



# Full wwPDB X-ray Structure Validation Report

May 21, 2014 – 02:05 AM EDT

PDB ID : 4KTR  
Title : Crystal structure of 2-O-alpha-glucosylglycerolphosphorylase in complex with isofagomine and glycerol  
Authors : Touhara, K.K.; Nihira, T.; Kitaoka, M.; Nakai, H.; Fushinobu, S.  
Deposited on : 2013-05-21  
Resolution : 2.30 Å(reported)

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

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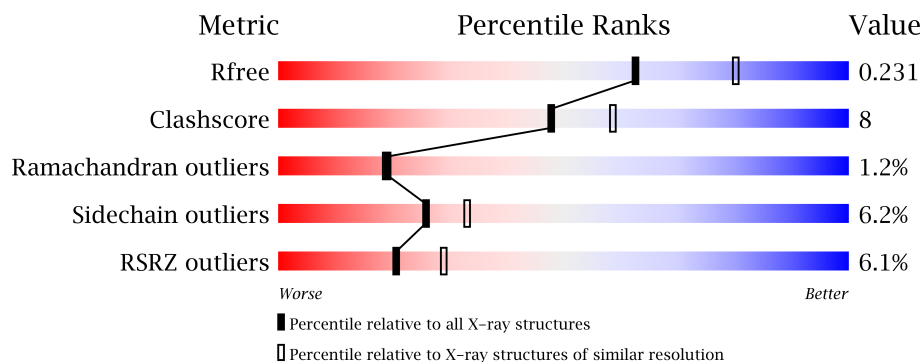
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	769	
1	B	769	
1	C	769	
1	D	769	
1	E	769	
1	F	769	
1	G	769	
1	H	769	

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

Mol	Type	Chain	Res	Geometry	Electron density
10	PE4	C	805	-	X
11	PE5	H	808	-	X
2	IFM	E	801	-	X
2	IFM	F	801	-	X
2	IFM	G	801	-	X
2	IFM	H	801	-	X
3	1PE	A	802	-	X
3	1PE	C	801	-	X
3	1PE	E	802	-	X
4	GOL	A	803	-	X
4	GOL	A	811	-	X
4	GOL	B	805	-	X
4	GOL	B	806	-	X
4	GOL	B	807	-	X
4	GOL	D	802	-	X
4	GOL	D	804	-	X
4	GOL	D	807	-	X
4	GOL	D	809	-	X
4	GOL	E	804	-	X
4	GOL	F	802	-	X
4	GOL	G	802	-	X
4	GOL	G	804	-	X
4	GOL	H	802	-	X
4	GOL	H	805	-	X
6	PGE	A	812	-	X
6	PGE	G	805	-	X
8	PG4	B	801	-	X
8	PG4	D	803	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 51264 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycoside hydrolase family 65 central catalytic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	0	0
			6093	3850	1036	1185	22			
1	B	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	C	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	D	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	E	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	F	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	G	762	Total	C	N	O	S	0	0	0
			6093	3850	1036	1185	22			
1	H	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
A	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
A	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
A	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
B	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
B	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
B	764	HIS	-	EXPRESSION TAG	UNP D6XZ22

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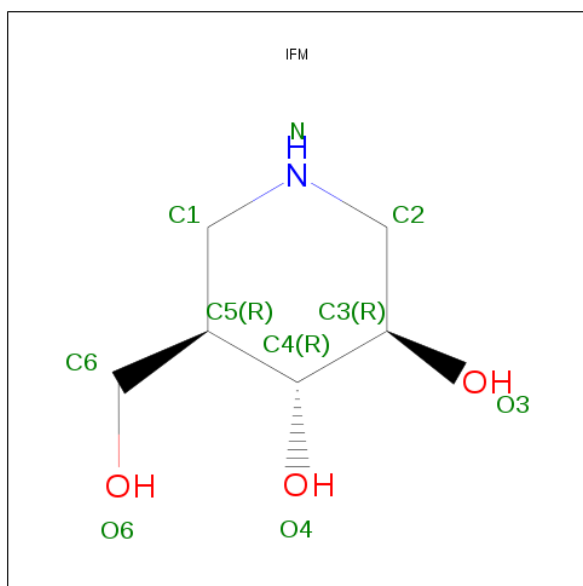
Chain	Residue	Modelled	Actual	Comment	Reference
B	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
C	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
C	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
C	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
D	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
D	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
D	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
E	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
E	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
E	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
F	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
F	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
F	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22

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Chain	Residue	Modelled	Actual	Comment	Reference
G	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
G	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
G	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
H	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
H	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
H	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	769	HIS	-	EXPRESSION TAG	UNP D6XZ22

- Molecule 2 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula:  $C_6H_{13}NO_3$ ).



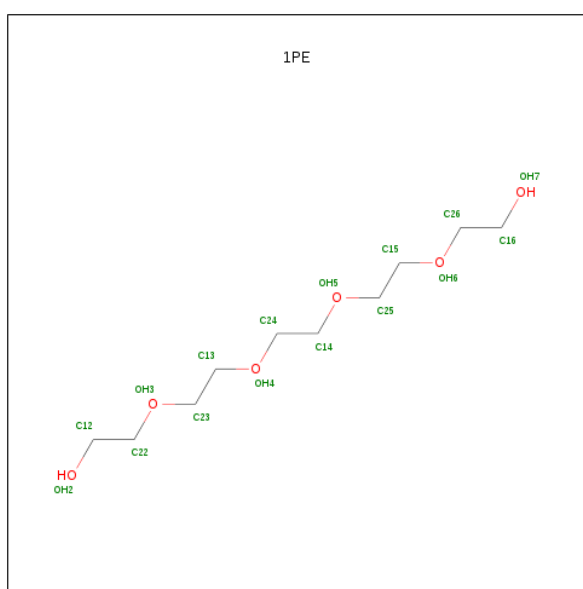
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	D	1	Total	C	N	O	0	0
			10	6	1	3		

