



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:52 PM BST

PDB ID : 3GXM  
Title : Crystal structure of acid-beta-glucosidase at pH 4.5, phosphate crystallization condition  
Authors : Lieberman, R.L.  
Deposited on : 2009-04-02  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

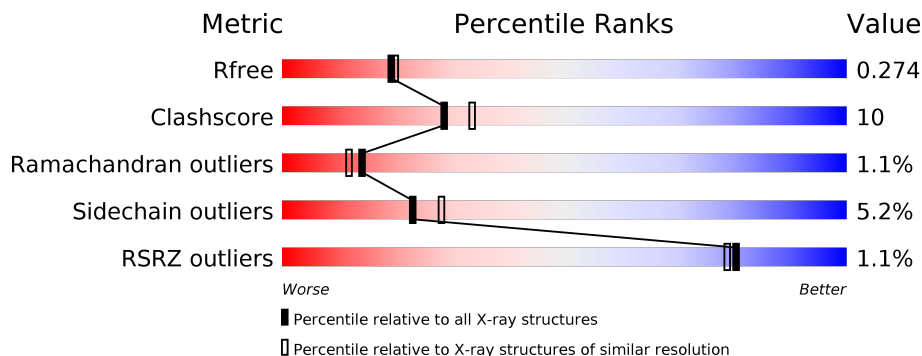
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	
1	B	497	
1	C	497	
1	D	497	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	498	X	-	-	-
3	SO4	A	506	-	-	X	-
3	SO4	B	503	-	-	X	-
3	SO4	C	504	-	-	X	-
3	SO4	D	502	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17060 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3930	2532	671	711	16	0	0	0
1	B	497	3930	2532	671	711	16	0	0	0
1	C	497	3930	2532	671	711	16	0	0	0
1	D	497	3930	2532	671	711	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

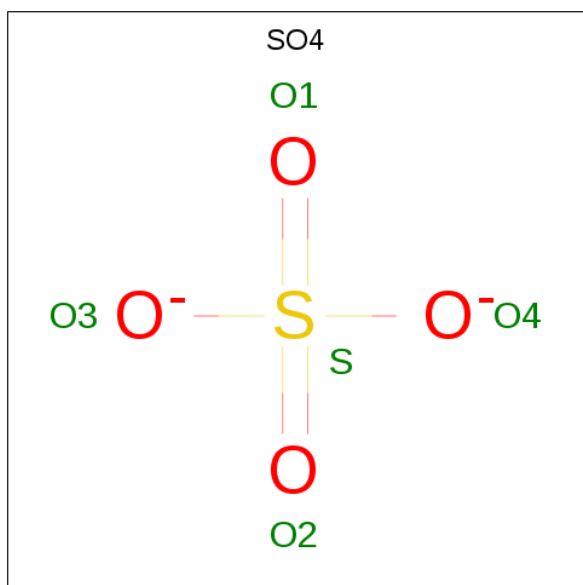
Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	variant	UNP P04062
B	495	HIS	ARG	variant	UNP P04062
C	495	HIS	ARG	variant	UNP P04062
D	495	HIS	ARG	variant	UNP P04062

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

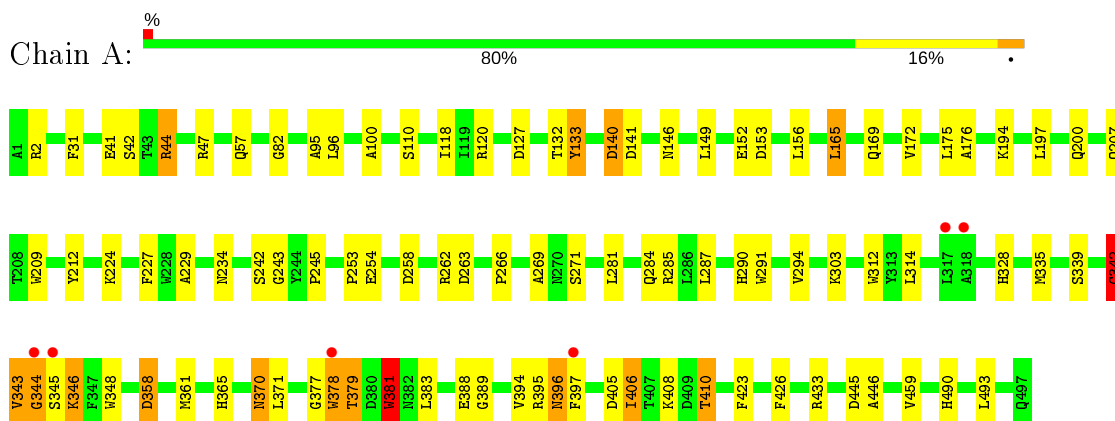
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	288	Total 288	O 288	0	0
4	B	272	Total 272	O 272	0	0
4	C	290	Total 290	O 290	0	0
4	D	294	Total 294	O 294	0	0

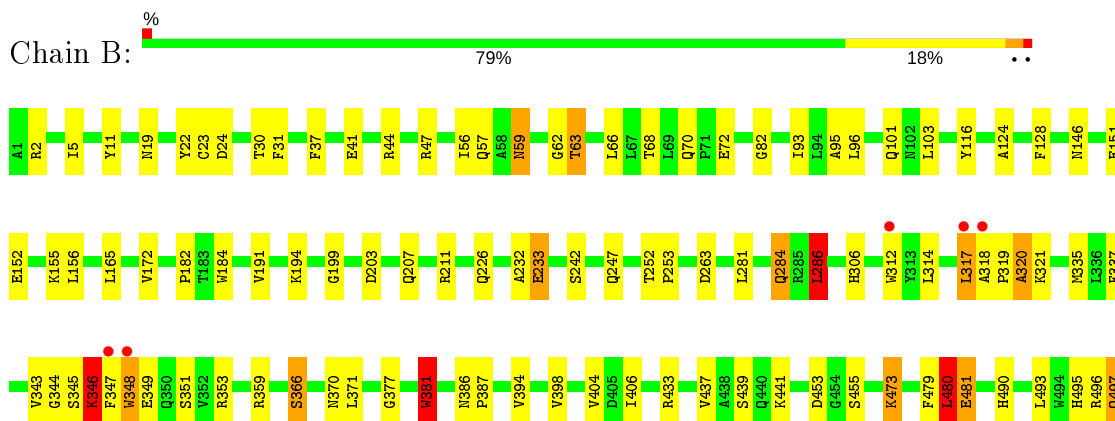
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

