



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:11 am BST

PDB ID : 6VMV  
Title : Crystal structure of the H767A mutant of GoxA soaked with glycine  
Authors : Yukl, E.T.  
Deposited on : 2020-01-28  
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 : 2.11  
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) : 2.11

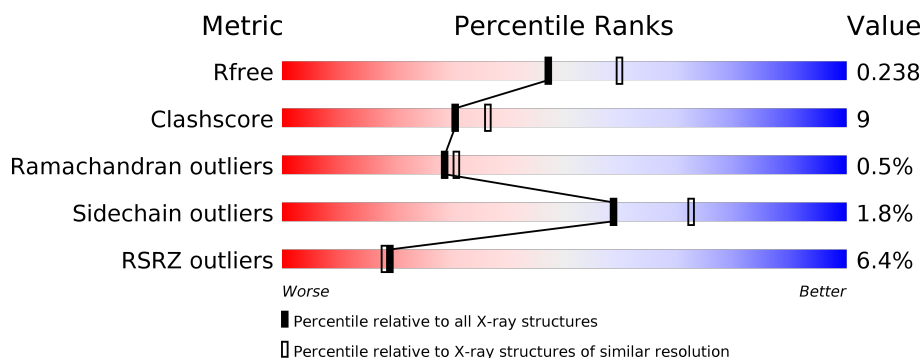
# 1 Overall quality at a glance

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	816	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 6%</div> </div> </div>
1	B	816	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	C	816	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	D	816	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div> </div>

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
3	SO4	A	902	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25765 atoms, of which 43 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 Glycine oxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	765	Total	C	H	N	O	S	0	14	0
			6149	3880	10	1043	1196	20			
1	B	778	Total	C	H	N	O	S	0	12	0
			6264	3947	11	1063	1222	21			
1	C	769	Total	C	H	N	O	S	0	6	0
			6146	3884	11	1043	1188	20			
1	D	778	Total	C	H	N	O	S	0	4	0
			6196	3908	11	1051	1206	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	ALA	HIS	engineered mutation	UNP A0A161XU12
B	767	ALA	HIS	engineered mutation	UNP A0A161XU12
C	767	ALA	HIS	engineered mutation	UNP A0A161XU12
D	767	ALA	HIS	engineered mutation	UNP A0A161XU12

- 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		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- 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	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	261	Total	O	0	0
			261	261		
4	B	206	Total	O	0	0
			206	206		
4	C	269	Total	O	0	0
			269	269		

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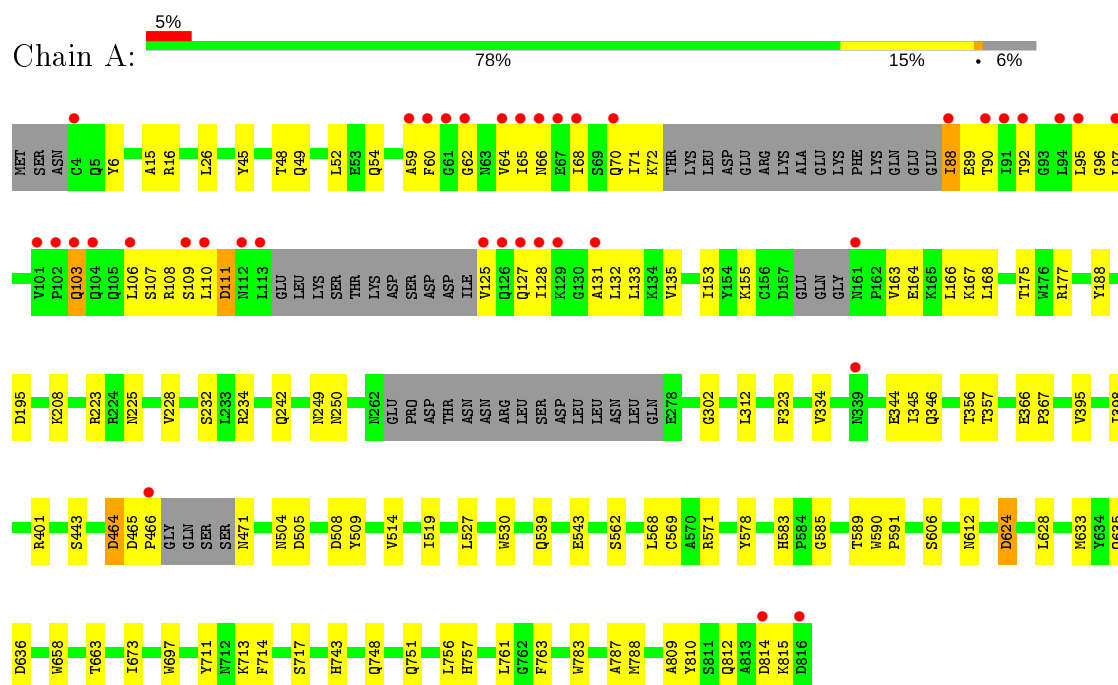
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	225	Total	O	0	0
			225	225		

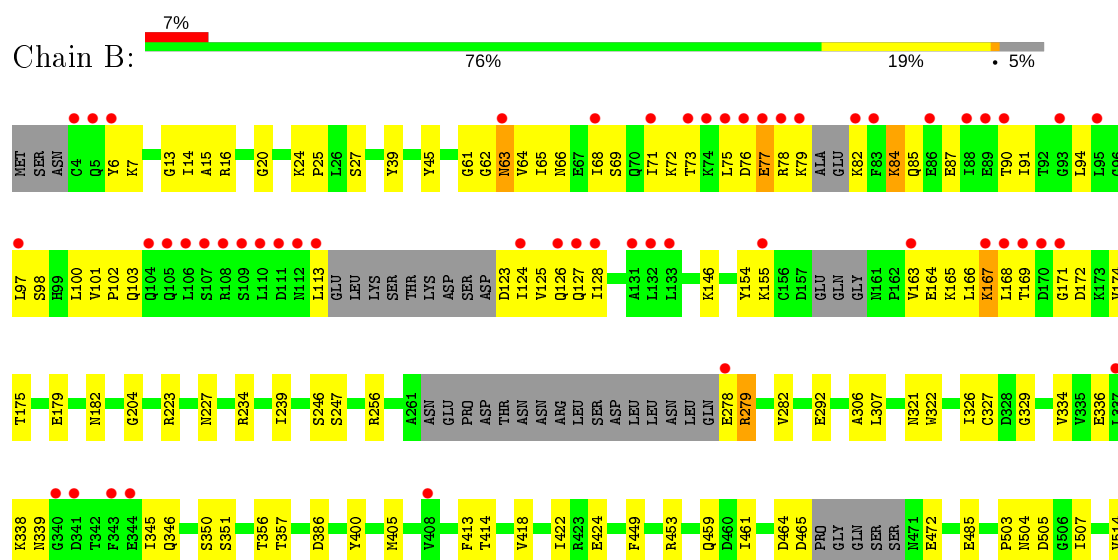
### 3 Residue-property plots [i](#)

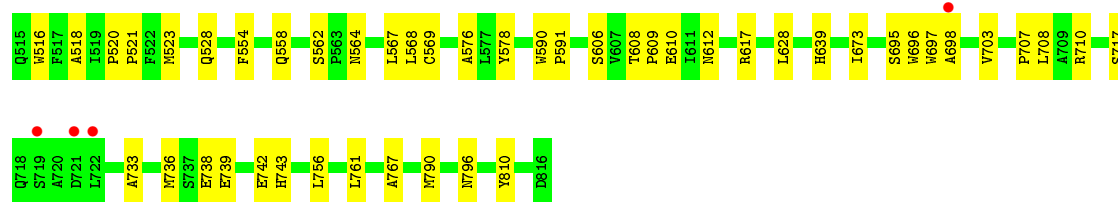
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