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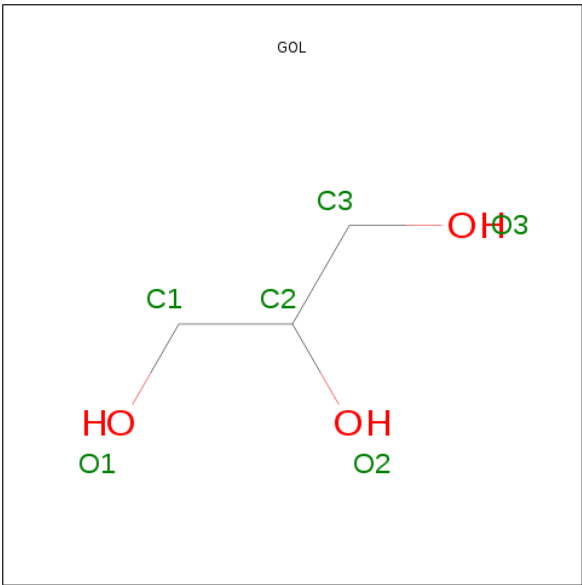
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			10	6	1	3		
2	F	1	Total	C	N	O	0	0
			10	6	1	3		
2	G	1	Total	C	N	O	0	0
			10	6	1	3		
2	H	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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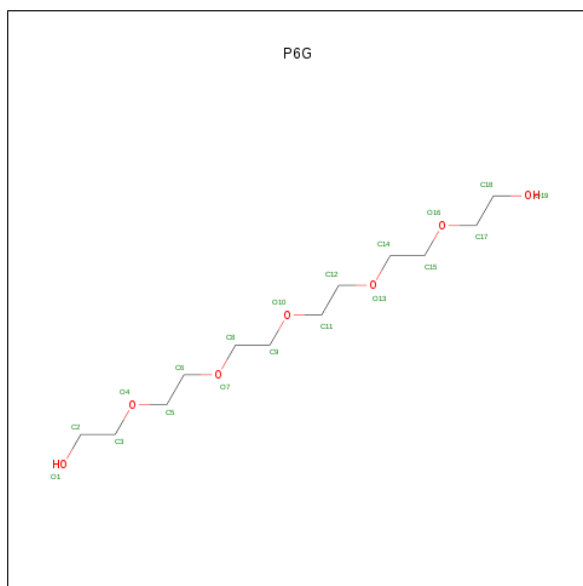
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0

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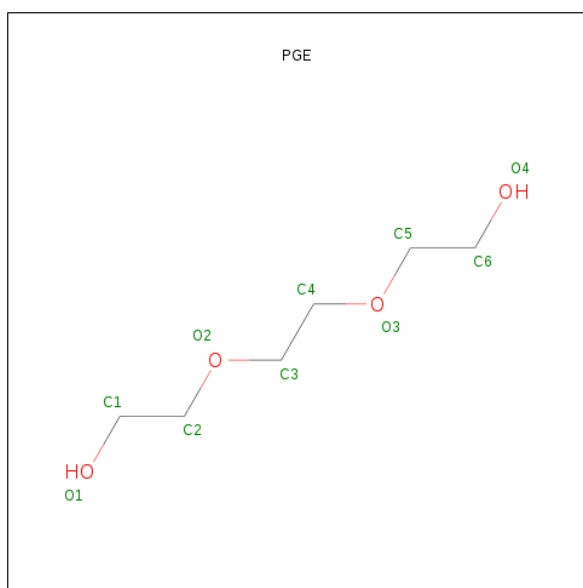
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		
5	E	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).

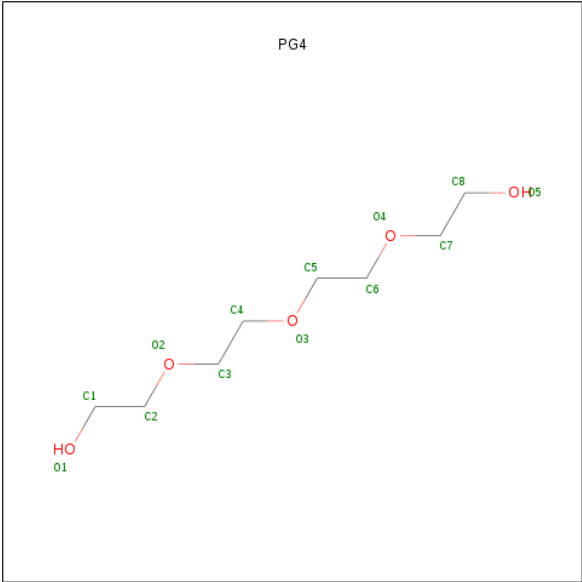


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

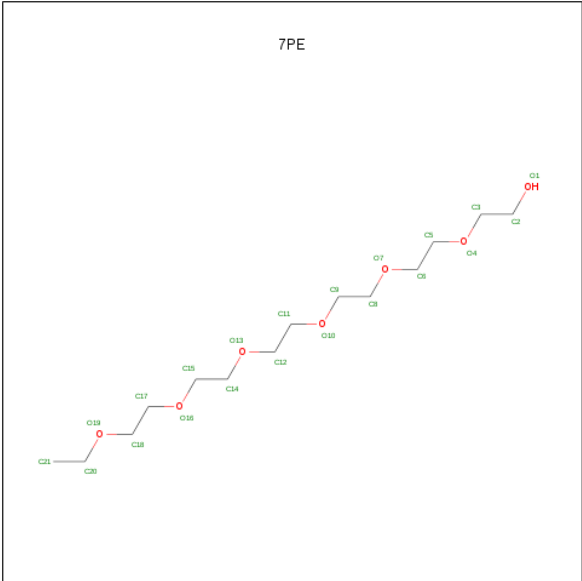
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Ca	0	0
			1	1		
7	D	2	Total	Ca	0	0
			2	2		
7	E	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



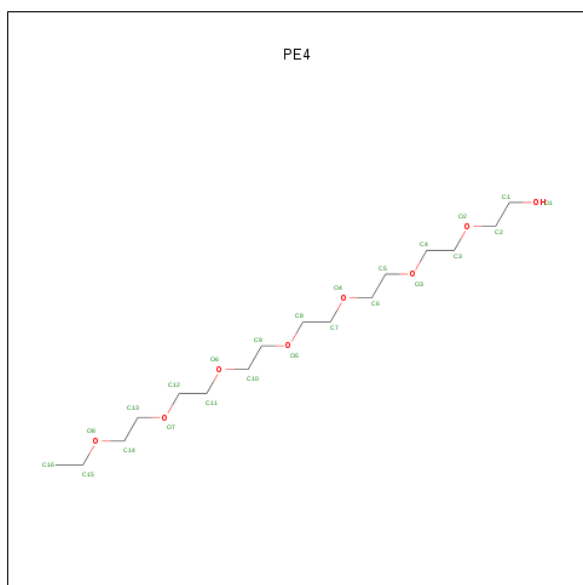
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		
8	D	1	Total	C	O	0	0
			13	8	5		
8	F	1	Total	C	O	0	0
			13	8	5		
8	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 2-(2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (three-letter code: 7PE) (formula: C<sub>14</sub>H<sub>30</sub>O<sub>7</sub>).