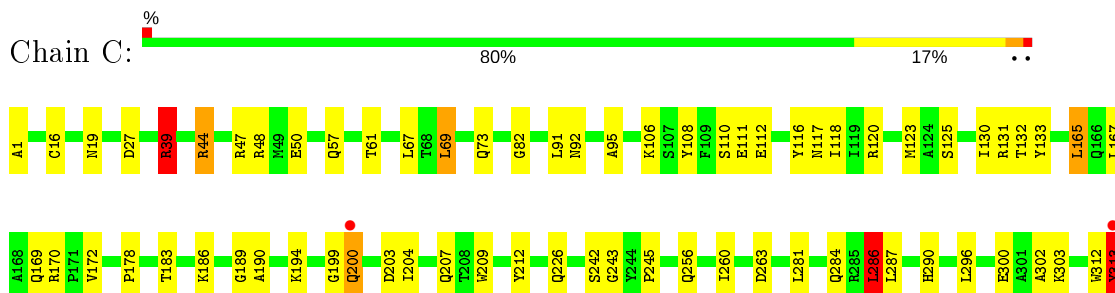
- Molecule 1: Glucosylceramidase



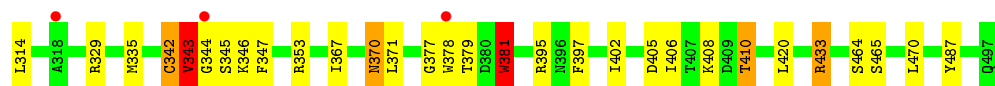
- Molecule 1: Glucosylceramidase



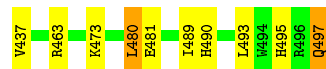
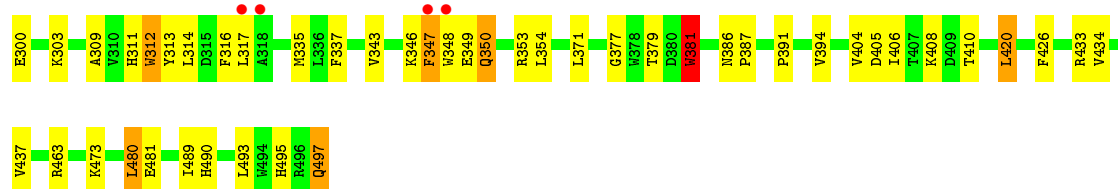
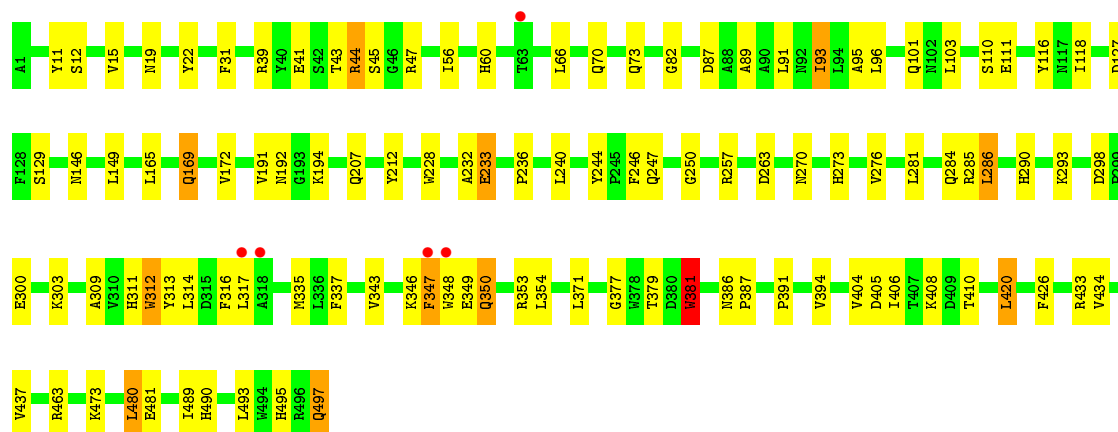
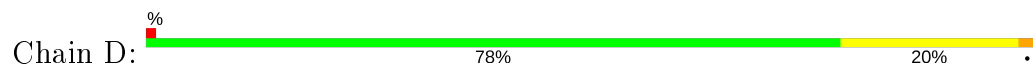
- Molecule 1: Glucosylceramidase







- Molecule 1: Glucosylceramidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.50 Å 91.78 Å 152.75 Å 90.00° 111.24° 90.00°	Depositor
Resolution (Å)	34.34 – 2.20 34.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (34.34-2.20) 96.1 (34.33-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.20 Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.220 , 0.276 0.220 , 0.274	Depositor DCC
$R_{free}$ test set	6970 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtrriage
Anisotropy	0.296	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 12.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.459 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4