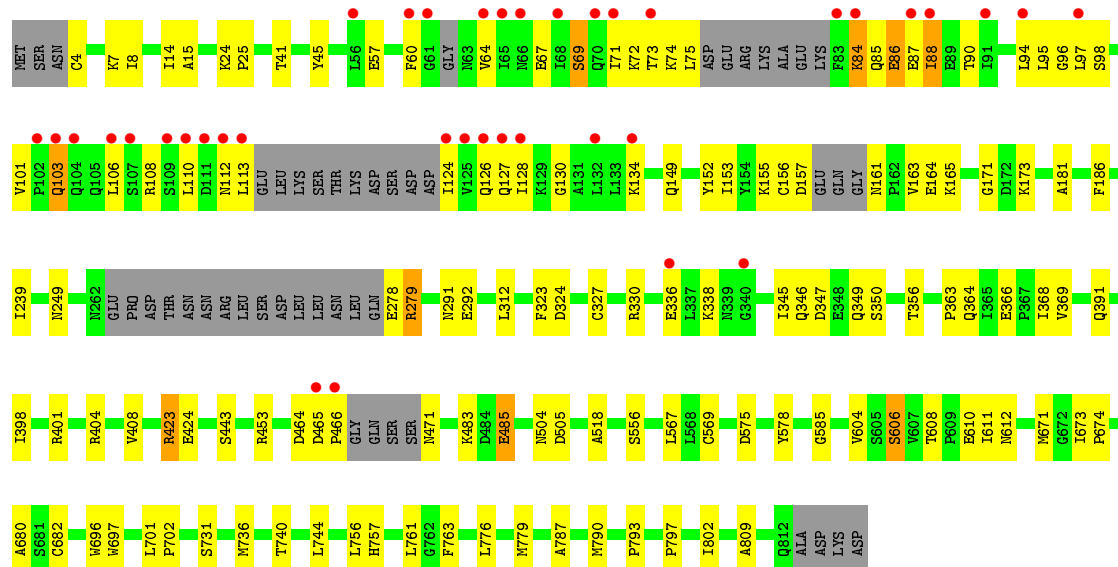
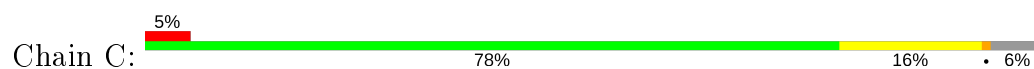


#### • Molecule 1: Glycine oxidase

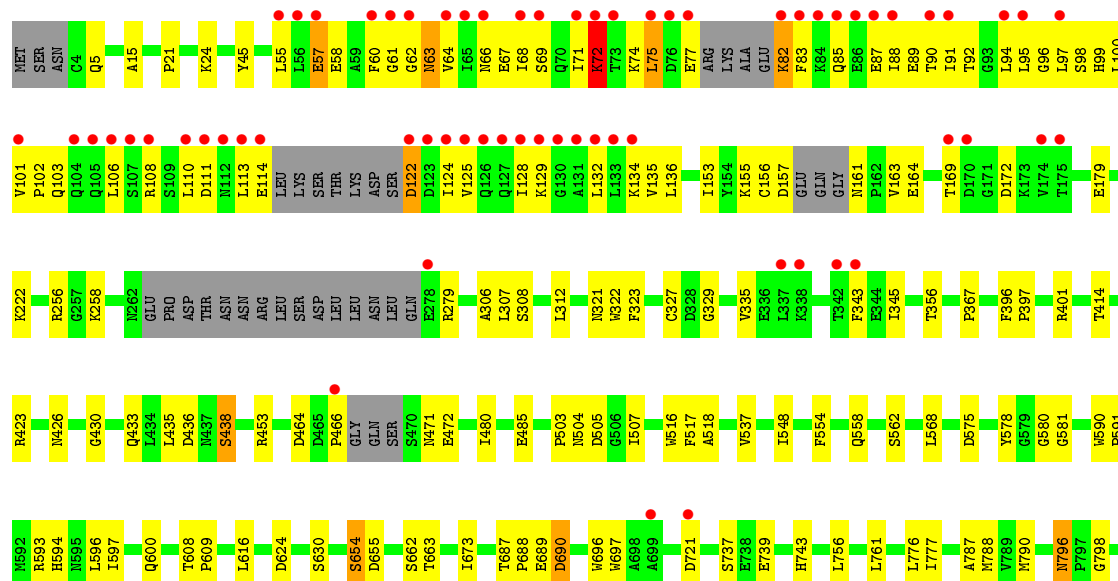
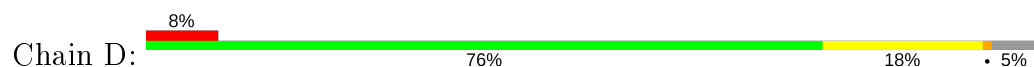




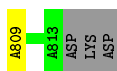
• Molecule 1: Glycine oxidase



• Molecule 1: Glycine oxidase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.97Å 93.08Å 187.64Å 90.00° 95.07° 90.00°	Depositor
Resolution (Å)	48.20 – 2.20 48.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.20-2.20) 98.7 (48.20-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.187 , 0.238 0.187 , 0.238	Depositor DCC
$R_{free}$ test set	1991 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.944	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: MG, SO4, TGH

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	0.63	0/6262	0.66	3/8528 (0.0%)
1	B	0.57	1/6376 (0.0%)	0.62	1/8672 (0.0%)
1	C	0.64	3/6258 (0.0%)	0.66	2/8517 (0.0%)
1	D	0.57	1/6309 (0.0%)	0.61	0/8586
All	All	0.60	5/25205 (0.0%)	0.64	6/34303 (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	2
1	C	0	1
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	CYS	CB-SG	-9.20	1.66	1.82
1	B	327	CYS	CB-SG	-8.83	1.67	1.82
1	D	327	CYS	CB-SG	-7.36	1.69	1.82
1	C	569	CYS	CB-SG	-5.28	1.73	1.81
1	C	186	PHE	CE2-CZ	5.03	1.47	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	ASP	CB-CG-OD1	7.03	124.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	671	MET	CG-SD-CE	5.69	109.30	100.20
1	A	624	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	324	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	195	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	571	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	ILE	Mainchain,Peptide
1	C	86	GLU	Peptide
1	D	72	LYS	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	6139	10	5890	91	0
1	B	6253	11	5996	122	0
1	C	6135	11	5904	113	0
1	D	6185	11	5935	126	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	0	0	2	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
4	A	261	0	0	2	0
4	B	206	0	0	7	0
4	C	269	0	0	5	0
4	D	225	0	0	6	0
All	All	25722	43	23725	445	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 9.

