
1:A:563:GLN:HE22	1:A:605:LEU:HD21	1.84	0.42
1:B:154:GLU:HG3	1:B:154:GLU:O	2.20	0.42
1:B:599:VAL:CG2	1:B:601:HIS:NE2	2.83	0.42
1:B:755:LEU:HB3	1:B:793:ILE:HD13	2.00	0.42
1:B:221:SER:HA	4:B:1129:HOH:O	2.19	0.42
1:B:421:CYS:HG	1:B:460:CYS:CB	2.31	0.42
1:B:547:ILE:HD12	1:B:630:TYR:CE2	2.54	0.42
1:B:586:TRP:CB	1:B:588:ILE:HD11	2.49	0.42
1:B:923:ALA:O	1:B:924:GLN:HG2	2.20	0.42
1:B:958:VAL:O	4:B:1102:HOH:O	2.22	0.42
1:A:738:SER:O	1:A:751:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:N	1:B:320:LEU:HD13	2.34	0.42
1:A:945:LEU:HD22	1:A:949:LEU:HD22	2.02	0.41
1:B:318:TYR:OH	1:B:320:LEU:HD22	2.20	0.41
1:B:592:TYR:CZ	1:B:601:HIS:HB2	2.56	0.41
1:A:109:ILE:HD11	1:A:149:ALA:HB2	2.03	0.41
1:A:690:GLU:C	1:A:696:LEU:HD11	2.39	0.41
1:A:74:ILE:HD12	1:A:74:ILE:N	2.35	0.41
1:B:889:LEU:C	1:B:889:LEU:HD12	2.41	0.41
1:B:550:LEU:HB3	4:B:1110:HOH:O	2.19	0.41
1:B:616:GLU:HG3	1:B:617:LYS:O	2.21	0.41
1:A:316:ILE:HD11	1:A:483:LYS:HG3	2.03	0.41
1:B:543:LEU:O	1:B:543:LEU:HD23	2.21	0.41
1:A:248:LEU:HD22	2:A:1001:NAG:H83	2.02	0.41
1:A:443:PRO:O	1:A:447:GLN:NE2	2.54	0.41
1:A:755:LEU:HB3	1:A:793:ILE:HD13	2.02	0.41
1:B:106:GLN:O	1:B:152:VAL:HG22	2.20	0.41
1:B:57:THR:CG2	1:B:58:ASN:HA	2.50	0.41
1:A:605:LEU:C	1:A:605:LEU:HD23	2.41	0.41
1:B:145:HIS:CD2	4:B:1111:HOH:O	2.73	0.41
1:A:106:GLN:O	1:A:152:VAL:HG22	2.20	0.41
1:A:890:GLY:HA3	1:A:928:LEU:HD21	2.02	0.41
1:B:200:GLU:HA	1:B:201:PRO:HA	1.91	0.41
2:A:1011:NAG:O7	4:A:1103:HOH:O	2.22	0.40
1:A:77:HIS:HD2	2:A:1004:NAG:H82	1.85	0.40
1:B:738:SER:O	1:B:751:ARG:HD2	2.21	0.40
1:B:877:ARG:HA	1:B:917:PHE:CE1	2.57	0.40
1:A:693:SER:OG	1:A:750:LEU:HD22	2.21	0.40
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.57	0.40
1:A:690:GLU:CG	1:A:696:LEU:CD2	3.00	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ASN:ND2	1:B:585:LEU:CD1[1_554]	1.90	0.30

## 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	864/967 (89%)	793 (92%)	57 (7%)	14 (2%)	11	44
1	B	854/967 (88%)	787 (92%)	55 (6%)	12 (1%)	13	47
All	All	1718/1934 (89%)	1580 (92%)	112 (6%)	26 (2%)	12	46

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	605	LEU
1	B	119	ASN
1	B	605	LEU
1	A	583	ARG
1	A	604	ILE
1	A	923	ALA
1	B	133	PRO
1	B	604	ILE
1	B	612	LEU
1	B	925	GLY
1	B	926	SER
1	A	451	ASP
1	B	451	ASP
1	A	57	THR
1	A	355	THR
1	A	920	SER
1	A	925	GLY
1	A	529	GLY
1	B	355	THR
1	B	610	ASP
1	B	744	SER
1	B	920	SER
1	A	133	PRO
1	A	570	VAL