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	0.74	1/4051 (0.0%)	0.77	1/5523 (0.0%)
1	B	0.74	0/4051	0.77	3/5523 (0.1%)
1	C	0.76	0/4051	0.84	6/5523 (0.1%)
1	D	0.74	0/4051	0.78	1/5523 (0.0%)
All	All	0.75	1/16204 (0.0%)	0.79	11/22092 (0.0%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	TRP	CB-CG	-6.36	1.38	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	LEU	CA-CB-CG	8.61	135.11	115.30
1	C	92	ASN	N-CA-C	-8.39	88.36	111.00
1	D	480	LEU	CA-CB-CG	7.49	132.53	115.30
1	A	165	LEU	CA-CB-CG	6.58	130.43	115.30
1	B	480	LEU	CA-CB-CG	6.05	129.21	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286	LEU	CA-CB-CG	5.67	128.34	115.30
1	C	39	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	313	TYR	C-N-CA	5.16	134.60	121.70
1	C	165	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	286	LEU	CB-CG-CD2	5.11	119.69	111.00
1	C	69	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	CYS	Peptide
1	B	344	GLY	Peptide
1	C	91	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3930	0	3843	78	0
1	B	3930	0	3843	78	0
1	C	3930	0	3843	69	0
1	D	3930	0	3843	90	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	40	0	0	7	0
3	B	35	0	0	5	0
3	C	35	0	0	4	0
3	D	30	0	0	4	0
4	A	288	0	0	8	0
4	B	272	0	0	7	0
4	C	290	0	0	11	0
4	D	294	0	0	13	0
All	All	17060	0	15424	303	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (303) 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:C:39:ARG:HH11	1:C:39:ARG:HG2	1.25	0.97
1:C:343:VAL:HB	1:C:344:GLY:HA2	1.51	0.93
1:D:11:TYR:HE2	1:D:353:ARG:HE	1.19	0.90
1:C:245:PRO:HG3	1:D:348:TRP:HB3	1.54	0.89
1:D:31:PHE:HD1	4:D:664:HOH:O	1.58	0.86
1:C:342:CYS:SG	1:C:343:VAL:N	2.48	0.86
1:A:44:ARG:HD2	3:A:506:SO4:O2	1.77	0.85
1:B:319:PRO:HA	1:B:320:ALA:HB2	1.61	0.82
1:B:70:GLN:NE2	1:B:437:VAL:HG21	1.94	0.82
1:C:243:GLY:O	1:D:348:TRP:CD1	2.36	0.78
1:D:95:ALA:CB	1:D:406:ILE:HD13	2.15	0.77
1:B:62:GLY:HA2	1:B:63:THR:OG1	1.84	0.76
1:B:495:HIS:HD2	4:B:853:HOH:O	1.68	0.75
1:D:284:GLN:HE22	1:D:313:TYR:HE1	1.34	0.75
1:C:169:GLN:HG3	1:C:170:ARG:H	1.52	0.75
1:B:5:ILE:HD12	1:B:22:TYR:CE2	2.23	0.73
1:B:96:LEU:HD21	1:B:404:VAL:HG13	1.70	0.72
1:D:270:ASN:ND2	4:D:614:HOH:O	2.21	0.72
1:D:56:ILE:HG12	1:D:480:LEU:HD22	1.72	0.72
1:D:149:LEU:O	4:D:665:HOH:O	2.08	0.72
1:D:312:TRP:HH2	1:D:316:PHE:C	1.93	0.71
1:A:207:GLN:NE2	1:A:263:ASP:OD1	2.22	0.71
1:A:194:LYS:HB2	1:A:242:SER:HA	1.71	0.71
1:A:132:THR:O	1:A:133:TYR:HB3	1.89	0.71
1:A:243:GLY:O	1:B:348:TRP:CD1	2.45	0.70
1:D:44:ARG:HD3	3:D:502:SO4:O4	1.91	0.70
1:B:68:THR:HG23	1:B:473:LYS:HB3	1.74	0.69
1:D:312:TRP:CH2	1:D:316:PHE:C	2.66	0.69
1:C:165:LEU:HD22	1:C:172:VAL:HB	1.75	0.68
1:C:44:ARG:HD3	3:C:504:SO4:O1	1.94	0.67
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.77	0.67
1:B:345:SER:O	1:B:346:LYS:C	2.32	0.67
1:C:120:ARG:HB2	1:C:379:THR:HG21	1.77	0.67
1:C:313:TYR:HE2	4:C:1068:HOH:O	1.76	0.67
1:C:300:GLU:HG2	4:C:755:HOH:O	1.95	0.66
1:C:313:TYR:HB3	1:C:314:LEU:HB2	1.77	0.66
1:A:342:CYS:SG	1:A:343:VAL:N	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:504:SO4:O1	1:B:441:LYS:NZ	2.30	0.65
1:C:44:ARG:CD	3:C:504:SO4:O1	2.44	0.65
1:D:60:HIS:HE1	4:D:955:HOH:O	1.79	0.65
1:B:194:LYS:HB2	1:B:242:SER:HA	1.79	0.64
1:B:207:GLN:NE2	1:B:263:ASP:OD1	2.30	0.64
1:D:93:ILE:O	1:D:101:GLN:HG2	1.97	0.64
1:A:328:HIS:HD2	4:A:1103:HOH:O	1.81	0.64
1:C:313:TYR:CE2	4:C:1068:HOH:O	2.49	0.64
1:D:314:LEU:HB2	1:D:343:VAL:HG12	1.79	0.64
1:B:319:PRO:CA	1:B:320:ALA:HB2	2.28	0.63
1:C:406:ILE:HG23	4:C:729:HOH:O	1.97	0.63
1:D:89:ALA:O	1:D:93:ILE:HG23	1.98	0.63
1:A:243:GLY:O	1:B:348:TRP:HD1	1.81	0.63
1:D:408:LYS:O	1:D:410:THR:HG23	2.00	0.62
1:B:31:PHE:HB3	4:B:935:HOH:O	1.99	0.62
1:A:408:LYS:HB3	1:A:410:THR:HG23	1.82	0.62
1:C:169:GLN:NE2	4:C:817:HOH:O	2.23	0.61
1:A:245:PRO:HD3	1:B:348:TRP:CG	2.36	0.61
1:D:44:ARG:CD	3:D:502:SO4:O4	2.49	0.61
1:A:209:TRP:CZ3	1:A:212:TYR:CD2	2.89	0.60
1:A:41:GLU:HG3	1:A:490:HIS:CD2	2.35	0.60
1:D:284:GLN:NE2	1:D:313:TYR:HE1	1.98	0.60
1:B:70:GLN:NE2	1:B:437:VAL:CG2	2.63	0.60
1:A:254:GLU:OE2	4:A:579:HOH:O	2.17	0.60
1:A:284:GLN:HG3	1:A:314:LEU:HD12	1.84	0.59
1:D:95:ALA:HB1	1:D:406:ILE:HD13	1.83	0.59
1:B:473:LYS:HG3	1:B:479:PHE:CE2	2.38	0.59
1:D:495:HIS:HD2	4:D:1066:HOH:O	1.84	0.59
1:A:343:VAL:HG13	1:A:344:GLY:H	1.67	0.59
1:B:62:GLY:CA	1:B:63:THR:OG1	2.49	0.59
1:C:39:ARG:HH11	1:C:39:ARG:CG	2.10	0.59
1:A:44:ARG:CD	3:A:506:SO4:O2	2.50	0.58
1:C:284:GLN:HB2	1:C:286:LEU:HD13	1.84	0.58
1:B:349:GLU:HG3	1:B:353:ARG:NH2	2.18	0.58
1:D:290:HIS:HA	1:D:293:LYS:HD2	1.86	0.58
1:D:165:LEU:HD22	1:D:172:VAL:HB	1.86	0.58
1:C:379:THR:HG22	4:C:719:HOH:O	2.03	0.58
1:D:386:ASN:HB2	1:D:387:PRO:HD2	1.86	0.58
1:B:226:GLN:HG3	3:B:502:SO4:O1	2.04	0.57
1:D:207:GLN:NE2	1:D:263:ASP:OD1	2.32	0.57
1:A:253:PRO:HB2	1:A:294:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:VAL:CB	1:C:344:GLY:HA2	2.32	0.57
1:D:349:GLU:HG2	1:D:353:ARG:NH1	2.18	0.57
1:A:396:ASN:HB2	4:A:745:HOH:O	2.04	0.56
1:C:284:GLN:CB	1:C:286:LEU:HD13	2.35	0.56
1:A:44:ARG:HB3	3:A:506:SO4:O2	2.05	0.56
1:C:408:LYS:O	1:C:410:THR:HG23	2.06	0.56
1:D:11:TYR:CE2	1:D:353:ARG:NE	2.64	0.56
1:B:284:GLN:HB2	1:B:286:LEU:HD13	1.86	0.56