All (445) 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:64:VAL:HG12	1:C:94:LEU:HD13	1.32	1.07
1:C:71:ILE:HG23	1:C:74:LYS:HD3	1.48	0.96
1:D:67:GLU:O	1:D:71:ILE:HG13	1.67	0.92
1:D:68:ILE:HA	1:D:71:ILE:HD12	1.52	0.91
1:D:155:LYS:O	1:D:163:VAL:HG12	1.73	0.89
1:D:72:LYS:HD2	1:D:72:LYS:O	1.74	0.88
1:B:64:VAL:HG13	1:B:94:LEU:CD1	2.04	0.88
1:C:86:GLU:O	1:C:86:GLU:CD	2.13	0.86
1:C:108:ARG:O	1:C:112:ASN:ND2	2.09	0.84
1:D:654:SER:OG	4:D:1001:HOH:O	1.95	0.84
1:B:62:GLY:HA2	1:B:64:VAL:N	1.94	0.83
1:B:169:THR:OG1	1:B:338:LYS:HE2	1.79	0.82
1:B:68:ILE:HD11	1:B:91:ILE:HG23	1.60	0.82
1:D:124:ILE:HG13	1:D:125:VAL:N	1.95	0.82
1:A:628:LEU:HA	1:A:633:MET:CE	2.11	0.80
1:C:443:SER:OG	4:C:1001:HOH:O	1.99	0.80
3:A:902:SO4:O2	1:D:423[B]:ARG:NH1	2.15	0.79
1:D:71:ILE:O	1:D:74:LYS:NZ	2.15	0.79
1:D:438:SER:OG	4:D:1002:HOH:O	2.01	0.79
1:D:122:ASP:CA	1:D:124:ILE:HG12	2.13	0.78
1:D:124:ILE:HG13	1:D:125:VAL:H	1.47	0.78
1:C:113:LEU:HD21	1:C:127:GLN:HE21	1.47	0.77
1:D:122:ASP:HA	1:D:124:ILE:HG12	1.65	0.77
1:D:110:LEU:HD21	1:D:132:LEU:HD21	1.66	0.76
1:C:84:LYS:O	1:C:88:ILE:HG12	1.86	0.76
1:B:562:SER:HB3	1:B:568:LEU:HD11	1.65	0.76
1:B:76:ASP:HB3	1:B:79:LYS:NZ	2.00	0.76
1:D:82:LYS:HD3	1:D:83:PHE:O	1.86	0.76
1:B:124:ILE:H	1:B:124:ILE:HD12	1.52	0.75
1:A:49:GLN:HE21	1:A:133:LEU:HD21	1.52	0.75
1:A:228[B]:VAL:HG22	1:A:234:ARG:HG2	1.69	0.74
1:D:655:ASP:OD1	4:D:1001:HOH:O	2.05	0.74
1:C:64:VAL:CG1	1:C:94:LEU:HD13	2.14	0.74
1:D:64:VAL:HG11	1:D:94:LEU:HB3	1.69	0.74
1:D:68:ILE:HG22	1:D:124:ILE:HD12	1.70	0.74
1:C:86:GLU:OE1	1:C:86:GLU:O	2.05	0.73
1:D:88:ILE:O	1:D:92:THR:HG23	1.89	0.73
1:D:169:THR:OG1	1:D:172:ASP:OD2	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HA	1:B:75:LEU:HB2	1.70	0.72
1:D:64:VAL:CG1	1:D:94:LEU:HB3	2.19	0.72
1:B:608:THR:HG23	1:B:609:PRO:HD2	1.71	0.72
1:D:122:ASP:HA	1:D:124:ILE:CG1	2.20	0.72
1:C:101:VAL:HG21	1:C:106:LEU:HD21	1.72	0.72
1:C:71:ILE:HG21	1:C:87:GLU:OE1	1.89	0.72
1:A:65:ILE:HA	1:A:68:ILE:HD11	1.71	0.71
1:C:84:LYS:HB3	1:C:87:GLU:HG2	1.70	0.71
1:D:24:LYS:NZ	4:D:1004:HOH:O	2.23	0.70
1:D:64:VAL:O	1:D:68:ILE:HG13	1.92	0.70
1:C:787:ALA:HB1	1:C:809:ALA:HB1	1.74	0.69
1:D:87:GLU:HA	1:D:90:THR:OG1	1.93	0.69
1:A:59:ALA:HB1	1:A:95:LEU:HD23	1.75	0.68
1:A:125:VAL:O	1:A:125:VAL:HG12	1.91	0.68
1:D:608:THR:HG23	1:D:609:PRO:HD2	1.75	0.68
1:B:62:GLY:HA2	1:B:63:ASN:C	2.13	0.67
1:C:71:ILE:HA	1:C:74:LYS:HB3	1.76	0.67
1:D:108:ARG:NH1	1:D:111:ASP:HB3	2.09	0.67
1:D:796:ASN:ND2	1:D:798:GLY:H	1.93	0.66
1:A:88:ILE:C	1:A:90:THR:H	1.98	0.66
1:C:126:GLN:OE1	1:C:126:GLN:HA	1.94	0.66
1:B:155:LYS:O	1:B:163:VAL:HG22	1.96	0.66
1:C:74:LYS:HG2	1:C:74:LYS:O	1.95	0.66
1:A:71:ILE:O	1:A:72:LYS:HB2	1.96	0.65
1:C:345:ILE:HG23	1:C:350:SER:OG	1.96	0.65
1:B:64:VAL:HG13	1:B:94:LEU:HD12	1.78	0.65
1:C:60:PHE:HA	1:C:64:VAL:HG21	1.78	0.65
1:C:249:ASN:ND2	4:C:1006:HOH:O	2.30	0.65
1:C:608:THR:HG22	1:C:610:GLU:H	1.62	0.65
1:B:708:LEU:HD13	1:B:810:TYR:CE2	2.31	0.65
1:A:88:ILE:C	1:A:90:THR:N	2.48	0.65
1:B:64:VAL:HG13	1:B:94:LEU:HD11	1.77	0.65
1:A:628:LEU:HA	1:A:633:MET:HE3	1.79	0.64
1:B:39:TYR:HH	1:B:400:TYR:HH	1.44	0.64
1:C:157:ASP:OD1	1:C:161:ASN:HB3	1.97	0.64
1:A:167:LYS:NZ	1:A:168:LEU:O	2.23	0.64
1:A:812:GLN:O	1:A:815:LYS:HD3	1.98	0.64
1:C:128:ILE:HD12	1:C:128:ILE:H	1.62	0.64
1:D:15:ALA:O	1:D:356:THR:HA	1.97	0.64
1:D:83:PHE:HE1	1:D:91:ILE:HD11	1.63	0.63
1:D:737:SER:OG	1:D:739:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:O	1:D:97:LEU:N	2.32	0.63
1:A:15:ALA:O	1:A:356:THR:HA	1.99	0.63
1:C:606[A]:SER:HB3	1:C:612:ASN:HA	1.80	0.63
1:C:608:THR:HB	1:C:611:ILE:HB	1.79	0.63
1:D:128:ILE:O	1:D:132:LEU:HG	1.99	0.63
1:C:330:ARG:HH22	1:C:346:GLN:HG2	1.63	0.62
1:B:124:ILE:O	1:B:128:ILE:HD12	2.00	0.62
1:A:312:LEU:HD11	1:C:312:LEU:HD11	1.80	0.62
1:A:125:VAL:HG13	1:A:127:GLN:HG3	1.82	0.62
1:A:108:ARG:HA	1:A:111:ASP:CB	2.31	0.61
1:A:64:VAL:O	1:A:68:ILE:HG12	2.01	0.61
1:A:635:GLN:HG2	1:A:658:TRP:CE2	2.36	0.61
1:B:292:GLU:O	4:B:1001:HOH:O	2.16	0.61
1:C:85:GLN:O	1:C:88:ILE:HB	2.01	0.60
1:B:6:TYR:CE1	1:B:155:LYS:HG2	2.36	0.60
1:C:152:TYR:CD2	1:C:165:LYS:HE2	2.36	0.60
1:B:174:VAL:O	1:B:246:SER:HB2	2.01	0.60
1:C:95:LEU:O	1:C:97:LEU:N	2.34	0.60
1:B:75:LEU:O	1:B:78:ARG:HG3	2.01	0.60
1:C:71:ILE:CG2	1:C:74:LYS:HD3	2.28	0.60
1:D:60:PHE:CE2	1:D:129:LYS:HG3	2.36	0.60
1:D:98:SER:CB	1:D:103:GLN:HG2	2.31	0.60
1:B:90:THR:O	1:B:94:LEU:HD23	2.01	0.60
1:C:98:SER:HB3	1:C:103:GLN:OE1	2.02	0.59
1:C:391:GLN:HB3	4:C:1194:HOH:O	2.01	0.59
1:D:89:GLU:O	1:D:92:THR:OG1	2.20	0.59
1:C:94:LEU:HD12	1:C:95:LEU:HG	1.83	0.59
1:A:48:THR:HB	4:A:1243:HOH:O	2.02	0.59
1:B:64:VAL:O	1:B:68:ILE:HG12	2.02	0.59
1:D:662:SER:OG	4:D:1003:HOH:O	2.16	0.59
1:C:466:PRO:HA	1:C:471:ASN:OD1	2.02	0.59
1:B:608:THR:HG22	1:B:610:GLU:H	1.67	0.59
1:B:71:ILE:O	1:B:75:LEU:HD23	2.02	0.58
1:C:113:LEU:HD21	1:C:127:GLN:NE2	2.17	0.58
1:D:88:ILE:HG23	1:D:110:LEU:HD12	1.84	0.58
1:A:814:ASP:OD1	1:D:690:ASP:HB3	2.04	0.58
1:C:71:ILE:HG23	1:C:74:LYS:HB3	1.84	0.58
1:C:86:GLU:OE1	1:C:90:THR:OG1	2.18	0.58
1:B:71:ILE:HG22	1:B:75:LEU:HD23	1.86	0.58
1:D:98:SER:OG	1:D:103:GLN:HG2	2.04	0.58
1:A:366:GLU:OE1	1:A:401:ARG:NE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASN:O	1:D:69:SER:HB3	2.04	0.58
1:B:278:GLU:N	4:B:1006:HOH:O	2.36	0.57
1:A:756:LEU:O	1:A:761[A]:LEU:HD12	2.05	0.57
1:C:71:ILE:HG22	1:C:71:ILE:O	2.04	0.57
1:B:256:ARG:NH2	4:B:1004:HOH:O	2.30	0.57
1:B:564[B]:ASN:N	1:B:564[B]:ASN:OD1	2.37	0.57
1:B:15:ALA:O	1:B:356:THR:HA	2.04	0.57
1:D:85:GLN:O	1:D:89:GLU:HB2	2.06	0.56
1:C:366:GLU:OE1	1:C:401:ARG:NE	2.35	0.56
1:D:335:VAL:HB	1:D:343:PHE:HB2	1.88	0.56
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.87	0.56
1:B:424:GLU:HB2	1:C:736:MET:HE2	1.86	0.56
1:B:82:LYS:HZ2	1:B:82:LYS:HB3	1.70	0.56
1:B:163:VAL:HG23	1:B:164:GLU:H	1.71	0.56
1:B:6:TYR:HB2	1:B:345:ILE:HD11	1.88	0.56
1:D:68:ILE:CD1	1:D:125:VAL:HG23	2.36	0.56
1:D:367:PRO:O	1:D:401:ARG:HD3	2.06	0.56
1:A:68:ILE:O	1:A:71:ILE:HB	2.06	0.55
1:B:554:PHE:O	1:B:558:GLN:HG2	2.07	0.55
1:C:69:SER:HA	1:C:72:LYS:HB3	1.87	0.55
1:C:680:ALA:HB3	1:C:776:LEU:HD22	1.89	0.55
1:D:453:ARG:HG2	1:D:518:ALA:HB2	1.89	0.55
1:B:76:ASP:HB3	1:B:79:LYS:HZ1	1.72	0.55
1:D:435:LEU:HD23	1:D:537:VAL:HG21	1.89	0.55
1:B:61:GLY:O	1:B:64:VAL:HG23	2.07	0.54
1:B:76:ASP:HB3	1:B:79:LYS:HZ2	1.69	0.54
1:D:562:SER:HB3	1:D:568:LEU:HD11	1.88	0.54
1:A:59:ALA:CB	1:A:95:LEU:HD23	2.36	0.54
1:A:71:ILE:O	1:A:72:LYS:CB	2.55	0.54
1:B:708:LEU:HD13	1:B:810:TYR:CZ	2.42	0.54
1:C:110:LEU:CD2	1:C:128:ILE:HG23	2.38	0.54
1:C:155:LYS:O	1:C:163:VAL:HG22	2.08	0.54