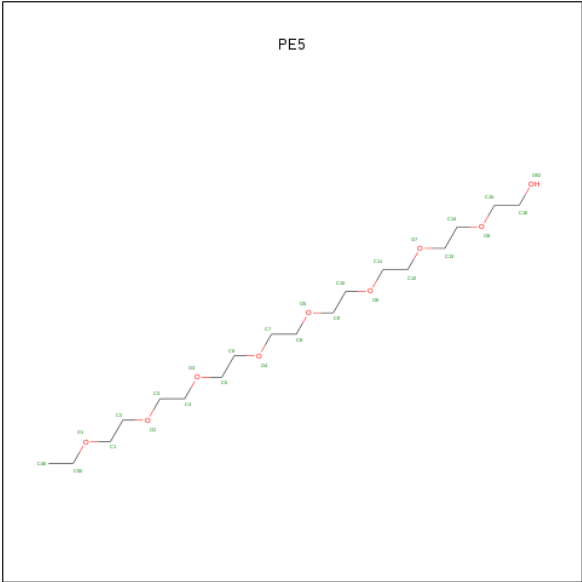
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			21	14	7		
9	D	1	Total	C	O	0	0
			21	14	7		

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			24	16	8		

- Molecule 11 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	O	0	0
			27	18	9		

- Molecule 12 is water.

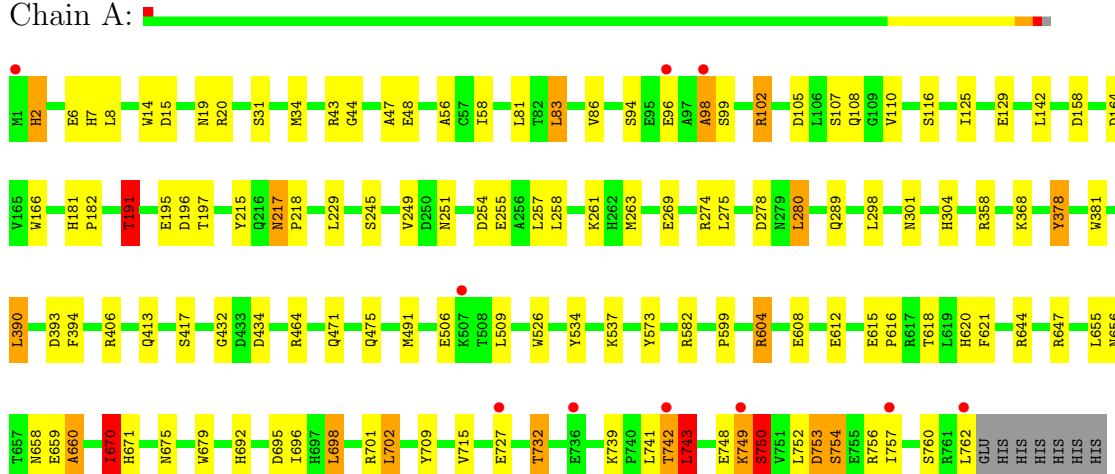
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	182	Total	O	0	0
			182	182		
12	B	303	Total	O	0	0
			303	303		
12	C	286	Total	O	0	0
			286	286		
12	D	348	Total	O	0	0
			348	348		
12	E	185	Total	O	0	0
			185	185		
12	F	247	Total	O	0	0
			247	247		
12	G	197	Total	O	0	0
			197	197		
12	H	218	Total	O	0	0
			218	218		

### 3 Residue-property plots

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

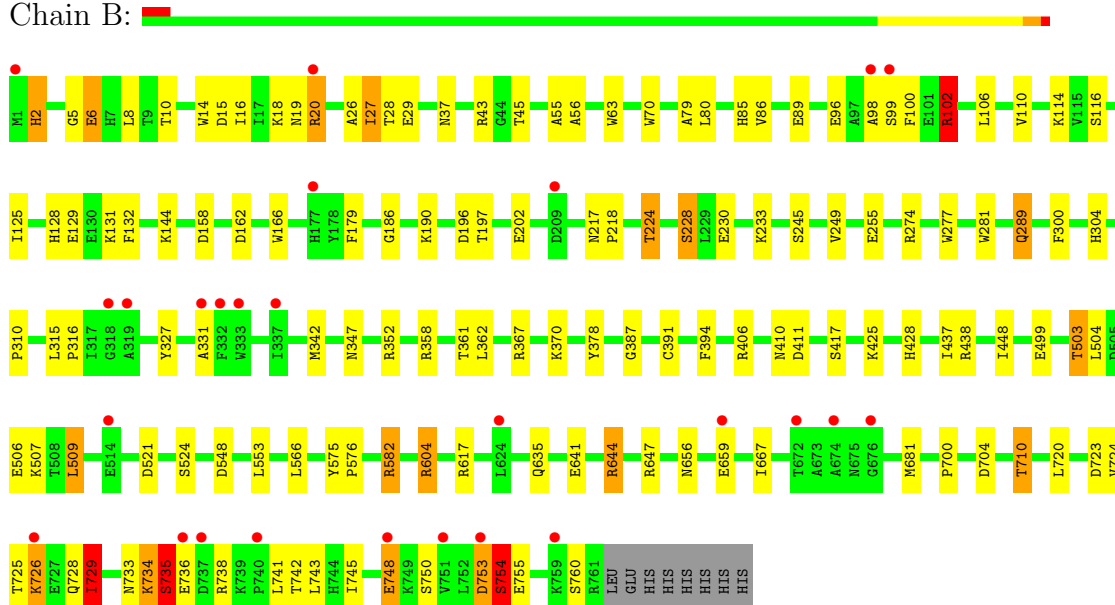
- Molecule 1: Glycoside hydrolase family 65 central catalytic

Chain A:



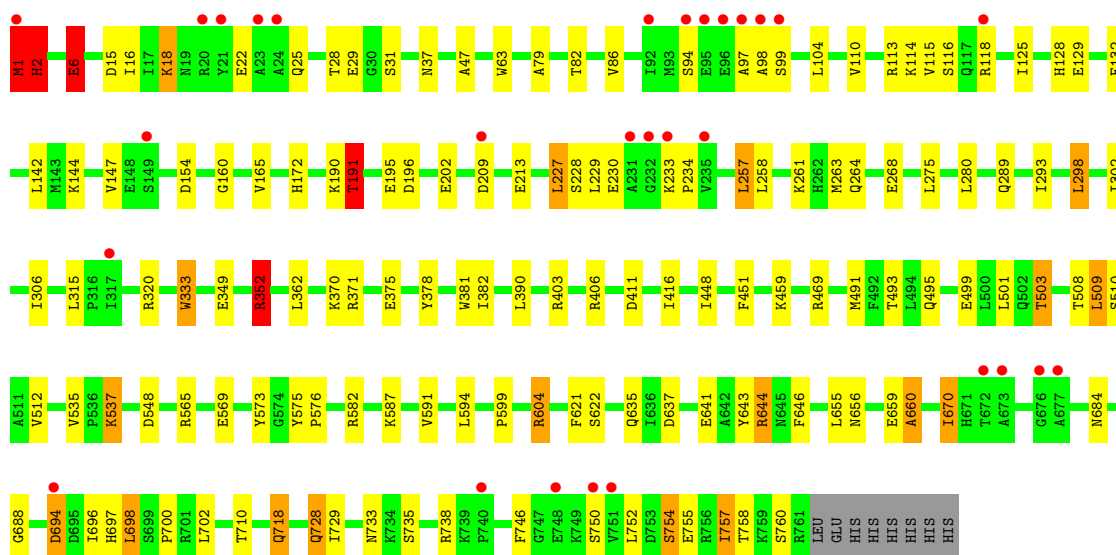
- Molecule 1: Glycoside hydrolase family 65 central catalytic

Chain B:



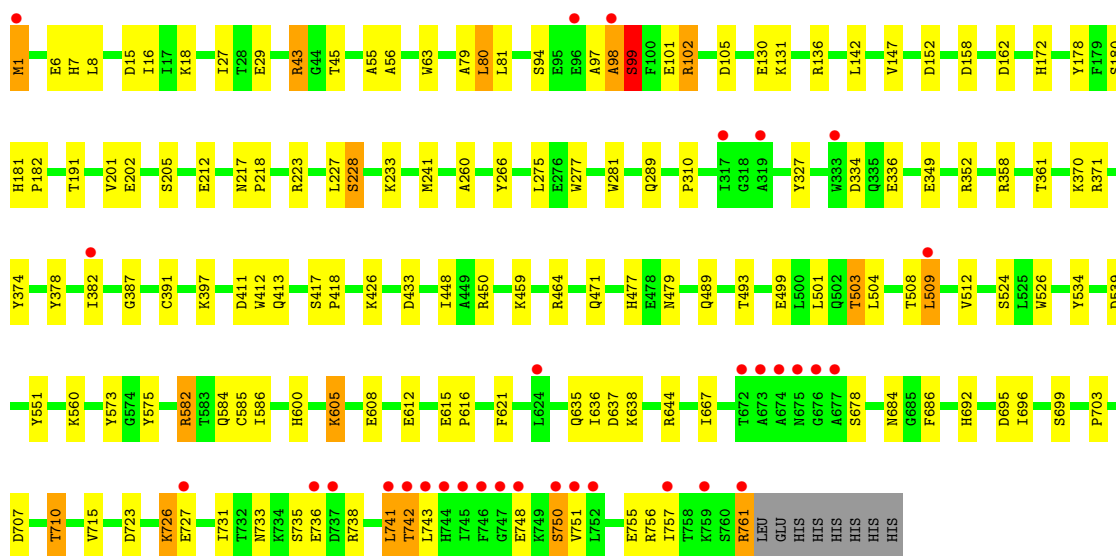
- Molecule 1: Glycoside hydrolase family 65 central catalytic

Chain C:



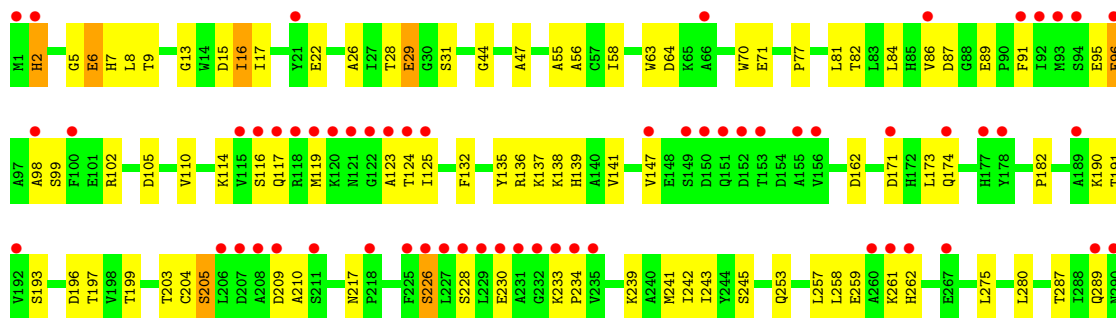
• Molecule 1: Glycoside hydrolase family 65 central catalytic

Chain D:

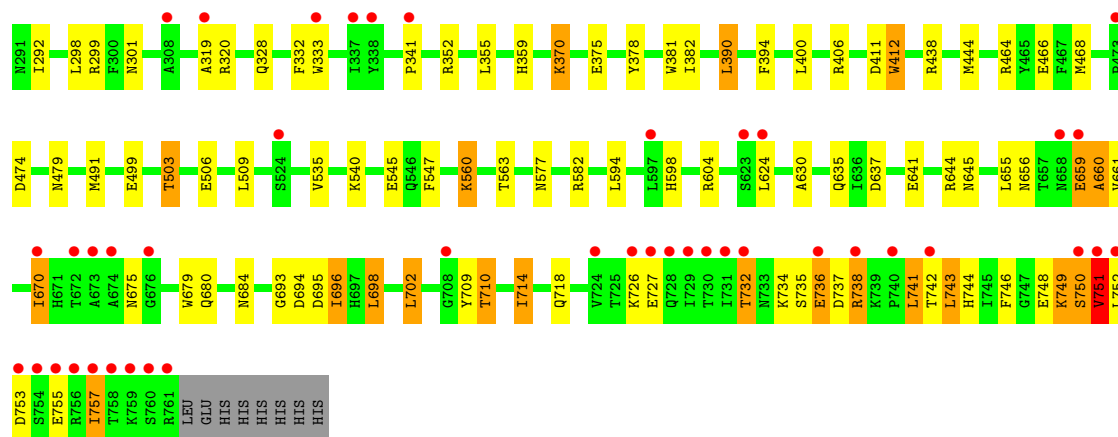


• Molecule 1: Glycoside hydrolase family 65 central catalytic

Chain E:

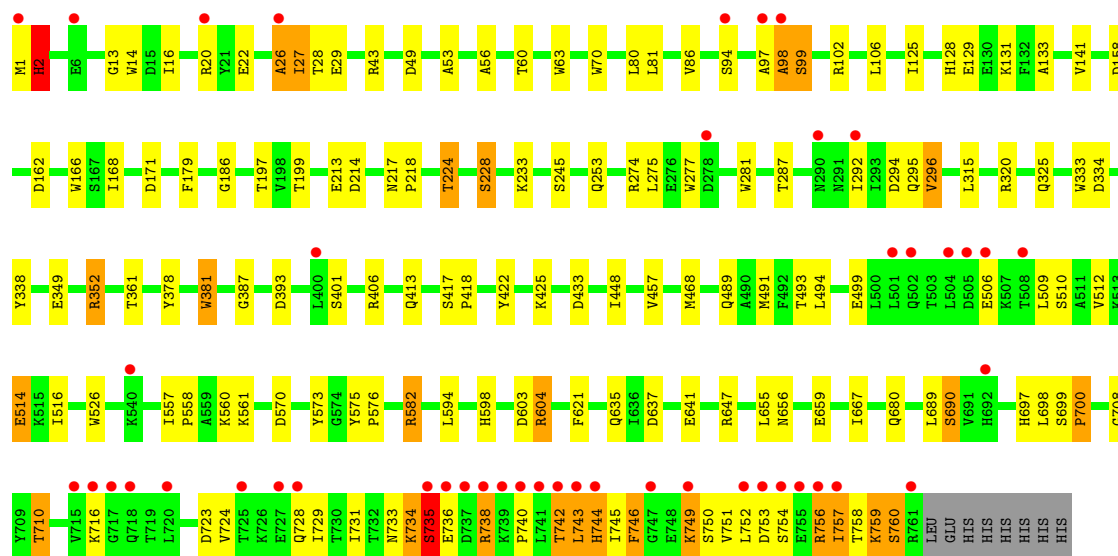






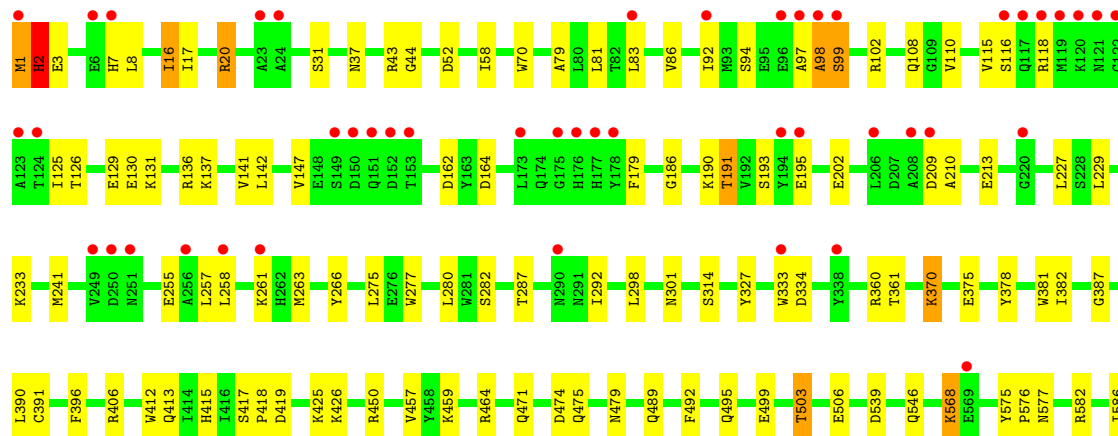
- Molecule 1: Glycoside hydrolase family 65 central catalytic

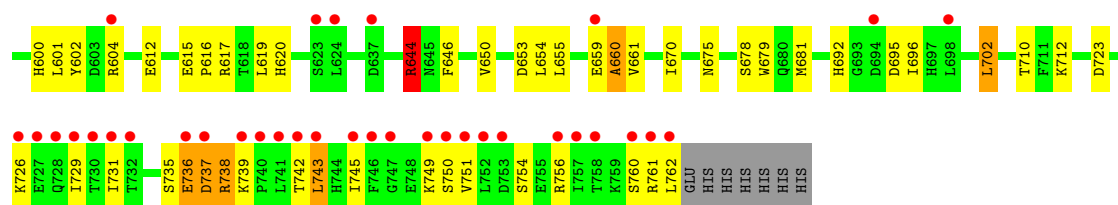
Chain F:



- Molecule 1: Glycoside hydrolase family 65 central catalytic

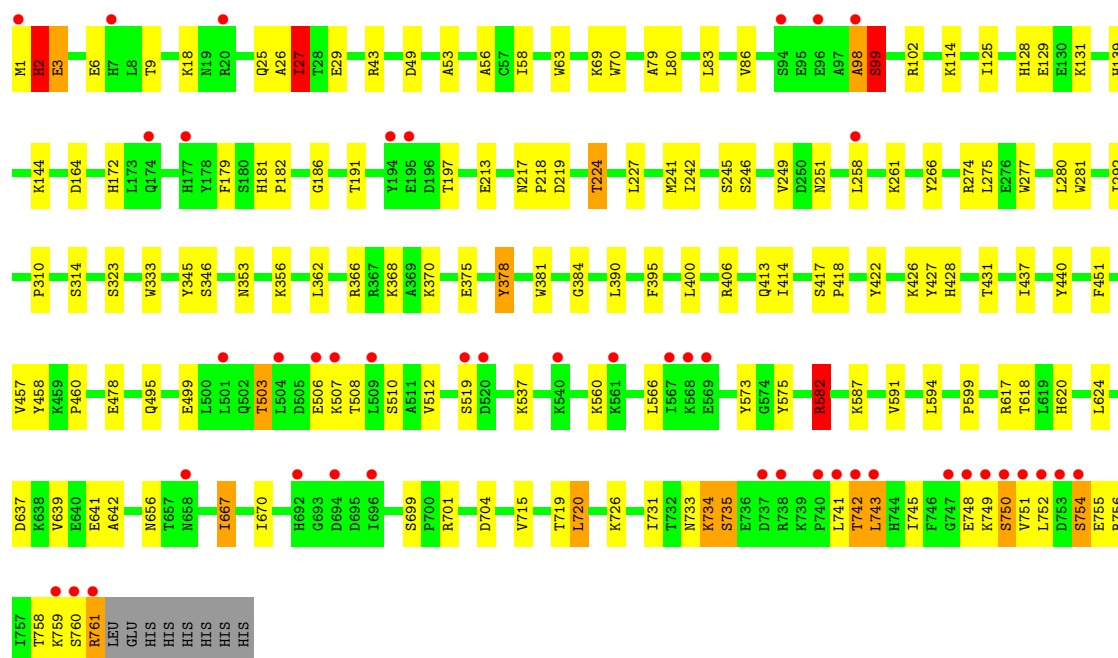
Chain G:





● Molecule 1: Glycoside hydrolase family 65 central catalytic

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.00Å 263.21Å 138.79Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	48.99 – 2.30 48.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.99-2.30) 99.8 (48.99-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.167 , 0.228 0.170 , 0.231	Depositor DCC
$R_{free}$ test set	16702 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 331431 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	51264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, PE4, PE5, CA, 1PE, PG4, P6G, IFM, 7PE

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	0.99	6/6236 (0.1%)	0.98	14/8456 (0.2%)
1	B	0.97	8/6228 (0.1%)	0.99	26/8445 (0.3%)
1	C	0.99	3/6228 (0.0%)	0.99	20/8445 (0.2%)
1	D	1.01	5/6228 (0.1%)	1.00	21/8445 (0.2%)
1	E	0.85	6/6228 (0.1%)	0.90	15/8445 (0.2%)
1	F	0.87	9/6228 (0.1%)	0.91	4/8445 (0.0%)
1	G	0.83	4/6236 (0.1%)	0.88	8/8456 (0.1%)
1	H	0.84	3/6228 (0.0%)	0.87	4/8445 (0.0%)
All	All	0.92	44/49840 (0.1%)	0.94	112/67582 (0.2%)

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	2
1	F	0	1
1	G	0	1
All	All	0	6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	TRP	CD2-CE2	7.43	1.50	1.41
1	B	754	SER	CB-OG	6.83	1.51	1.42
1	E	70	TRP	CD2-CE2	6.81	1.49	1.41
1	F	333	TRP	CD2-CE2	6.40	1.49	1.41
1	F	63	TRP	CD2-CE2	6.39	1.49	1.41
1	C	333	TRP	CD2-CE2	6.38	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	333	TRP	CD2-CE2	6.30	1.49	1.41
1	F	166	TRP	CD2-CE2	6.25	1.48	1.41
1	F	281	TRP	CD2-CE2	6.19	1.48	1.41
1	E	412	TRP	CD2-CE2	6.19	1.48	1.41
1	G	333	TRP	CD2-CE2	6.05	1.48	1.41
1	B	70	TRP	CD2-CE2	6.01	1.48	1.41
1	H	281	TRP	CD2-CE2	5.96	1.48	1.41
1	A	14	TRP	CD2-CE2	5.94	1.48	1.41
1	B	14	TRP	CD2-CE2	5.85	1.48	1.41
1	B	166	TRP	CD2-CE2	5.84	1.48	1.41
1	G	70	TRP	CD2-CE2	5.82	1.48	1.41
1	H	63	TRP	CD2-CE2	5.80	1.48	1.41
1	F	70	TRP	CD2-CE2	5.80	1.48	1.41
1	B	304	HIS	CG-CD2	5.78	1.45	1.35
1	D	277	TRP	CD2-CE2	5.76	1.48	1.41
1	B	281	TRP	CD2-CE2	5.75	1.48	1.41
1	E	679	TRP	CD2-CE2	5.74	1.48	1.41
1	A	381	TRP	CD2-CE2	5.73	1.48	1.41
1	E	63	TRP	CD2-CE2	5.66	1.48	1.41
1	A	679	TRP	CD2-CE2	5.51	1.48	1.41
1	B	277	TRP	CD2-CE2	5.50	1.48	1.41
1	D	526	TRP	CD2-CE2	5.49	1.48	1.41
1	F	14	TRP	CD2-CE2	5.41	1.47	1.41
1	G	277	TRP	CD2-CE2	5.40	1.47	1.41
1	G	679	TRP	CD2-CE2	5.38	1.47	1.41
1	D	281	TRP	CD2-CE2	5.35	1.47	1.41
1	D	678	SER	CB-OG	5.30	1.49	1.42
1	F	526	TRP	CD2-CE2	5.25	1.47	1.41
1	F	381	TRP	CD2-CE2	5.22	1.47	1.41
1	C	63	TRP	CD2-CE2	5.19	1.47	1.41
1	E	381	TRP	CD2-CE2	5.17	1.47	1.41
1	B	63	TRP	CD2-CE2	5.17	1.47	1.41
1	C	381	TRP	CD2-CE2	5.17	1.47	1.41
1	F	277	TRP	CD2-CE2	5.15	1.47	1.41
1	A	166	TRP	CD2-CE2	5.11	1.47	1.41
1	E	333	TRP	CD2-CE2	5.09	1.47	1.41
1	A	191	THR	CB-CG2	-5.05	1.35	1.52
1	A	526	TRP	CD2-CE2	5.03	1.47	1.41