1:D:87:ASP:HB2	1:D:129:SER:HA	1.87	0.56
1:D:463:ARG:NH2	4:D:948:HOH:O	2.38	0.56
1:A:44:ARG:NH1	3:A:506:SO4:O1	2.40	0.55
1:B:346:LYS:O	1:B:349:GLU:O	2.24	0.55
1:C:284:GLN:HG3	1:C:314:LEU:HD12	1.88	0.55
1:D:192:ASN:HB2	1:D:244:TYR:O	2.07	0.55
1:B:151:GLU:HB2	1:C:130:ILE:HD11	1.88	0.55
1:C:408:LYS:O	1:C:410:THR:CG2	2.55	0.55
1:D:312:TRP:HH2	1:D:317:LEU:N	2.04	0.55
1:C:117:ASN:HA	1:C:172:VAL:HG22	1.88	0.55
1:D:91:LEU:HD23	1:D:391:PRO:HG3	1.87	0.55
1:A:426:PHE:HB3	1:A:493:LEU:HD21	1.88	0.54
1:B:347:PHE:CE1	1:B:348:TRP:HZ3	2.24	0.54
1:C:183:THR:O	1:C:189:GLY:HA2	2.06	0.54
1:A:287:LEU:HB3	1:A:291:TRP:CD1	2.42	0.54
1:B:211:ARG:HD2	4:B:983:HOH:O	2.07	0.54
1:B:95:ALA:CB	1:B:406:ILE:HD13	2.38	0.54
1:C:39:ARG:NH1	1:C:39:ARG:HG2	2.02	0.54
1:A:266:PRO:HB2	4:A:909:HOH:O	2.07	0.54
1:B:70:GLN:HE22	1:B:437:VAL:HG21	1.68	0.54
1:A:358:ASP:HA	1:A:361:MET:HE2	1.90	0.54
1:B:232:ALA:O	1:B:233:GLU:HB2	2.09	0.53
1:D:312:TRP:CH2	1:D:316:PHE:O	2.61	0.53
1:B:371:LEU:O	1:B:433:ARG:HD2	2.08	0.53
1:D:349:GLU:OE1	1:D:353:ARG:HD2	2.07	0.53
1:A:339:SER:O	1:A:379:THR:HG22	2.08	0.53
1:B:57:GLN:HG3	1:B:481:GLU:OE1	2.08	0.53
1:C:82:GLY:HA3	1:C:118:ILE:O	2.09	0.53
1:C:245:PRO:CG	1:D:348:TRP:HB3	2.35	0.53
1:A:396:ASN:CB	4:A:745:HOH:O	2.58	0.52
1:A:245:PRO:HD3	1:B:348:TRP:HB3	1.92	0.52
1:A:120:ARG:NH2	1:A:234:ASN:OD1	2.35	0.52
1:A:152:GLU:HA	1:A:156:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:SER:HB3	3:D:502:SO4:O2	2.11	0.51
1:B:93:ILE:O	1:B:101:GLN:HG2	2.10	0.51
1:C:106:LYS:HG2	1:C:167:LEU:HD22	1.93	0.51
1:A:408:LYS:O	1:A:410:THR:HG23	2.09	0.51
1:B:44:ARG:CD	3:B:503:SO4:O3	2.58	0.51
1:B:19:ASN:O	1:B:103:LEU:HD12	2.11	0.51
1:D:381:TRP:HA	1:D:381:TRP:HE3	1.76	0.51
1:A:82:GLY:HA3	1:A:118:ILE:O	2.11	0.50
1:C:116:TYR:OH	1:C:420:LEU:HD13	2.11	0.50
1:D:381:TRP:HA	1:D:381:TRP:CE3	2.45	0.50
1:A:140:ASP:N	1:A:140:ASP:OD1	2.43	0.50
1:B:44:ARG:HD2	3:B:503:SO4:O3	2.12	0.50
1:B:306:HIS:ND1	3:B:505:SO4:O1	2.43	0.50
1:B:319:PRO:CA	1:B:320:ALA:CB	2.89	0.50
1:A:365:HIS:HD2	1:A:445:ASP:OD2	1.94	0.50
1:B:319:PRO:HA	1:B:320:ALA:CB	2.39	0.50
1:D:426:PHE:HB3	1:D:493:LEU:HD21	1.94	0.50
1:C:19:ASN:HB2	4:C:516:HOH:O	2.12	0.49
1:C:377:GLY:C	1:C:378:TRP:CE3	2.85	0.49
1:D:12:SER:OG	3:D:499:SO4:O2	2.20	0.49
1:A:120:ARG:HB2	1:A:379:THR:HG21	1.95	0.49
1:D:116:TYR:OH	1:D:420:LEU:HD13	2.11	0.49
1:C:286:LEU:HD22	1:C:287:LEU:HG	1.94	0.49
1:A:405:ASP:OD2	4:A:953:HOH:O	2.19	0.49
1:A:245:PRO:CG	1:B:348:TRP:HB3	2.43	0.49
1:A:389:GLY:O	1:A:396:ASN:HB3	2.13	0.49
1:B:182:PRO:HB3	1:B:184:TRP:NE1	2.28	0.49
1:C:209:TRP:O	1:C:212:TYR:HB3	2.12	0.49
1:D:19:ASN:O	1:D:103:LEU:HD12	2.13	0.49
1:C:44:ARG:HD2	3:C:504:SO4:O1	2.13	0.49
1:C:194:LYS:HB2	1:C:242:SER:HA	1.95	0.48
1:B:496:ARG:O	1:B:497:GLN:HB3	2.13	0.48
1:D:232:ALA:O	1:D:233:GLU:HB2	2.13	0.48
1:D:15:VAL:HG11	1:D:354:LEU:HD22	1.96	0.48
1:A:269:ALA:HB2	4:A:1175:HOH:O	2.14	0.48
1:D:257:ARG:HD2	1:D:298:ASP:OD2	2.14	0.48
1:B:347:PHE:CE1	1:B:348:TRP:CZ3	3.01	0.48
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.95	0.48
1:C:194:LYS:NZ	4:C:527:HOH:O	2.46	0.48
1:D:95:ALA:HB3	1:D:406:ILE:HD13	1.95	0.48
1:B:82:GLY:HA2	1:B:116:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HG	1:C:470:LEU:HD11	1.95	0.48
1:A:95:ALA:HB3	1:A:406:ILE:HG22	1.96	0.48
1:C:381:TRP:CE3	1:C:381:TRP:HA	2.48	0.48
1:B:453:ASP:OD1	1:B:455:SER:OG	2.31	0.47
1:B:41:GLU:HG3	1:B:490:HIS:CD2	2.49	0.47
1:D:22:TYR:CD2	1:D:22:TYR:C	2.87	0.47
1:C:245:PRO:HD3	1:D:348:TRP:CD2	2.49	0.47
1:C:256:GLN:O	1:C:260:ILE:HG13	2.15	0.47
1:D:96:LEU:HD21	1:D:404:VAL:HG13	1.97	0.47
1:B:387:PRO:HD3	1:B:404:VAL:O	2.15	0.47
1:B:312:TRP:CZ2	1:B:318:ALA:HB3	2.50	0.47
1:B:191:VAL:O	1:B:247:GLN:HA	2.15	0.47
1:C:381:TRP:HA	1:C:381:TRP:HE3	1.80	0.47
1:A:371:LEU:HD23	1:A:378:TRP:HH2	1.80	0.47
1:D:495:HIS:CD2	4:D:1066:HOH:O	2.65	0.47
1:B:146:ASN:ND2	4:B:1122:HOH:O	2.47	0.46
1:D:314:LEU:HB2	1:D:343:VAL:CG1	2.45	0.46
1:D:497:GLN:HG2	4:D:1044:HOH:O	2.14	0.46
1:A:141:ASP:OD2	1:A:146:ASN:HB2	2.15	0.46
1:D:386:ASN:HB2	1:D:387:PRO:CD	2.44	0.46
1:C:131:ARG:NH1	4:C:543:HOH:O	2.44	0.46
1:A:245:PRO:CD	1:B:348:TRP:HB3	2.46	0.46
1:C:132:THR:O	1:C:133:TYR:HB3	2.13	0.46
1:A:96:LEU:HB3	1:A:100:ALA:HB3	1.98	0.46
1:D:300:GLU:OE2	1:D:303:LYS:HE2	2.15	0.46
1:A:243:GLY:N	4:A:567:HOH:O	2.41	0.46
1:A:346:LYS:HG2	1:A:348:TRP:CH2	2.51	0.46
1:C:47:ARG:HD3	1:C:50:GLU:OE1	2.16	0.46
1:A:31:PHE:HE1	1:A:493:LEU:HD13	1.80	0.46
1:B:72:GLU:HB2	4:B:538:HOH:O	2.16	0.46
1:C:329:ARG:NH1	4:C:603:HOH:O	2.42	0.45
1:D:284:GLN:NE2	1:D:313:TYR:CE1	2.81	0.45
1:D:66:LEU:HD11	1:D:473:LYS:HB2	1.97	0.45
1:A:312:TRP:CZ2	1:A:378:TRP:CD1	3.04	0.45
1:B:381:TRP:HA	1:B:381:TRP:CE3	2.51	0.45
1:A:42:SER:HA	1:A:47:ARG:O	2.16	0.45
1:B:199:GLY:HA3	1:B:203:ASP:OD2	2.16	0.45
1:C:353:ARG:NH1	3:C:500:SO4:O1	2.50	0.45
1:D:191:VAL:O	1:D:247:GLN:HA	2.16	0.45
1:A:175:LEU:HD12	1:A:229:ALA:O	2.16	0.45
1:B:314:LEU:HB2	1:B:343:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:GLN:HB3	1:D:286:LEU:HG	1.98	0.45
1:D:31:PHE:HB2	1:D:495:HIS:CE1	2.52	0.45
1:B:351:SER:O	1:B:359:ARG:NH1	2.45	0.45
1:B:497:GLN:HB3	4:B:789:HOH:O	2.16	0.45