1:C:15:ALA:O	1:C:356:THR:HA	2.08	0.54
1:A:110:LEU:HD21	1:A:128:ILE:HG23	1.90	0.54
1:C:756:LEU:O	1:C:761[A]:LEU:HD12	2.08	0.54
1:D:68:ILE:CG2	1:D:124:ILE:HD12	2.38	0.53
1:B:227:ASN:HB3	4:B:1198:HOH:O	2.08	0.53
1:C:606[A]:SER:HB2	1:C:608:THR:O	2.09	0.53
1:B:174:VAL:HG12	1:B:247:SER:OG	2.08	0.53
1:D:5:GLN:HG2	1:D:343:PHE:CD1	2.43	0.53
1:B:503:PRO:HB3	1:B:507:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:HG2	1:B:518:ALA:HB2	1.90	0.53
1:D:102:PRO:O	1:D:106:LEU:HD12	2.07	0.53
1:A:177:ARG:NH1	1:A:242:GLN:OE1	2.42	0.53
1:B:167:LYS:HD3	1:B:169:THR:HG23	1.89	0.53
1:C:163:VAL:HG23	1:C:164:GLU:HG2	1.90	0.53
1:A:26:LEU:HD21	1:A:52:LEU:HD23	1.90	0.53
1:A:395[A]:VAL:HG13	1:A:527:LEU:HD12	1.91	0.52
1:B:606[A]:SER:HB3	1:B:612:ASN:HA	1.91	0.52
1:C:69:SER:HA	1:C:72:LYS:CB	2.40	0.52
1:A:590:TRP:CG	1:A:591:PRO:HD3	2.45	0.52
1:B:767:ALA:O	1:C:483:LYS:HD3	2.10	0.52
1:A:109:SER:OG	1:A:131:ALA:HB1	2.10	0.52
1:D:122:ASP:HA	1:D:124:ILE:CD1	2.39	0.52
1:D:110:LEU:CD2	1:D:132:LEU:HD21	2.38	0.52
1:D:62:GLY:O	1:D:64:VAL:N	2.42	0.52
1:A:106:LEU:O	1:A:109:SER:HB3	2.10	0.52
1:B:485[A]:GLU:CD	1:B:485[A]:GLU:H	2.14	0.51
1:D:98:SER:HB3	1:D:103:GLN:HG2	1.93	0.51
1:D:83:PHE:CE1	1:D:91:ILE:HD11	2.43	0.51
1:D:122:ASP:OD1	1:D:124:ILE:HD11	2.10	0.51
1:D:157:ASP:OD1	1:D:161:ASN:HB3	2.11	0.51
1:D:624:ASP:OD2	1:D:630:SER:OG	2.27	0.51
1:A:228[B]:VAL:HG22	1:A:228[B]:VAL:O	2.11	0.51
1:B:717[B]:SER:OG	1:B:796[B]:ASN:HB2	2.11	0.51
1:D:122:ASP:O	1:D:125:VAL:HG12	2.10	0.51
1:A:814:ASP:OD1	1:D:690:ASP:CB	2.59	0.51
1:A:128:ILE:HG22	1:A:132:LEU:HD11	1.92	0.51
1:B:459:GLN:O	1:B:461:ILE:HG23	2.11	0.51
1:A:92:THR:OG1	1:A:103:GLN:NE2	2.44	0.51
1:C:504:ASN:CG	1:C:505:ASP:H	2.14	0.51
1:D:45:TYR:CD2	1:D:790:MET:HG2	2.46	0.51
1:C:423[A]:ARG:HH11	1:C:423[A]:ARG:HB3	1.76	0.51
1:D:436:ASP:OD1	1:D:438:SER:HB3	2.10	0.50
1:C:8:ILE:HG13	1:C:345:ILE:HG21	1.93	0.50
1:B:204:GLY:O	1:B:521:PRO:HD2	2.11	0.50
1:C:156:CYS:HG	1:C:161:ASN:N	2.10	0.50
1:D:88:ILE:HG23	1:D:110:LEU:CD1	2.41	0.50
1:B:696:TRP:HB3	1:B:697:TGH:CD2	2.41	0.50
1:C:453:ARG:HG2	1:C:518:ALA:HB2	1.93	0.50
1:A:108:ARG:HA	1:A:111:ASP:HB2	1.93	0.50
1:B:155:LYS:CE	1:B:166:LEU:HA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:797:PRO:HB3	1:C:802:ILE:O	2.11	0.50
1:A:108:ARG:HA	1:A:111:ASP:HB3	1.93	0.50
1:D:426:ASN:HD21	1:D:548:ILE:HG22	1.77	0.50
1:D:122:ASP:HA	1:D:124:ILE:HD11	1.94	0.50
1:C:291:ASN:OD1	1:C:292:GLU:N	2.45	0.50
1:C:680:ALA:HB3	1:C:776:LEU:CD2	2.42	0.50
1:B:449:PHE:CZ	1:B:528[B]:GLN:HG3	2.46	0.49
1:C:88:ILE:HD13	1:C:88:ILE:H	1.78	0.49
1:B:167:LYS:HE3	1:B:169:THR:HG22	1.92	0.49
1:A:743:HIS:HD2	3:A:902:SO4:O1	1.96	0.49
1:D:74:LYS:O	1:D:77:GLU:HB3	2.12	0.49
1:B:278:GLU:HA	1:B:278:GLU:OE1	2.13	0.49
1:C:364:GLN:O	1:C:404:ARG:NH2	2.44	0.49
1:C:278:GLU:OE1	4:C:1002:HOH:O	2.20	0.49
1:D:55:LEU:HD13	1:D:55:LEU:O	2.13	0.49
1:D:590:TRP:O	1:D:593:ARG:HG2	2.12	0.49
1:D:64:VAL:HG12	1:D:94:LEU:HB3	1.94	0.49
1:B:69:SER:O	1:B:73:THR:HG23	2.13	0.49
1:D:57:GLU:OE1	1:D:58:GLU:HG3	2.12	0.48
1:B:707:PRO:HG2	1:B:710:ARG:HG2	1.95	0.48
1:B:77:GLU:HA	1:B:77:GLU:OE1	2.13	0.48
1:C:110:LEU:HD21	1:C:128:ILE:HG23	1.95	0.48
1:C:85:GLN:HA	1:C:88:ILE:HG12	1.94	0.48
1:A:539:GLN:O	1:A:543:GLU:HG2	2.13	0.48
1:D:82:LYS:N	1:D:114:GLU:HA	2.29	0.48
1:D:312:LEU:HD13	1:D:777:ILE:HD13	1.95	0.48
1:A:54:GLN:HA	1:A:54:GLN:NE2	2.29	0.48
1:A:65:ILE:HD12	1:A:65:ILE:C	2.34	0.48
1:B:346:GLN:HA	1:B:351:SER:OG	2.13	0.48
1:C:4:CYS:SG	1:C:7:LYS:HE3	2.54	0.48
1:D:696:TRP:HB3	1:D:697:TGH:CD2	2.44	0.48
1:A:49:GLN:NE2	1:A:133:LEU:HD21	2.24	0.47
1:B:20:GLY:O	1:B:146:LYS:HE2	2.14	0.47
1:B:520:PRO:HG2	1:B:523[B]:MET:HG3	1.96	0.47
1:A:208:LYS:HB3	1:A:208:LYS:HE2	1.52	0.47
1:A:398[B]:ILE:HD12	1:A:519:ILE:HG21	1.96	0.47
1:B:756:LEU:O	1:B:761:LEU:HD12	2.14	0.47
1:C:130:GLY:O	1:C:134:LYS:HG3	2.14	0.47
1:D:101:VAL:HB	1:D:106:LEU:HD11	1.96	0.47
1:A:395[A]:VAL:HG21	1:A:530:TRP:HB2	1.95	0.47
1:B:154:TYR:CZ	1:B:165:LYS:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PHE:CD2	1:B:414:THR:HG23	2.49	0.47
1:A:128:ILE:HG22	1:A:132:LEU:CD1	2.44	0.47
1:B:98:SER:HB3	1:B:103:GLN:NE2	2.29	0.47
1:C:101:VAL:CG2	1:C:106:LEU:HD21	2.42	0.47
1:C:84:LYS:HB3	1:C:87:GLU:CG	2.41	0.47
1:B:101:VAL:HG13	1:B:102:PRO:HD2	1.97	0.47
1:C:585:GLY:HA2	1:C:697:TGH:CZ2	2.44	0.47
1:C:88:ILE:HD13	1:C:88:ILE:N	2.29	0.47
1:D:597:ILE:O	1:D:597:ILE:HG13	2.14	0.47
1:C:60:PHE:CA	1:C:64:VAL:HG21	2.43	0.47
1:A:585:GLY:HA2	1:A:697:TGH:CZ2	2.45	0.47
1:D:153:ILE:HD12	1:D:345:ILE:HD12	1.97	0.47
1:B:171:GLY:HA3	1:B:338:LYS:HB3	1.97	0.47
1:B:16:ARG:HG2	1:B:357:THR:OG1	2.15	0.47
1:B:77:GLU:OE1	1:B:77:GLU:CA	2.63	0.47
1:A:589:THR:HG23	1:A:591:PRO:HD2	1.97	0.46
1:B:155:LYS:HE2	1:B:166:LEU:HA	1.97	0.46
1:B:76:ASP:HA	1:B:79:LYS:HG3	1.95	0.46
1:C:45:TYR:CD2	1:C:790:MET:HG2	2.49	0.46
1:D:503:PRO:HB3	1:D:507:ILE:HD13	1.97	0.46
1:A:514:VAL:HG12	1:A:514:VAL:O	2.15	0.46
1:B:738:GLU:O	1:B:742:GLU:HG2	2.16	0.46
1:A:464:ASP:O	1:A:465:ASP:C	2.53	0.46
1:A:814:ASP:HA	1:A:815:LYS:O	2.15	0.46
1:B:24:LYS:N	1:B:25:PRO:HD2	2.30	0.46
1:B:576:ALA:HB3	4:B:1085:HOH:O	2.13	0.46
1:C:112:ASN:O	1:C:113:LEU:HB2	2.15	0.46
1:D:222:LYS:NZ	4:D:1008:HOH:O	2.35	0.46
1:C:124:ILE:CG2	1:C:124:ILE:O	2.64	0.46
1:D:163:VAL:HG13	1:D:164:GLU:N	2.30	0.46
4:C:1238:HOH:O	1:D:472:GLU:HG2	2.16	0.46
1:A:163:VAL:HG23	1:A:164:GLU:HG2	1.98	0.46
1:B:72:LYS:NZ	1:B:124:ILE:HD11	2.30	0.46
1:D:21:PRO:HB3	1:D:100:LEU:HD23	1.97	0.46
1:D:75:LEU:O	1:D:75:LEU:HG	2.16	0.46
1:B:307:LEU:HB2	1:B:321:ASN:OD1	2.16	0.46
1:D:55:LEU:HD13	1:D:55:LEU:C	2.36	0.46
1:C:84:LYS:HE2	1:C:85:GLN:H	1.81	0.46
1:D:99:HIS:CD2	1:D:99:HIS:H	2.33	0.46
1:A:107:SER:O	1:A:111:ASP:N	2.45	0.46
1:A:590:TRP:CD2	1:A:591:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:NH2	1:C:346:GLN:HG2	2.29	0.46
1:D:568:LEU:HD23	1:D:616:LEU:HD21	1.98	0.46
1:B:182:ASN:HB2	1:B:326:ILE:O	2.17	0.45
1:A:323:PHE:HA	1:A:673:ILE:HD11	1.99	0.45
1:A:443:SER:OG	4:A:1001:HOH:O	2.21	0.45
1:A:751:GLN:HG3	1:D:414:THR:HG21	1.99	0.45
1:B:179:GLU:HB2	1:B:628:LEU:HG	1.99	0.45
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.98	0.45
1:A:787:ALA:HA	1:A:810:TYR:O	2.17	0.45
1:C:73:THR:C	1:C:75:LEU:H	2.20	0.45
1:B:567:LEU:HD23	1:B:567:LEU:N	2.31	0.45
1:A:153:ILE:HD12	1:A:345:ILE:CD1	2.47	0.45
1:A:562:SER:HB3	1:A:568:LEU:HD11	1.99	0.45
1:A:713:LYS:HB3	1:A:748:GLN:HG3	1.99	0.45
1:B:673:ILE:O	1:B:673:ILE:HG23	2.16	0.45
1:C:24:LYS:N	1:C:25:PRO:CD	2.80	0.45
1:C:465:ASP:HA	1:C:466:PRO:HD2	1.46	0.45