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Mol	Chain	Res	Type
1	A	55	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	782/870 (90%)	721 (92%)	61 (8%)	15	45
1	B	774/870 (89%)	708 (92%)	66 (8%)	12	41
All	All	1556/1740 (89%)	1429 (92%)	127 (8%)	13	43

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	60	GLU
1	A	67	LEU
1	A	71	SER
1	A	92	VAL
1	A	94	SER
1	A	99	VAL
1	A	109	ILE
1	A	110	LEU
1	A	132	LYS
1	A	145	HIS
1	A	157	THR
1	A	194	LEU
1	A	196	VAL
1	A	203	GLN
1	A	237	PRO
1	A	322	LYS
1	A	339	TRP
1	A	350	LEU
1	A	355	THR
1	A	383	MET
1	A	389	ILE

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Mol	Chain	Res	Type
1	A	395	PHE
1	A	419	ASN
1	A	423	GLU
1	A	433	SER
1	A	436	ILE
1	A	446	ILE
1	A	447	GLN
1	A	452	GLU
1	A	469	LEU
1	A	478	ILE
1	A	533	GLU
1	A	543	LEU
1	A	547	ILE
1	A	557	CYS
1	A	568	GLN
1	A	571	PHE
1	A	588	ILE
1	A	593	SER
1	A	595	SER
1	A	611	THR
1	A	653	LEU
1	A	658	ASP
1	A	676	THR
1	A	686	TYR
1	A	698	GLU
1	A	722	LEU
1	A	727	LEU
1	A	744	SER
1	A	762	ASN
1	A	784	LEU
1	A	792	LYS
1	A	802	THR
1	A	811	GLN
1	A	814	LEU
1	A	915	LYS
1	A	916	LEU
1	A	920	SER
1	A	924	GLN
1	A	928	LEU
1	B	57	THR
1	B	61	ARG
1	B	67	LEU

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Mol	Chain	Res	Type
1	B	71	SER
1	B	92	VAL
1	B	94	SER
1	B	99	VAL
1	B	109	ILE
1	B	110	LEU
1	B	135	LYS
1	B	139	VAL
1	B	145	HIS
1	B	154	GLU
1	B	194	LEU
1	B	203	GLN
1	B	233	LEU
1	B	245	GLU
1	B	320	LEU
1	B	322	LYS
1	B	339	TRP
1	B	350	LEU
1	B	367	VAL
1	B	383	MET
1	B	389	ILE
1	B	395	PHE
1	B	419	ASN
1	B	426	THR
1	B	433	SER
1	B	452	GLU
1	B	469	LEU
1	B	476	LYS
1	B	478	ILE
1	B	498	SER
1	B	533	GLU
1	B	534	VAL
1	B	535	LYS
1	B	547	ILE
1	B	554	GLN
1	B	557	CYS
1	B	560	ARG
1	B	583	ARG
1	B	585	LEU
1	B	595	SER
1	B	606	LYS
1	B	610	ASP

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Mol	Chain	Res	Type
1	B	614	LEU
1	B	617	LYS
1	B	625	VAL
1	B	632	ILE
1	B	642	GLN
1	B	652	THR
1	B	658	ASP
1	B	686	TYR
1	B	700	LEU
1	B	722	LEU
1	B	727	LEU
1	B	744	SER
1	B	762	ASN
1	B	784	LEU
1	B	785	ASN
1	B	884	LEU
1	B	920	SER
1	B	924	GLN
1	B	927	HIS
1	B	928	LEU
1	B	960	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	544	GLN
1	A	601	HIS
1	A	912	GLN
1	B	119	ASN
1	B	301	GLN
1	B	456	ASN
1	B	501	ASN
1	B	785	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