1:A:197:LEU:HD11	1:A:209:TRP:CD1	2.51	0.45
1:B:366:SER:O	1:B:370:ASN:ND2	2.49	0.45
1:C:207:GLN:NE2	1:C:263:ASP:OD1	2.30	0.45
1:D:273:HIS:O	1:D:276:VAL:HG23	2.17	0.45
1:D:312:TRP:HH2	1:D:316:PHE:O	1.96	0.45
1:D:371:LEU:O	1:D:433:ARG:HD2	2.16	0.45
1:B:381:TRP:HA	1:B:381:TRP:HE3	1.82	0.45
1:D:285:ARG:NH1	4:D:540:HOH:O	2.50	0.45
1:A:41:GLU:HG3	1:A:490:HIS:NE2	2.32	0.44
1:B:59:ASN:ND2	4:B:987:HOH:O	2.50	0.44
1:B:5:ILE:HD12	1:B:22:TYR:CD2	2.51	0.44
1:C:312:TRP:HZ2	1:C:378:TRP:HE1	1.64	0.44
1:A:209:TRP:O	1:A:212:TYR:HB3	2.17	0.44
1:A:377:GLY:C	1:A:378:TRP:CE3	2.91	0.44
1:C:125:SER:HB3	1:C:133:TYR:CE2	2.52	0.44
1:B:284:GLN:CB	1:B:286:LEU:HD13	2.47	0.44
1:D:312:TRP:HH2	1:D:317:LEU:HA	1.83	0.44
1:B:23:CYS:HB2	1:B:103:LEU:HD13	2.00	0.44
1:B:56:ILE:HG12	1:B:480:LEU:HD22	1.99	0.44
1:C:199:GLY:HA3	1:C:203:ASP:OD2	2.18	0.44
1:D:236:PRO:O	1:D:250:GLY:HA2	2.18	0.44
1:B:11:TYR:CD2	1:B:353:ARG:NH1	2.86	0.44
1:D:312:TRP:HH2	1:D:317:LEU:CA	2.30	0.44
1:A:408:LYS:O	1:A:410:THR:CG2	2.66	0.44
1:C:108:TYR:CE1	1:C:402:ILE:HD12	2.53	0.44
1:D:73:GLN:O	1:D:434:VAL:HA	2.18	0.44
1:A:381:TRP:HA	1:A:381:TRP:CE3	2.52	0.44
1:A:290:HIS:ND1	3:A:505:SO4:O3	2.51	0.44
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.48	0.44
1:A:245:PRO:HB2	1:A:394:VAL:HG11	2.00	0.43
1:C:110:SER:OG	1:C:112:GLU:HG2	2.17	0.43
1:A:127:ASP:N	1:A:127:ASP:OD1	2.52	0.43
1:C:1:ALA:HB2	1:C:27:ASP:OD1	2.18	0.43
1:D:337:PHE:CE1	1:D:377:GLY:HA3	2.54	0.43
1:A:31:PHE:CE1	1:A:493:LEU:HD13	2.53	0.43
1:A:423:PHE:CZ	1:A:459:VAL:HG11	2.53	0.43
1:B:337:PHE:CE1	1:B:377:GLY:HA3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:MET:SD	1:C:178:PRO:HD3	2.58	0.43
1:D:347:PHE:C	1:D:347:PHE:CD2	2.92	0.43
1:A:381:TRP:HA	1:A:381:TRP:HE3	1.84	0.43
1:C:95:ALA:HB3	1:C:406:ILE:HG22	2.00	0.43
1:D:463:ARG:NH1	4:D:988:HOH:O	2.52	0.43
1:A:395:ARG:HD3	1:A:397:PHE:CZ	2.53	0.43
1:D:41:GLU:HG3	1:D:490:HIS:CD2	2.54	0.43
1:C:200:GLN:N	1:C:203:ASP:OD2	2.44	0.43
1:D:82:GLY:HA2	1:D:116:TYR:CD1	2.54	0.43
1:D:169:GLN:HG2	4:D:578:HOH:O	2.19	0.43
1:C:296:LEU:HA	1:C:302:ALA:HB2	2.00	0.43
1:A:95:ALA:CB	1:A:406:ILE:CG2	2.97	0.43
1:C:290:HIS:HB2	4:C:724:HOH:O	2.18	0.43
1:C:16:CYS:SG	1:C:48:ARG:HG3	2.59	0.42
1:B:95:ALA:HB1	1:B:406:ILE:HD13	2.01	0.42
1:A:370:ASN:HB3	1:A:378:TRP:HZ2	1.85	0.42
1:A:44:ARG:NH2	3:A:503:SO4:O2	2.51	0.42
1:B:128:PHE:CZ	1:B:398:VAL:HG22	2.55	0.42
1:A:383:LEU:HA	1:A:383:LEU:HD23	1.86	0.42
1:A:406:ILE:HD13	1:A:406:ILE:H	1.84	0.42
1:D:70:GLN:HE22	1:D:437:VAL:HG21	1.83	0.42
1:C:120:ARG:CB	1:C:379:THR:HG21	2.46	0.42
1:D:41:GLU:HG3	1:D:490:HIS:NE2	2.34	0.42
1:A:312:TRP:HZ2	1:A:378:TRP:CD1	2.38	0.42
1:B:312:TRP:HZ2	1:B:318:ALA:HB3	1.83	0.42
1:B:252:THR:HB	1:B:253:PRO:HD2	2.01	0.41
1:C:312:TRP:HH2	1:C:367:ILE:HG13	1.85	0.41
1:A:95:ALA:CB	1:A:406:ILE:HG22	2.50	0.41
1:B:44:ARG:HD3	3:B:503:SO4:O3	2.19	0.41
1:A:446:ALA:HA	1:A:459:VAL:O	2.20	0.41
1:C:186:LYS:HD3	1:C:190:ALA:O	2.19	0.41
1:D:346:LYS:O	1:D:349:GLU:O	2.39	0.41
1:A:149:LEU:HB3	1:A:153:ASP:HB2	2.01	0.41
1:B:2:ARG:O	1:B:24:ASP:HA	2.19	0.41
1:D:313:TYR:CD1	1:D:313:TYR:N	2.88	0.41
1:D:207:GLN:HE22	1:D:263:ASP:HA	1.85	0.41
1:D:348:TRP:CD1	1:D:349:GLU:HG3	2.55	0.41
1:D:405:ASP:OD2	1:D:408:LYS:HD2	2.21	0.41
1:A:165:LEU:HD22	1:A:172:VAL:HB	2.02	0.41
1:A:245:PRO:HD3	1:B:348:TRP:CB	2.51	0.41
1:B:37:PHE:CG	1:B:480:LEU:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:THR:HG23	1:D:47:ARG:HB2	2.01	0.41
1:C:370:ASN:HB3	1:C:378:TRP:HZ2	1.85	0.41
1:D:11:TYR:HE2	1:D:353:ARG:NE	2.00	0.41
1:D:194:LYS:HE3	1:D:240:LEU:O	2.21	0.41
1:D:309:ALA:HA	1:D:337:PHE:O	2.20	0.41
1:D:346:LYS:HB3	1:D:349:GLU:HB2	2.01	0.41
1:D:95:ALA:HB3	1:D:406:ILE:CD1	2.50	0.41
1:A:176:ALA:HB2	1:A:227:PHE:CE2	2.56	0.41
1:A:371:LEU:CD2	1:A:378:TRP:HH2	2.33	0.41
1:D:70:GLN:NE2	1:D:437:VAL:HG21	2.35	0.41
1:D:146:ASN:ND2	4:D:1141:HOH:O	2.54	0.41
1:A:258:ASP:O	1:A:262:ARG:HG2	2.22	0.40
1:A:284:GLN:HG3	1:A:314:LEU:HB2	2.04	0.40
1:C:405:ASP:OD2	1:C:408:LYS:HE2	2.20	0.40
1:C:371:LEU:O	1:C:433:ARG:HD2	2.21	0.40
1:D:350:GLN:HG2	4:D:637:HOH:O	2.21	0.40
1:D:127:ASP:HB3	1:D:246:PHE:CG	2.56	0.40
1:A:209:TRP:CE3	1:A:209:TRP:HA	2.56	0.40
1:C:465:SER:HA	1:C:487:TYR:CE1	2.56	0.40
1:B:66:LEU:HB3	1:B:439:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	495/497 (100%)	457 (92%)	32 (6%)	6 (1%)	13 10
1	B	495/497 (100%)	468 (94%)	19 (4%)	8 (2%)	9 7
1	C	495/497 (100%)	460 (93%)	31 (6%)	4 (1%)	19 19
1	D	495/497 (100%)	471 (95%)	20 (4%)	4 (1%)	19 19
All	All	1980/1988 (100%)	1856 (94%)	102 (5%)	22 (1%)	14 12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	GLU
1	B	320	ALA
1	B	346	LYS
1	C	343	VAL
1	D	233	GLU
1	B	381	TRP
1	D	350	GLN
1	A	133	TYR
1	A	343	VAL
1	A	381	TRP
1	B	63	THR
1	C	313	TYR
1	C	381	TRP
1	D	281	LEU
1	A	281	LEU
1	A	344	GLY
1	A	345	SER
1	B	124	ALA
1	B	281	LEU
1	B	317	LEU
1	C	281	LEU
1	D	381	TRP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/424 (100%)	401 (95%)	23 (5%)	22	26
1	B	424/424 (100%)	405 (96%)	19 (4%)	27	34
1	C	424/424 (100%)	399 (94%)	25 (6%)	19	23
1	D	424/424 (100%)	403 (95%)	21 (5%)	24	30
All	All	1696/1696 (100%)	1608 (95%)	88 (5%)	23	28