1:B:13:GLY:O	1:B:14:ILE:HD13	2.17	0.45
1:B:733:ALA:O	1:B:736:MET:HG2	2.17	0.45
1:A:711:TYR:HA	1:A:714:PHE:CE2	2.52	0.44
1:B:125:VAL:HG23	1:B:126:GLN:N	2.32	0.44
1:B:338:LYS:HG3	1:B:339:ASN:OD1	2.17	0.44
1:C:173:LYS:HG2	1:C:336:GLU:HB2	2.00	0.44
1:A:54:GLN:HA	1:A:54:GLN:HE21	1.83	0.44
1:A:95:LEU:O	1:A:97:LEU:N	2.49	0.44
1:D:504:ASN:CG	1:D:505:ASP:H	2.20	0.44
1:D:594:HIS:O	1:D:597:ILE:HG22	2.17	0.44
1:B:590:TRP:N	1:B:591:PRO:CD	2.81	0.44
1:D:72:LYS:HE2	1:D:124:ILE:HG22	1.98	0.44
1:D:179:GLU:O	1:D:329:GLY:HA3	2.17	0.44
1:D:756:LEU:O	1:D:761:LEU:HD23	2.17	0.44
1:A:606:SER:HB2	1:A:612[A]:ASN:HA	1.99	0.44
1:B:179:GLU:O	1:B:329:GLY:HA3	2.16	0.44
1:C:181:ALA:HA	1:C:239:ILE:O	2.18	0.44
1:D:430:GLY:O	1:D:433:GLN:HG3	2.18	0.44
1:B:78:ARG:HG3	1:B:79:LYS:N	2.33	0.44
1:A:16:ARG:HG2	1:A:357:THR:OG1	2.17	0.44
1:A:302:GLY:HA3	1:A:783:TRP:CZ2	2.53	0.44
1:C:101:VAL:HG23	1:C:106:LEU:HD11	2.00	0.44
1:C:57:GLU:HA	1:C:60:PHE:HB2	2.00	0.44
1:A:66:ASN:O	1:A:70:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:TYR:CB	1:B:345:ILE:HD11	2.48	0.44
1:C:398[B]:ILE:HD13	1:C:398[B]:ILE:HA	1.87	0.44
1:B:239:ILE:HD13	1:B:282:VAL:HG21	2.00	0.43
1:B:84:LYS:H	1:B:87:GLU:CD	2.21	0.43
1:A:249:ASN:OD1	1:A:250:ASN:N	2.51	0.43
1:B:65:ILE:O	1:B:68:ILE:HB	2.18	0.43
1:C:278:GLU:O	1:C:279:ARG:HB2	2.17	0.43
1:C:8:ILE:HG12	1:C:153:ILE:HD13	1.99	0.43
1:D:101:VAL:HG11	1:D:135:VAL:CG1	2.48	0.43
1:D:307:LEU:HB2	1:D:321:ASN:OD1	2.17	0.43
1:A:167:LYS:C	1:A:167:LYS:HD3	2.39	0.43
1:A:367:PRO:O	1:A:401:ARG:HD3	2.19	0.43
1:C:757:HIS:HA	1:C:763:PHE:CZ	2.54	0.43
1:A:223:ARG:HD3	1:A:234:ARG:CZ	2.48	0.43
1:B:84:LYS:HG3	1:B:85:GLN:N	2.34	0.43
1:C:673:ILE:HD12	1:C:674:PRO:HA	2.00	0.43
1:C:408:VAL:HB	1:C:702:PRO:HB3	2.00	0.43
1:C:761[B]:LEU:HD21	1:C:779:MET:HE2	2.01	0.43
1:C:124:ILE:O	1:C:128:ILE:HD12	2.19	0.43
1:C:41:THR:HB	1:C:793:PRO:HD3	2.01	0.43
1:D:88:ILE:CG2	1:D:110:LEU:HD12	2.49	0.43
1:D:743:HIS:ND1	3:D:903:SO4:O4	2.30	0.43
1:B:113:LEU:HD22	1:B:127:GLN:HE22	1.83	0.43
1:B:45:TYR:CD2	1:B:790:MET:HG2	2.54	0.43
1:C:466:PRO:HB3	1:C:471:ASN:OD1	2.18	0.43
1:B:514:VAL:O	1:B:514:VAL:HG12	2.18	0.43
1:C:696:TRP:HB3	1:C:697:TGH:CD2	2.49	0.43
1:B:175:THR:HB	1:B:334:VAL:CG1	2.49	0.43
1:C:485:GLU:H	1:C:485:GLU:CD	2.23	0.43
1:C:85:GLN:HA	1:C:88:ILE:CG1	2.49	0.43
1:D:108:ARG:NH1	1:D:111:ASP:CB	2.79	0.43
1:D:580:GLY:HA2	1:D:581:GLY:C	2.39	0.43
1:D:689:GLU:CD	1:D:689:GLU:H	2.22	0.43
1:A:175:THR:HB	1:A:334[A]:VAL:CG1	2.49	0.43
1:B:739:GLU:HG2	1:B:743:HIS:CE1	2.54	0.43
1:C:347:ASP:OD2	1:C:349:GLN:HB2	2.19	0.43
1:D:113:LEU:O	1:D:114:GLU:HB2	2.18	0.43
1:D:504:ASN:HB2	1:D:517:PHE:N	2.34	0.43
1:A:504:ASN:CG	1:A:505:ASP:H	2.23	0.42
1:C:110:LEU:HD22	1:C:128:ILE:HG23	2.01	0.42
1:C:368:ILE:HG23	1:C:369:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ILE:HG23	1:B:350[A]:SER:OG	2.19	0.42
1:B:68:ILE:HD11	1:B:91:ILE:CG2	2.41	0.42
1:B:7:LYS:HA	1:B:350[A]:SER:OG	2.19	0.42
1:A:624:ASP:HB3	1:A:663:THR:HG22	2.01	0.42
1:A:188:TYR:OH	1:A:636:ASP:HB2	2.18	0.42
1:C:45:TYR:CE2	1:C:363:PRO:HG2	2.54	0.42
1:A:395[A]:VAL:HG13	1:A:527:LEU:CD1	2.49	0.42
1:B:418:VAL:O	1:B:422:ILE:HG13	2.18	0.42
1:B:405:MET:CE	1:B:698:ALA:HB3	2.50	0.42
1:D:108:ARG:HH12	1:D:111:ASP:CB	2.33	0.42
1:D:466:PRO:HA	1:D:471:ASN:HB3	2.02	0.42
1:C:45:TYR:CD2	1:C:363:PRO:HG2	2.55	0.42
1:D:590:TRP:CG	1:D:591:PRO:HD3	2.55	0.42
1:B:223:ARG:HD3	1:B:234:ARG:CZ	2.49	0.42
1:B:386:ASP:N	1:B:386:ASP:OD1	2.50	0.42
1:A:509:TYR:CD1	1:B:639:HIS:HB3	2.54	0.42
1:D:101:VAL:HG21	1:D:136:LEU:HD23	2.01	0.42
1:D:624:ASP:HB3	1:D:663:THR:HG22	2.00	0.42
1:A:466:PRO:HA	1:A:471:ASN:N	2.34	0.42
1:C:71:ILE:HA	1:C:74:LYS:CB	2.47	0.42
1:D:5:GLN:NE2	1:D:343:PHE:CE1	2.88	0.42
1:D:61:GLY:HA2	1:D:62:GLY:HA2	1.55	0.42
1:D:776:LEU:HD23	1:D:776:LEU:N	2.35	0.42
1:A:225:ASN:O	1:A:228[B]:VAL:HG13	2.19	0.42
1:C:85:GLN:CA	1:C:88:ILE:HG12	2.49	0.42
1:B:503:PRO:HD2	1:B:696:TRP:HA	2.02	0.41
1:C:279:ARG:HH11	1:C:279:ARG:HG2	1.85	0.41
1:A:125:VAL:O	1:A:125:VAL:CG1	2.61	0.41
4:B:1135:HOH:O	1:C:740:THR:HG22	2.20	0.41
1:A:6:TYR:CE2	1:A:166:LEU:HD13	2.55	0.41
1:A:508:ASP:OD2	1:A:583:HIS:NE2	2.53	0.41
1:B:617:ARG:HG3	4:B:1069:HOH:O	2.20	0.41
1:C:163:VAL:HG23	1:C:164:GLU:N	2.35	0.41
1:D:696:TRP:HB3	1:D:697:TGH:CE3	2.50	0.41
1:B:39:TYR:OH	1:B:400:TYR:OH	2.17	0.41
1:B:590:TRP:CG	1:B:591:PRO:HD3	2.55	0.41
1:C:14:ILE:O	1:C:149:GLN:HB2	2.20	0.41
1:D:687:THR:HB	1:D:688:PRO:HD2	2.02	0.41
1:B:65:ILE:HD12	1:B:66:ASN:N	2.36	0.41
1:C:323:PHE:HA	1:C:673:ILE:HD11	2.03	0.41
1:C:94:LEU:HD12	1:C:95:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:TYR:HB2	1:D:788:MET:HG2	2.03	0.41
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.86	0.41
1:C:84:LYS:HG3	1:C:85:GLN:N	2.35	0.41
1:D:306:ALA:HB2	1:D:322:TRP:CE2	2.55	0.41
1:A:132:LEU:O	1:A:135:VAL:HG12	2.21	0.41
1:B:339:ASN:N	1:B:339:ASN:OD1	2.53	0.41
1:B:6:TYR:O	1:B:350[A]:SER:OG	2.36	0.41
1:D:480:ILE:HG21	1:D:507:ILE:HD11	2.01	0.41
1:B:695[B]:SER:HB3	1:B:703:VAL:HG21	2.02	0.41
1:D:554:PHE:O	1:D:558:GLN:HG2	2.20	0.41
1:A:344:GLU:HB3	1:A:346:GLN:HG3	2.02	0.41
1:B:695[A]:SER:HB2	1:B:703:VAL:HG21	2.02	0.41
1:A:757:HIS:HA	1:A:763:PHE:CZ	2.56	0.41
1:A:45:TYR:HB2	1:A:788:MET:HG2	2.03	0.41
1:B:172:ASP:OD2	1:B:338:LYS:HG2	2.20	0.41
1:B:97:LEU:HD22	1:B:100:LEU:HD12	2.03	0.41
1:B:306:ALA:HB2	1:B:322:TRP:CE2	2.56	0.41
1:B:564[A]:ASN:ND2	1:B:567:LEU:HG	2.36	0.41
1:D:72:LYS:HE2	1:D:124:ILE:CG2	2.51	0.41
1:A:155:LYS:O	1:A:163:VAL:HG22	2.20	0.40
1:B:155:LYS:HE3	1:B:166:LEU:HA	2.03	0.40
1:D:132:LEU:N	1:D:132:LEU:HD23	2.36	0.40
1:D:156:CYS:HB3	1:D:161:ASN:N	2.36	0.40
1:D:396:PHE:N	1:D:397:PRO:CD	2.84	0.40
1:D:504:ASN:HB2	1:D:516:TRP:C	2.41	0.40
1:D:323:PHE:HA	1:D:673:ILE:HD11	2.04	0.40
1:B:504:ASN:HB2	1:B:516:TRP:C	2.40	0.40
1:C:736:MET:SD	1:C:744:LEU:HD12	2.61	0.40
1:D:101:VAL:CG2	1:D:136:LEU:HD23	2.51	0.40
1:D:71:ILE:C	1:D:74:LYS:NZ	2.75	0.40
1:A:128:ILE:HD12	1:A:128:ILE:H	1.86	0.40
1:B:24:LYS:HA	1:B:27:SER:OG	2.22	0.40
1:C:567:LEU:HD11	1:C:604:VAL:HG11	2.02	0.40
1:C:682:CYS:SG	1:C:701:LEU:HD12	2.60	0.40
1:D:596:LEU:HA	1:D:596:LEU:HD23	1.91	0.40
1:B:113:LEU:HD13	1:B:127:GLN:NE2	2.36	0.40
1:C:171:GLY:HA3	1:C:338:LYS:HE3	2.03	0.40
1:D:91:ILE:HD13	1:D:128:ILE:CD1	2.52	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	766/816 (94%)	733 (96%)	28 (4%)	5 (1%)	22	22
1	B	777/816 (95%)	750 (96%)	25 (3%)	2 (0%)	41	46
1	C	760/816 (93%)	732 (96%)	24 (3%)	4 (0%)	29	31
1	D	769/816 (94%)	734 (95%)	32 (4%)	3 (0%)	34	37
All	All	3072/3264 (94%)	2949 (96%)	109 (4%)	14 (0%)	29	31