20 ligands are 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	NAG	A	1001	1,2	14,14,15	0.61	0	15,19,21	1.78	3 (20%)
2	NAG	A	1002	3,2	14,14,15	0.69	0	15,19,21	1.75	4 (26%)
3	MAN	A	1003	2	11,11,12	0.50	0	13,15,17	1.74	3 (23%)
2	NAG	A	1004	1,2	14,14,15	0.57	0	15,19,21	1.15	1 (6%)
2	NAG	A	1005	2	14,14,15	0.54	0	15,19,21	1.22	1 (6%)
2	NAG	A	1006	1	14,14,15	0.44	0	15,19,21	1.72	4 (26%)
2	NAG	A	1007	1	14,14,15	0.58	0	15,19,21	0.66	0
2	NAG	A	1008	1	14,14,15	0.57	0	15,19,21	2.05	4 (26%)
2	NAG	A	1009	1	14,14,15	0.67	0	15,19,21	0.96	1 (6%)
2	NAG	A	1010	1	14,14,15	0.84	1 (7%)	15,19,21	2.36	2 (13%)
2	NAG	A	1011	1	14,14,15	0.72	0	15,19,21	0.72	0
2	NAG	A	1012	1	14,14,15	0.88	0	15,19,21	0.49	0
3	MAN	B	1001	3,2	11,11,12	0.64	0	13,15,17	1.75	3 (23%)
3	MAN	B	1002	3	11,11,12	0.53	0	13,15,17	2.43	4 (30%)
2	NAG	B	1003	1,2	14,14,15	0.71	0	15,19,21	2.20	3 (20%)
2	NAG	B	1004	3,2	14,14,15	0.53	0	15,19,21	2.03	5 (33%)
2	NAG	B	1005	1,2	14,14,15	0.57	0	15,19,21	1.11	1 (6%)
2	NAG	B	1006	2	14,14,15	0.65	0	15,19,21	1.42	3 (20%)
2	NAG	B	1007	1	14,14,15	0.80	0	15,19,21	1.14	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	1008	1	14,14,15	0.59	0	15,19,21	1.14	1 (6%)