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	44	ARG
1	A	57	GLN
1	A	110	SER
1	A	140	ASP
1	A	169	GLN
1	A	200	GLN
1	A	224	LYS
1	A	271	SER
1	A	285	ARG
1	A	303	LYS
1	A	335	MET
1	A	342	CYS
1	A	346	LYS
1	A	358	ASP
1	A	370	ASN
1	A	379	THR
1	A	381	TRP
1	A	388	GLU
1	A	396	ASN
1	A	406	ILE
1	A	410	THR
1	A	433	ARG
1	B	30	THR
1	B	47	ARG
1	B	59	ASN
1	B	155	LYS
1	B	284	GLN
1	B	286	LEU
1	B	317	LEU
1	B	321	LYS
1	B	335	MET
1	B	346	LYS
1	B	348	TRP
1	B	366	SER
1	B	381	TRP
1	B	394	VAL
1	B	473	LYS
1	B	480	LEU
1	B	481	GLU
1	B	493	LEU
1	B	497	GLN
1	C	39	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	44	ARG
1	C	57	GLN
1	C	61	THR
1	C	69	LEU
1	C	73	GLN
1	C	111	GLU
1	C	200	GLN
1	C	204	ILE
1	C	226	GLN
1	C	286	LEU
1	C	303	LYS
1	C	335	MET
1	C	342	CYS
1	C	343	VAL
1	C	345	SER
1	C	346	LYS
1	C	347	PHE
1	C	370	ASN
1	C	381	TRP
1	C	395	ARG
1	C	397	PHE
1	C	410	THR
1	C	433	ARG
1	C	464	SER
1	D	39	ARG
1	D	44	ARG
1	D	93	ILE
1	D	110	SER
1	D	111	GLU
1	D	118	ILE
1	D	169	GLN
1	D	212	TYR
1	D	228	TRP
1	D	286	LEU
1	D	311	HIS
1	D	312	TRP
1	D	335	MET
1	D	347	PHE
1	D	379	THR
1	D	381	TRP
1	D	394	VAL
1	D	420	LEU