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	C	88	ILE
1	D	63	ASN
1	D	96	GLY
1	A	62	GLY
1	A	111	ASP
1	B	63	ASN
1	A	60	PHE
1	C	103	GLN
1	C	279	ARG
1	D	279	ARG
1	B	279	ARG
1	A	96	GLY
1	C	96	GLY

### 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	676/710 (95%)	670 (99%)	6 (1%)	78	88
1	B	687/710 (97%)	675 (98%)	12 (2%)	60	74
1	C	674/710 (95%)	660 (98%)	14 (2%)	53	67
1	D	679/710 (96%)	659 (97%)	20 (3%)	42	54
All	All	2716/2840 (96%)	2664 (98%)	52 (2%)	59	71

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	232	SER
1	A	464	ASP
1	A	569	CYS
1	A	578	TYR
1	A	717	SER
1	B	77	GLU
1	B	84	LYS
1	B	123	ASP
1	B	167	LYS
1	B	279	ARG
1	B	336	GLU
1	B	464	ASP
1	B	465	ASP
1	B	472[A]	GLU
1	B	472[B]	GLU
1	B	569	CYS
1	B	578	TYR
1	C	67	GLU
1	C	69	SER
1	C	84	LYS
1	C	423[A]	ARG
1	C	423[B]	ARG
1	C	424	GLU
1	C	464	ASP
1	C	485	GLU
1	C	556	SER
1	C	575	ASP
1	C	578	TYR
1	C	606[A]	SER
1	C	606[B]	SER
1	C	731	SER
1	D	57	GLU