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	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	3,2	-	0/6/23/26	0/1/1/1
3	MAN	A	1003	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1004	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
3	MAN	B	1001	3,2	-	0/2/19/22	0/1/1/1
3	MAN	B	1002	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1003	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1005	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1006	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1008	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1010	NAG	C1-C2	2.44	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	NAG	O5-C1-C2	-3.73	106.28	111.47
2	B	1004	NAG	C2-N2-C7	-3.53	117.80	122.94
2	A	1008	NAG	C4-C3-C2	-3.07	106.52	111.02
2	B	1004	NAG	C4-C3-C2	-2.98	106.65	111.02
2	B	1003	NAG	O5-C1-C2	-2.83	107.54	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	MAN	C2-C3-C4	-2.52	106.49	110.88
2	A	1001	NAG	C3-C4-C5	-2.51	105.79	110.22
2	A	1002	NAG	C2-N2-C7	-2.50	119.29	122.94
2	B	1003	NAG	C3-C4-C5	-2.48	105.85	110.22
3	A	1003	MAN	C6-C5-C4	-2.38	107.43	113.00
3	B	1001	MAN	O3-C3-C2	-2.35	105.75	110.02
2	A	1008	NAG	C2-N2-C7	-2.34	119.53	122.94
2	B	1006	NAG	C2-N2-C7	-2.26	119.65	122.94
2	A	1001	NAG	O5-C1-C2	-2.22	108.38	111.47
2	A	1002	NAG	C6-C5-C4	-2.20	107.85	113.00
2	A	1006	NAG	O5-C1-C2	-2.18	108.44	111.47
2	A	1006	NAG	C4-C3-C2	-2.06	108.00	111.02
2	B	1007	NAG	C3-C4-C5	-2.06	106.59	110.22
2	A	1006	NAG	C6-C5-C4	-2.05	108.21	113.00
2	B	1004	NAG	C1-C2-N2	2.23	114.29	110.49
2	A	1009	NAG	C1-O5-C5	2.28	115.31	112.17
2	B	1008	NAG	C1-O5-C5	2.29	115.32	112.17
2	A	1004	NAG	C4-C3-C2	2.53	114.72	111.02
2	B	1006	NAG	O5-C1-C2	2.77	115.33	111.47
3	B	1002	MAN	O5-C1-C2	2.97	115.45	110.79
3	A	1003	MAN	C1-C2-C3	3.00	113.46	109.65
2	B	1004	NAG	O4-C4-C3	3.04	116.96	110.36
2	A	1005	NAG	C1-O5-C5	3.07	116.40	112.17
3	B	1002	MAN	C1-C2-C3	3.19	113.69	109.65
2	B	1005	NAG	C1-O5-C5	3.22	116.60	112.17
3	B	1001	MAN	O4-C4-C3	3.24	117.42	110.36
2	A	1008	NAG	O5-C1-C2	3.41	116.22	111.47
2	A	1010	NAG	O5-C1-C2	3.43	116.24	111.47
2	B	1006	NAG	C1-O5-C5	3.53	117.03	112.17
3	B	1001	MAN	C1-C2-C3	3.69	114.33	109.65
2	A	1002	NAG	C1-O5-C5	3.74	117.32	112.17
2	B	1004	NAG	C1-O5-C5	4.04	117.73	112.17
3	A	1003	MAN	C1-O5-C5	4.08	117.79	112.17
2	A	1006	NAG	C1-O5-C5	4.73	118.69	112.17
2	A	1001	NAG	C1-O5-C5	5.00	119.05	112.17
2	A	1008	NAG	C1-O5-C5	5.57	119.84	112.17
2	B	1003	NAG	C1-O5-C5	6.86	121.63	112.17
3	B	1002	MAN	C1-O5-C5	6.92	121.71	112.17
2	A	1010	NAG	C1-O5-C5	7.59	122.63	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	1	0
2	A	1004	NAG	1	0
2	A	1006	NAG	2	0
2	A	1011	NAG	6	0
2	A	1012	NAG	1	0
3	B	1001	MAN	2	0
3	B	1002	MAN	1	0
2	B	1007	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	871/967 (90%)	-0.28	4 (0%)	90 73	33, 69, 108, 146	0
1	B	862/967 (89%)	-0.02	35 (4%)	38 16	20, 78, 116, 135	0
All	All	1733/1934 (89%)	-0.15	39 (2%)	61 31	20, 73, 113, 146	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	610	ASP	7.8
1	B	611	THR	6.7
1	B	615	PRO	6.5
1	B	612	LEU	5.2
1	B	617	LYS	5.0
1	B	558	SER	4.8
1	A	528	LEU	4.8
1	B	554	GLN	4.1
1	B	614	LEU	3.9
1	B	613	ASP	3.9
1	B	559	LEU	3.8
1	B	557	CYS	3.6
1	B	621	VAL	3.4
1	A	530	GLU	3.4
1	B	532	ALA	3.3
1	A	529	GLY	3.3
1	B	598	ASN	3.3
1	B	596	SER	3.2
1	B	609	THR	3.1
1	B	648	ASN	3.1
1	B	556	GLY	3.0
1	B	606	LYS	3.0
1	B	616	GLU	3.0
1	B	649	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	570	VAL	2.9
1	B	618	THR	2.8
1	B	569	GLY	2.7
1	B	555	ASP	2.6
1	A	559	LEU	2.5
1	B	607	SER	2.5
1	B	440	ALA	2.4
1	B	561	LEU	2.4
1	B	603	HIS	2.3
1	B	595	SER	2.3
1	B	608	LYS	2.3
1	B	72	VAL	2.2
1	B	623	PHE	2.2
1	B	602	ARG	2.0
1	B	502	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	1001	14/15	0.96	0.17	0.21	40,70,99,123	0
2	NAG	B	1005	14/15	0.90	0.17	0.16	55,102,112,134	0
2	NAG	B	1003	14/15	0.92	0.19	-0.18	26,88,112,113	0
2	NAG	A	1006	14/15	0.90	0.19	-0.34	84,132,146,148	0
2	NAG	A	1004	14/15	0.95	0.18	-0.53	46,67,83,93	0
2	NAG	A	1002	14/15	0.94	0.15	-	69,100,122,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	1008	14/15	0.84	0.21	-	72,135,184,187	0
2	NAG	B	1007	14/15	0.76	0.25	-	125,162,193,205	0
2	NAG	B	1006	14/15	0.85	0.21	-	89,120,146,147	0
2	NAG	A	1008	14/15	0.73	0.26	-	109,152,178,178	0
2	NAG	A	1007	14/15	0.84	0.19	-	80,133,164,185	0
2	NAG	A	1011	14/15	0.85	0.25	-	114,133,166,168	0
2	NAG	A	1005	14/15	0.91	0.17	-	46,103,145,150	0
3	MAN	B	1001	11/12	0.78	0.13	-	100,151,166,167	0
2	NAG	B	1004	14/15	0.92	0.17	-	99,122,163,191	0
2	NAG	A	1009	14/15	0.49	0.26	-	92,170,183,186	0
3	MAN	B	1002	11/12	0.84	0.31	-	106,144,168,193	0
2	NAG	A	1010	14/15	0.86	0.16	-	103,153,172,186	0
2	NAG	A	1012	14/15	0.81	0.27	-	109,156,196,208	0
3	MAN	A	1003	11/12	0.77	0.18	-	81,145,174,188	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.