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Mol	Chain	Res	Type
1	D	481	GLU
1	D	489	ILE
1	D	497	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	223	HIS
1	A	306	HIS
1	A	328	HIS
1	A	365	HIS
1	A	495	HIS
1	A	497	GLN
1	B	59	ASN
1	B	60	HIS
1	B	146	ASN
1	B	169	GLN
1	B	200	GLN
1	B	274	HIS
1	B	350	GLN
1	B	396	ASN
1	B	495	HIS
1	C	328	HIS
1	C	495	HIS
1	D	60	HIS
1	D	146	ASN
1	D	169	GLN
1	D	226	GLN
1	D	311	HIS
1	D	350	GLN
1	D	362	GLN
1	D	365	HIS
1	D	495	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 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
3	SO4	B	501	-	4,4,4	0.34	0	6,6,6	0.44	0
3	SO4	A	506	-	4,4,4	0.18	0	6,6,6	0.46	0
3	SO4	D	500	-	4,4,4	0.28	0	6,6,6	0.50	0
3	SO4	C	503	-	4,4,4	0.50	0	6,6,6	0.27	0
3	SO4	D	503	-	4,4,4	0.42	0	6,6,6	0.33	0
3	SO4	C	500	-	4,4,4	0.26	0	6,6,6	0.35	0
3	SO4	A	503	-	4,4,4	0.40	0	6,6,6	0.43	0
3	SO4	C	504	-	4,4,4	0.26	0	6,6,6	0.58	0
2	NAG	C	498	1	14,14,15	0.94	1 (7%)	17,19,21	1.72	5 (29%)
2	NAG	B	498	1	14,14,15	0.60	0	17,19,21	1.56	4 (23%)
3	SO4	B	499	-	4,4,4	0.23	0	6,6,6	0.59	0
3	SO4	B	503	-	4,4,4	0.32	0	6,6,6	0.85	0
3	SO4	A	500	-	4,4,4	0.44	0	6,6,6	0.57	0
3	SO4	D	502	-	4,4,4	0.32	0	6,6,6	0.54	0
2	NAG	D	498	1	14,14,15	0.58	0	17,19,21	2.56	4 (23%)
2	NAG	A	498	1	14,14,15	0.73	0	17,19,21	1.33	2 (11%)
3	SO4	A	501	-	4,4,4	0.34	0	6,6,6	0.37	0
3	SO4	A	505	-	4,4,4	0.44	0	6,6,6	0.30	0
3	SO4	A	502	-	4,4,4	0.37	0	6,6,6	0.30	0
3	SO4	B	502	-	4,4,4	0.54	0	6,6,6	0.47	0
3	SO4	A	504	-	4,4,4	0.42	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	D	499	-	4,4,4	0.30	0	6,6,6	0.51	0
3	SO4	B	504	-	4,4,4	0.41	0	6,6,6	0.20	0
3	SO4	D	504	-	4,4,4	0.35	0	6,6,6	0.34	0
3	SO4	C	501	-	4,4,4	0.35	0	6,6,6	0.72	0
3	SO4	B	500	-	4,4,4	0.29	0	6,6,6	0.31	0
3	SO4	C	499	-	4,4,4	0.27	0	6,6,6	0.45	0
3	SO4	C	505	-	4,4,4	0.39	0	6,6,6	0.33	0
3	SO4	D	501	-	4,4,4	0.41	0	6,6,6	0.40	0
3	SO4	A	499	-	4,4,4	0.27	0	6,6,6	0.32	0
3	SO4	B	505	-	4,4,4	0.46	0	6,6,6	0.30	0
3	SO4	C	502	-	4,4,4	0.35	0	6,6,6	0.38	0