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Mol	Chain	Res	Type
1	D	63	ASN
1	D	72	LYS
1	D	75	LEU
1	D	82	LYS
1	D	122	ASP
1	D	134	LYS
1	D	256	ARG
1	D	258	LYS
1	D	308	SER
1	D	438	SER
1	D	464	ASP
1	D	485	GLU
1	D	575	ASP
1	D	578	TYR
1	D	600	GLN
1	D	654	SER
1	D	690	ASP
1	D	721	ASP
1	D	796	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	54	GLN
1	A	66	ASN
1	A	103	GLN
1	A	105	GLN
1	A	139	HIS
1	A	743	HIS
1	B	63	ASN
1	B	105	GLN
1	B	546	ASN
1	C	42	ASN
1	C	104	GLN
1	C	127	GLN
1	D	63	ASN
1	D	66	ASN
1	D	99	HIS
1	D	262	ASN
1	D	346	GLN
1	D	612	ASN

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Mol	Chain	Res	Type
1	D	796	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	TGH	C	697	1	15,22,23	2.12	5 (33%)	13,31,33	3.81	6 (46%)
1	TGH	D	697	1	15,22,23	2.42	6 (40%)	13,31,33	3.64	7 (53%)
1	TGH	A	697	1	15,22,23	2.07	5 (33%)	13,31,33	4.53	7 (53%)
1	TGH	B	697	1	15,22,23	1.82	4 (26%)	13,31,33	2.12	4 (30%)

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
1	TGH	C	697	1	-	3/8/14/16	0/2/2/2
1	TGH	D	697	1	-	1/8/14/16	0/2/2/2
1	TGH	A	697	1	-	1/8/14/16	0/2/2/2
1	TGH	B	697	1	-	1/8/14/16	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TGH	CE3-CZ3	5.48	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	697	TGH	CE3-CZ3	4.38	1.45	1.36
1	A	697	TGH	CE3-CZ3	4.28	1.45	1.36
1	D	697	TGH	CZ2-CE2	4.20	1.50	1.42
1	C	697	TGH	CE3-CZ3	4.20	1.45	1.36
1	D	697	TGH	CZ3-CH2	3.70	1.45	1.39
1	A	697	TGH	CZ2-CE2	3.60	1.49	1.42
1	C	697	TGH	CB-CA	-3.58	1.45	1.53
1	C	697	TGH	CH2-CZ2	3.55	1.50	1.40
1	B	697	TGH	CB-CA	-3.39	1.46	1.53
1	C	697	TGH	CZ2-CE2	3.18	1.48	1.42
1	A	697	TGH	CB-CA	-3.11	1.46	1.53
1	D	697	TGH	CH2-CZ2	2.96	1.49	1.40
1	A	697	TGH	CH2-CZ2	2.82	1.48	1.40
1	D	697	TGH	CB-CA	-2.76	1.47	1.53
1	A	697	TGH	CZ3-CH2	2.56	1.44	1.39
1	C	697	TGH	CZ3-CH2	2.54	1.44	1.39
1	B	697	TGH	CH2-CZ2	2.20	1.46	1.40
1	D	697	TGH	CE3-CD2	2.12	1.46	1.42
1	B	697	TGH	CZ2-CE2	2.01	1.46	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	697	TGH	CZ2-CH2-N1	9.33	126.96	117.26
1	A	697	TGH	CZ2-CH2-N1	9.19	126.81	117.26
1	A	697	TGH	CZ3-CH2-CZ2	-7.87	114.82	119.80
1	D	697	TGH	CZ3-CE3-CD2	-7.35	110.91	121.13
1	A	697	TGH	CZ3-CE3-CD2	-6.96	111.46	121.13
1	D	697	TGH	CZ2-CH2-N1	6.67	124.19	117.26
1	A	697	TGH	CE3-CZ3-CH2	5.56	129.95	120.08
1	C	697	TGH	CZ3-CH2-CZ2	-5.53	116.30	119.80
1	D	697	TGH	CE3-CZ3-CH2	5.06	129.06	120.08
1	D	697	TGH	CZ3-CH2-CZ2	-4.95	116.67	119.80
1	A	697	TGH	CH2-N1-C2	-4.59	114.64	123.16
1	C	697	TGH	CZ3-CE3-CD2	-4.44	114.96	121.13
1	B	697	TGH	CZ2-CH2-N1	4.36	121.79	117.26
1	B	697	TGH	CZ3-CE3-CD2	-3.91	115.69	121.13
1	C	697	TGH	CE3-CZ3-CH2	3.80	126.83	120.08
1	C	697	TGH	CZ3-CH2-N1	-3.56	116.60	122.25
1	C	697	TGH	CH2-N1-C2	-3.48	116.70	123.16
1	D	697	TGH	CH2-N1-C2	-2.95	117.68	123.16
1	A	697	TGH	CE3-CD2-CG	-2.89	129.11	134.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	697	TGH	CZ3-CH2-N1	-2.47	118.34	122.25
1	D	697	TGH	CE3-CD2-CG	-2.41	129.99	134.42
1	B	697	TGH	CE3-CD2-CG	-2.36	130.09	134.42
1	B	697	TGH	CZ3-CH2-N1	-2.09	118.93	122.25
1	D	697	TGH	CZ3-CH2-N1	-2.05	118.99	122.25

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	697	TGH	CZ3-CH2-N1-C2
1	A	697	TGH	CZ3-CH2-N1-C2
1	D	697	TGH	CZ3-CH2-N1-C2
1	B	697	TGH	CZ3-CH2-N1-C2
1	C	697	TGH	O1-C2-N1-CH2
1	C	697	TGH	CZ2-CH2-N1-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	697	TGH	2	0
1	D	697	TGH	2	0
1	A	697	TGH	1	0
1	B	697	TGH	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	SO4	C	902	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	D	902	-	4,4,4	0.16	0	6,6,6	0.11	0
3	SO4	A	903	-	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	B	902	-	4,4,4	0.12	0	6,6,6	0.36	0
3	SO4	C	903	-	4,4,4	0.20	0	6,6,6	0.23	0
3	SO4	A	904	-	4,4,4	0.14	0	6,6,6	0.16	0
3	SO4	A	905	-	4,4,4	0.22	0	6,6,6	0.27	0
3	SO4	D	903	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	A	902	-	4,4,4	0.12	0	6,6,6	0.25	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	903	SO4	1	0
3	A	902	SO4	2	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	764/816 (93%)	0.04	38 (4%) 28 27	26, 40, 96, 138	0
1	B	777/816 (95%)	0.21	57 (7%) 15 14	31, 50, 107, 160	0
1	C	768/816 (94%)	0.06	38 (4%) 29 28	26, 42, 101, 150	0
1	D	777/816 (95%)	0.19	65 (8%) 11 9	26, 48, 111, 161	0
All	All	3086/3264 (94%)	0.13	198 (6%) 19 18	26, 45, 105, 161	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	11.2
1	D	113	LEU	7.5
1	B	83	PHE	7.1
1	A	65	ILE	7.1
1	A	68	ILE	6.5
1	B	124	ILE	6.3
1	D	73	THR	6.3
1	C	110	LEU	6.2
1	A	113	LEU	6.2
1	D	68	ILE	6.2
1	D	71	ILE	6.1
1	C	83	PHE	5.9
1	C	94	LEU	5.8
1	D	61	GLY	5.8
1	B	75	LEU	5.5
1	A	94	LEU	5.3
1	C	124	ILE	5.0
1	B	88	ILE	4.8
1	B	128	ILE	4.8
1	B	719	SER	4.7
1	D	62	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	4.6
1	B	107	SER	4.6
1	A	62	GLY	4.6
1	A	60	PHE	4.6
1	B	111	ASP	4.5
1	D	91	ILE	4.5
1	D	82	LYS	4.5
1	A	64	VAL	4.5
1	B	89	GLU	4.5
1	B	68	ILE	4.4
1	B	86	GLU	4.4
1	B	113	LEU	4.3
1	D	122	ASP	4.3
1	C	65	ILE	4.3
1	B	108	ARG	4.3
1	D	112	ASN	4.2
1	D	75	LEU	4.2
1	D	124	ILE	4.2
1	A	128	ILE	4.2
1	B	132	LEU	4.1
1	C	465	ASP	4.1
1	D	123	ASP	4.1
1	D	110	LEU	4.1
1	B	343	PHE	4.0
1	D	56	LEU	4.0
1	C	127	GLN	3.9
1	D	127	GLN	3.9
1	D	466	PRO	3.8
1	C	113	LEU	3.8
1	B	169	THR	3.8
1	D	108	ARG	3.8
1	B	127	GLN	3.8
1	D	87	GLU	3.7
1	C	91	ILE	3.7
1	A	90	THR	3.7
1	C	109	SER	3.6
1	D	114	GLU	3.6
1	B	163	VAL	3.6
1	C	104	GLN	3.6
1	B	4	CYS	3.6
1	D	133	LEU	3.6
1	A	106	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	68	ILE	3.6
1	B	6	TYR	3.6
1	D	126	GLN	3.5
1	A	125	VAL	3.5
1	B	82	LYS	3.5
1	D	131	ALA	3.5
1	D	77	GLU	3.5
1	D	338	LYS	3.5
1	D	97	LEU	3.4
1	A	127	GLN	3.4
1	B	73	THR	3.4
1	C	125	VAL	3.4
1	D	90	THR	3.4
1	D	66	ASN	3.3
1	A	88	ILE	3.3
1	A	109	SER	3.3
1	A	91	ILE	3.3
1	A	126	GLN	3.2
1	B	167	LYS	3.2
1	D	95	LEU	3.2
1	A	92	THR	3.2
1	D	94	LEU	3.2
1	A	61	GLY	3.2
1	D	130	GLY	3.2
1	D	88	ILE	3.2
1	D	129	LYS	3.2
1	D	337	LEU	3.2
1	C	73	THR	3.2
1	D	72	LYS	3.1
1	B	171	GLY	3.1
1	B	71	ILE	3.1
1	D	76	ASP	3.1
1	A	97	LEU	3.0
1	B	104	GLN	3.0
1	B	112	ASN	3.0
1	C	64	VAL	3.0
1	C	88	ILE	3.0
1	B	74	LYS	3.0
1	A	466	PRO	2.9
1	D	169	THR	2.9
1	D	57	GLU	2.9
1	D	104	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	70	GLN	2.9
1	D	128	ILE	2.9
1	C	126	GLN	2.8
1	D	86	GLU	2.8
1	A	101	VAL	2.8
1	A	103	GLN	2.8
1	B	170	ASP	2.8
1	D	125	VAL	2.8
1	A	112	ASN	2.8
1	C	97	LEU	2.8
1	A	95	LEU	2.8
1	A	816	ASP	2.7
1	B	721	ASP	2.7
1	A	161	ASN	2.7
1	B	337	LEU	2.7
1	D	721	ASP	2.7
1	C	70	GLN	2.7
1	B	93	GLY	2.7
1	B	131	ALA	2.7
1	D	65	ILE	2.7
1	C	84	LYS	2.7
1	B	341	ASP	2.6
1	B	76	ASP	2.6
1	C	107	SER	2.6
1	B	106	LEU	2.6
1	B	168	LEU	2.6
1	A	104	GLN	2.6
1	B	110	LEU	2.5
1	D	60	PHE	2.5
1	B	77	GLU	2.5
1	D	111	ASP	2.5
1	C	112	ASN	2.5
1	B	155	LYS	2.5
1	B	340	GLY	2.5
1	C	103	GLN	2.5
1	A	814	ASP	2.5
1	C	111	ASP	2.5
1	C	66	ASN	2.4
1	A	110	LEU	2.4
1	C	60	PHE	2.4
1	D	64	VAL	2.4
1	C	102	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	126	GLN	2.4
1	A	4	CYS	2.4
1	C	132	LEU	2.4
1	D	106	LEU	2.4
1	C	61	GLY	2.4
1	D	699	ALA	2.4
1	D	69	SER	2.4
1	D	134	LYS	2.4
1	B	5	GLN	2.4
1	D	107	SER	2.4
1	D	278	GLU	2.4
1	D	175	THR	2.3
1	D	342	THR	2.3
1	C	336	GLU	2.3
1	D	55	LEU	2.3
1	B	97	LEU	2.3
1	B	105	GLN	2.3
1	D	101	VAL	2.3
1	D	174	VAL	2.3
1	B	63	ASN	2.3
1	D	85	GLN	2.3
1	B	90	THR	2.2
1	B	133	LEU	2.2
1	D	343	PHE	2.2
1	C	71	ILE	2.2
1	C	128	ILE	2.2
1	C	466	PRO	2.2
1	B	408	VAL	2.2
1	C	87	GLU	2.2
1	B	79	LYS	2.2
1	D	170	ASP	2.2
1	A	66	ASN	2.2
1	C	106	LEU	2.2
1	D	132	LEU	2.2
1	B	109	SER	2.1
1	B	722	LEU	2.1
1	B	344	GLU	2.1
1	B	698	ALA	2.1
1	C	340	GLY	2.1
1	C	134	LYS	2.1
1	A	339	ASN	2.1
1	A	102	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	278	GLU	2.1
1	A	129	LYS	2.1
1	A	131	ALA	2.1
1	A	67	GLU	2.0
1	B	78	ARG	2.0
1	B	95	LEU	2.0
1	C	56	LEU	2.0
1	D	84	LYS	2.0
1	D	105	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TGH	C	697	21/22	0.93	0.17	26,44,79,85	0
1	TGH	A	697	21/22	0.93	0.16	23,36,66,71	0
1	TGH	B	697	21/22	0.93	0.20	31,51,95,103	0
1	TGH	D	697	21/22	0.96	0.15	26,47,89,97	0

## 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. 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	A	904	5/5	0.83	0.28	138,139,141,144	0
3	SO4	A	903	5/5	0.87	0.28	108,112,114,115	0
2	MG	C	901	1/1	0.89	0.13	41,41,41,41	0
3	SO4	D	902	5/5	0.90	0.24	106,108,115,117	0
2	MG	B	901	1/1	0.93	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	902	5/5	0.94	0.20	91,97,99,101	0
3	SO4	C	902	5/5	0.94	0.14	102,104,105,106	0
3	SO4	D	903	5/5	0.96	0.14	101,103,105,108	0
3	SO4	C	903	5/5	0.97	0.13	75,77,85,88	0
3	SO4	A	905	5/5	0.97	0.09	65,69,82,86	0
2	MG	D	901	1/1	0.97	0.12	43,43,43,43	0
2	MG	A	901	1/1	0.98	0.12	36,36,36,36	0
3	SO4	A	902	5/5	0.98	0.12	88,92,97,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.