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	498	1	-	0/6/23/26	0/1/1/1
2	NAG	B	498	1	-	0/6/23/26	0/1/1/1
2	NAG	C	498	1	-	1/6/23/26	0/1/1/1
2	NAG	D	498	1	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	498	NAG	C1-C2	2.12	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	498	NAG	C1-O5-C5	8.69	123.97	112.19
2	C	498	NAG	C1-O5-C5	3.81	117.35	112.19
2	B	498	NAG	O5-C1-C2	-3.24	106.18	111.29
2	D	498	NAG	C1-C2-N2	-3.03	105.31	110.49
2	C	498	NAG	O5-C1-C2	-3.02	106.51	111.29
2	C	498	NAG	C1-C2-N2	2.69	115.09	110.49
2	B	498	NAG	C3-C4-C5	-2.66	105.49	110.24
2	A	498	NAG	O5-C1-C2	-2.58	107.21	111.29
2	B	498	NAG	O4-C4-C5	2.51	115.53	109.30
2	D	498	NAG	O4-C4-C5	2.40	115.26	109.30
2	A	498	NAG	C1-O5-C5	2.34	115.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	498	NAG	C1-O5-C5	2.34	115.36	112.19
2	C	498	NAG	C8-C7-N2	2.13	119.71	116.10
2	D	498	NAG	O3-C3-C4	-2.09	105.52	110.35
2	C	498	NAG	O7-C7-C8	-2.01	118.33	122.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	498	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	498	NAG	O5-C5-C6-O6
2	D	498	NAG	C4-C5-C6-O6
2	C	498	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	SO4	4	0
3	C	500	SO4	1	0
3	A	503	SO4	1	0
3	C	504	SO4	3	0
3	B	503	SO4	3	0
3	D	502	SO4	3	0
3	A	505	SO4	1	0
3	B	502	SO4	1	0
3	A	504	SO4	1	0
3	D	499	SO4	1	0
3	B	505	SO4	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	497/497 (100%)	-0.32	6 (1%) 79 77	9, 23, 41, 49	1 (0%)
1	B	497/497 (100%)	-0.38	5 (1%) 82 81	10, 23, 39, 62	1 (0%)
1	C	497/497 (100%)	-0.30	5 (1%) 82 81	11, 23, 42, 49	1 (0%)
1	D	497/497 (100%)	-0.34	5 (1%) 82 81	11, 22, 40, 60	1 (0%)
All	All	1988/1988 (100%)	-0.33	21 (1%) 80 79	9, 23, 40, 62	4 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	TRP	5.4
1	B	317	LEU	5.0
1	C	344	GLY	4.4
1	A	344	GLY	4.2
1	A	317	LEU	4.1
1	C	318	ALA	3.6
1	A	318	ALA	3.6
1	A	378	TRP	3.4
1	D	63	THR	3.4
1	D	317	LEU	3.3
1	B	347	PHE	3.1
1	A	397	PHE	3.0
1	D	348	TRP	3.0
1	D	347	PHE	3.0
1	B	318	ALA	2.8
1	C	378	TRP	2.8
1	C	200	GLN	2.6
1	D	318	ALA	2.6
1	A	345	SER	2.6
1	C	313	TYR	2.4
1	B	312	TRP	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	505	5/5	0.89	0.13	63,63,64,64	0
2	NAG	B	498	14/15	0.92	0.10	32,34,36,38	0
2	NAG	A	498	14/15	0.92	0.13	21,27,30,33	0
3	SO4	A	503	5/5	0.92	0.17	58,59,59,62	0
2	NAG	C	498	14/15	0.93	0.12	21,28,31,31	0
3	SO4	A	504	5/5	0.93	0.14	67,67,67,67	0
2	NAG	D	498	14/15	0.93	0.10	29,33,34,34	0
3	SO4	A	505	5/5	0.94	0.10	68,68,68,68	0
3	SO4	C	505	5/5	0.94	0.15	59,59,61,63	0
3	SO4	B	502	5/5	0.94	0.12	43,45,46,47	0
3	SO4	C	503	5/5	0.95	0.12	55,55,56,56	0
3	SO4	D	504	5/5	0.95	0.18	60,61,61,61	0
3	SO4	A	506	5/5	0.96	0.12	44,44,46,47	0
3	SO4	D	503	5/5	0.97	0.12	48,49,50,52	0
3	SO4	B	501	5/5	0.97	0.12	36,39,42,42	0
3	SO4	B	504	5/5	0.97	0.11	64,65,65,66	0
3	SO4	A	501	5/5	0.97	0.11	37,38,39,40	0
3	SO4	C	501	5/5	0.97	0.10	35,36,37,38	0
3	SO4	C	504	5/5	0.97	0.11	39,41,43,44	0
3	SO4	D	501	5/5	0.97	0.11	40,41,42,43	0
3	SO4	B	503	5/5	0.97	0.13	45,47,48,49	0
3	SO4	D	502	5/5	0.98	0.10	42,43,45,45	0
3	SO4	B	500	5/5	0.98	0.08	41,42,43,44	0
3	SO4	B	499	5/5	0.98	0.12	30,31,32,34	0
3	SO4	A	502	5/5	0.98	0.12	46,47,48,49	0
3	SO4	D	500	5/5	0.98	0.11	37,37,39,41	0
3	SO4	C	502	5/5	0.98	0.09	46,48,48,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	500	5/5	0.99	0.12	30,31,32,33	0
3	SO4	D	499	5/5	0.99	0.11	28,28,32,33	0
3	SO4	A	499	5/5	0.99	0.14	27,29,30,33	0
3	SO4	A	500	5/5	0.99	0.07	30,31,33,33	0
3	SO4	C	499	5/5	0.99	0.12	34,35,36,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.