All (112) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ARG	NE-CZ-NH2	12.77	126.69	120.30
1	D	102	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	A	670	ILE	CG1-CB-CG2	-11.80	85.43	111.40
1	E	438	ARG	NE-CZ-NH1	-9.91	115.35	120.30
1	B	644	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	E	438	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	C	406	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	C	352	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	C	406	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	406	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	E	406	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	B	644	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	D	16	ILE	CG1-CB-CG2	-7.81	94.23	111.40
1	A	15	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	406	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	E	406	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	D	43	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	B	102	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	B	102	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	C	411	ASP	CB-CG-OD2	7.12	124.71	118.30
1	D	43	ARG	NE-CZ-NH2	7.05	123.82	120.30
1	B	729	ILE	CB-CA-C	-6.97	97.66	111.60
1	D	539	ASP	CB-CG-OD1	6.93	124.53	118.30
1	C	670	ILE	CG1-CB-CG2	-6.90	96.21	111.40
1	H	582	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	D	15	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	367	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	390	LEU	CB-CG-CD1	6.64	122.28	111.00
1	C	698	LEU	CA-CB-CG	6.59	130.45	115.30
1	B	358	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	D	223	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	617	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	B	15	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	521	ASP	CB-CG-OD1	6.44	124.10	118.30
1	C	644	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	F	393	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	565	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	698	LEU	CA-CB-CG	6.33	129.85	115.30
1	G	464	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	G	644	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	F	433	ASP	CB-CG-OD1	6.17	123.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	320	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	G	702	LEU	CA-CB-CG	6.14	129.42	115.30
1	D	158	ASP	CB-CG-OD1	6.13	123.81	118.30
1	E	105	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	8	LEU	CA-CB-CG	6.06	129.23	115.30
1	E	390	LEU	CB-CG-CD1	6.00	121.20	111.00
1	B	548	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	644	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	358	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	158	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	433	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	411	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	753	ASP	N-CA-C	-5.76	95.44	111.00
1	D	358	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	743	LEU	CA-CB-CG	5.74	128.49	115.30
1	H	406	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	274	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	105	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	362	LEU	CA-CB-CG	5.67	128.34	115.30
1	H	617	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	C	644	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	B	162	ASP	CB-CG-OD1	5.54	123.28	118.30
1	G	450	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	667	ILE	CG1-CB-CG2	5.50	123.49	111.40
1	A	280	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	257	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	362	LEU	CA-CB-CG	5.47	127.88	115.30
1	D	102	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	403	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	566	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	358	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	406	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	433	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	E	320	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	B	8	LEU	CA-CB-CG	5.37	127.65	115.30
1	E	670	ILE	CG1-CB-CG2	-5.37	99.59	111.40
1	D	371	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	G	539	ASP	CB-CG-OD1	5.35	123.12	118.30
1	G	43	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	B	438	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	191	THR	N-CA-CB	-5.31	100.21	110.30
1	C	548	ASP	CB-CG-OD1	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	LEU	CA-CB-CG	5.29	127.46	115.30
1	C	411	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	102	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	G	406	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	698	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	393	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	411	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	274	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	H	227	LEU	CA-CB-CG	5.24	127.36	115.30
1	E	299	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	644	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	105	ASP	CB-CG-OD1	5.18	122.97	118.30
1	F	406	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	743	LEU	CA-CB-CG	5.12	127.06	115.30
1	B	162	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	C	469	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	E	464	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	15	ASP	CB-CG-OD1	5.07	122.86	118.30
1	E	355	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	A	8	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	C	298	LEU	CB-CG-CD2	5.06	119.60	111.00
1	E	702	LEU	CA-CB-CG	5.05	126.92	115.30
1	E	299	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	227	LEU	CB-CA-C	-5.03	100.64	110.20
1	G	164	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	A	698	LEU	CB-CG-CD1	5.02	119.54	111.00
1	E	411	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	647	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	641	GLU	OE1-CD-OE2	5.01	129.32	123.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	HIS	Peptide
1	A	748	GLU	Peptide
1	C	1	MET	Peptide
1	C	694	ASP	Peptide
1	F	26	ALA	Peptide
1	G	1	MET	Peptide



## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6093	0	5855	81	0
1	B	6085	0	5844	94	0
1	C	6085	0	5844	88	0
1	D	6085	0	5844	76	0
1	E	6085	0	5844	108	0
1	F	6085	0	5844	113	0
1	G	6093	0	5855	96	0
1	H	6085	0	5844	104	0
2	A	10	0	13	4	0
2	D	10	0	12	3	0
2	E	10	0	13	0	0
2	F	10	0	13	2	0
2	G	10	0	13	3	0
2	H	10	0	13	1	0
3	A	16	0	22	0	0
3	C	16	0	22	1	0
3	E	16	0	22	2	0
4	A	48	0	64	12	0
4	B	36	0	47	9	0
4	C	36	0	48	2	0
4	D	54	0	72	14	0
4	E	24	0	32	1	0
4	F	18	0	24	2	0
4	G	18	0	24	4	0
4	H	30	0	40	10	0
5	A	19	0	26	3	0
5	E	19	0	26	5	0
6	A	10	0	14	7	0
6	C	10	0	14	0	0
6	F	10	0	14	2	0
6	G	10	0	14	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	B	13	0	18	1	0
8	D	13	0	18	1	0
8	F	13	0	18	0	0
8	H	13	0	18	1	0
9	B	21	0	30	5	0
9	D	21	0	30	3	0
10	C	24	0	34	6	0
11	H	27	0	38	12	0
12	A	182	0	0	8	0
12	B	303	0	0	8	0
12	C	286	0	0	10	0
12	D	348	0	0	11	0
12	E	185	0	0	8	0
12	F	247	0	0	13	0
12	G	197	0	0	3	0
12	H	218	0	0	7	0
All	All	51264	0	47580	765	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (765) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:801:IFM:H2C2	12:D:1243:HOH:O	1.38	1.23
2:A:801:IFM:H2C2	12:A:917:HOH:O	1.35	1.21
1:B:352:ARG:HD3	12:B:1019:HOH:O	1.45	1.17
1:A:278:ASP:HB3	12:A:1031:HOH:O	1.45	1.14
1:F:756:ARG:HG3	1:F:756:ARG:HH11	1.09	1.12
4:D:806:GOL:H2	12:D:1202:HOH:O	1.51	1.09
1:E:468:MET:HE1	12:E:974:HOH:O	1.51	1.08
1:E:737:ASP:HA	1:E:738:ARG:CB	1.85	1.06
1:H:599:PRO:HB3	11:H:808:PE5:H142	1.38	1.06
1:D:310:PRO:O	4:D:812:GOL:H11	1.59	1.03
1:H:213:GLU:HB3	1:H:224:THR:HG22	1.40	1.02
1:G:737:ASP:HA	1:G:738:ARG:HB2	1.40	1.00
1:F:604:ARG:HB3	1:F:604:ARG:HH11	1.27	1.00
1:E:737:ASP:HA	1:E:738:ARG:HB3	1.41	0.99
1:E:6:GLU:HG2	12:E:1030:HOH:O	1.59	0.99
11:H:808:PE5:H42	11:H:808:PE5:H72	1.45	0.97
1:B:734:LYS:O	1:B:735:SER:HB2	1.66	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:637:ASP:HB3	12:D:1053:HOH:O	1.63	0.96
1:A:608:GLU:OE2	4:A:805:GOL:H12	1.66	0.96
1:F:98:ALA:O	1:F:99:SER:HB2	1.62	0.95
1:F:604:ARG:HB3	1:F:604:ARG:NH1	1.82	0.94
1:A:604:ARG:HD2	12:A:1059:HOH:O	1.67	0.94
1:E:226:SER:HB3	1:H:704:ASP:OD2	1.69	0.93
1:H:499:GLU:O	1:H:503:THR:HB	1.69	0.93
1:G:710:THR:HG22	1:G:723:ASP:OD2	1.69	0.93
1:B:26:ALA:O	1:B:27:ILE:CB	2.18	0.91
1:C:1:MET:HG3	1:C:2:HIS:HB2	1.51	0.91
1:C:499:GLU:O	1:C:503:THR:HB	1.71	0.91
1:B:327:TYR:H	4:B:804:GOL:H32	1.37	0.90
1:F:753:ASP:HB2	12:F:979:HOH:O	1.70	0.90
1:B:644:ARG:HD3	12:D:1128:HOH:O	1.69	0.89
1:B:26:ALA:O	1:B:27:ILE:HB	1.71	0.88
1:H:164:ASP:OD1	4:H:807:GOL:H2	1.75	0.87
1:A:217:ASN:HB2	1:A:218:PRO:HD2	1.57	0.86
1:F:510:SER:O	1:F:514:GLU:HG2	1.75	0.86
4:H:804:GOL:H12	12:H:986:HOH:O	1.74	0.86
1:G:108:GLN:HG3	1:G:110:VAL:HG23	1.56	0.85
1:C:18:LYS:HE3	1:C:29:GLU:OE1	1.76	0.85
1:C:352:ARG:HD2	12:C:1073:HOH:O	1.77	0.84
1:B:604:ARG:HG2	9:B:802:7PE:H211	1.59	0.84
1:G:413:GLN:HE22	1:G:475:GLN:HE22	1.24	0.83
1:B:228:SER:HB3	1:E:644:ARG:HH22	1.41	0.83
1:C:18:LYS:CE	1:C:29:GLU:OE1	2.27	0.82
1:E:732:THR:HG23	12:E:1064:HOH:O	1.78	0.82
1:E:684:ASN:HB3	5:E:803:P6G:H91	1.60	0.82
1:F:560:LYS:HG3	12:F:1068:HOH:O	1.79	0.81
1:F:756:ARG:O	1:F:757:ILE:HB	1.78	0.81
1:G:737:ASP:HA	1:G:738:ARG:CB	2.11	0.81
1:C:191:THR:HG23	12:C:954:HOH:O	1.79	0.80
1:A:83:LEU:HD12	6:A:812:PGE:H62	1.64	0.80
1:F:731:ILE:O	1:F:757:ILE:HG22	1.80	0.80
1:F:749:LYS:HE2	12:F:1073:HOH:O	1.81	0.80
1:H:224:THR:HG23	12:H:995:HOH:O	1.82	0.80
1:E:352:ARG:HD3	12:E:956:HOH:O	1.82	0.80
1:B:734:LYS:O	1:B:735:SER:CB	2.29	0.80
1:G:731:ILE:HD13	1:G:743:LEU:HD23	1.62	0.80
1:H:219:ASP:OD1	4:H:807:GOL:H11	1.82	0.79
1:G:735:SER:C	1:G:737:ASP:H	1.84	0.79
1:E:499:GLU:O	1:E:503:THR:HB	1.83	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:738:ARG:O	1:E:738:ARG:HG3	1.83	0.78
1:H:217:ASN:HB2	1:H:218:PRO:HD2	1.64	0.78
1:C:128:HIS:HB3	12:C:1164:HOH:O	1.84	0.78
1:E:210:ALA:HB1	1:E:226:SER:O	1.83	0.78
1:G:413:GLN:HE22	1:G:475:GLN:NE2	1.81	0.78
1:C:459:LYS:HZ3	4:D:809:GOL:H32	1.49	0.77
1:E:230:GLU:HB2	1:E:233:LYS:HD2	1.67	0.77
1:A:83:LEU:HD12	6:A:812:PGE:C6	2.14	0.77
1:C:22:GLU:OE1	1:C:25:GLN:HG3	1.83	0.77
1:B:499:GLU:O	1:B:503:THR:HB	1.84	0.77
8:B:801:PG4:H21	12:B:976:HOH:O	1.85	0.77
1:A:107:SER:HB2	4:A:808:GOL:H11	1.67	0.77
10:C:805:PE4:H131	10:C:805:PE4:O6	1.84	0.76
1:C:459:LYS:NZ	4:D:809:GOL:H32	1.99	0.76
1:A:158:ASP:OD2	6:A:812:PGE:H6	1.85	0.75
3:E:802:1PE:H222	12:E:1006:HOH:O	1.85	0.75
1:E:737:ASP:HA	1:E:738:ARG:HB2	1.68	0.75
2:F:801:IFM:H2C1	4:F:802:GOL:O3	1.87	0.75
1:F:756:ARG:HG3	1:F:756:ARG:NH1	1.88	0.75
1:D:374:TYR:OH	4:D:809:GOL:H12	1.86	0.75
1:F:352:ARG:HD3	12:F:1034:HOH:O	1.87	0.75
1:H:213:GLU:HB3	1:H:224:THR:CG2	2.16	0.75
1:D:742:THR:HG22	1:D:751:VAL:HG13	1.69	0.75
1:H:582:ARG:HH21	1:H:582:ARG:HG2	1.50	0.74
1:G:142:LEU:HD21	1:G:263:MET:HE1	1.68	0.74
1:A:742:THR:O	1:A:743:LEU:HB2	1.86	0.74
1:B:644:ARG:HH12	1:D:228:SER:HB3	1.51	0.74
1:H:114:LYS:HG3	1:H:128:HIS:CD2	2.23	0.74
1:E:190:LYS:HE2	12:E:1044:HOH:O	1.87	0.73
1:A:659:GLU:O	1:A:660:ALA:HB3	1.88	0.73
1:D:136:ARG:HD3	12:D:1041:HOH:O	1.88	0.73
1:H:1:MET:HA	1:H:292:ILE:HG21	1.70	0.73
1:F:756:ARG:CG	1:F:756:ARG:HH11	1.95	0.73
1:H:2:HIS:O	1:H:3:GLU:HB3	1.87	0.73
1:H:656:ASN:HA	12:H:1075:HOH:O	1.88	0.73
1:H:733:ASN:HD22	1:H:741:LEU:HD11	1.51	0.72
1:A:83:LEU:CD1	6:A:812:PGE:O4	2.37	0.72
1:F:745:ILE:O	1:F:746:PHE:HB2	1.88	0.72
1:G:94:SER:O	1:G:97:ALA:HB2	1.90	0.72
1:F:98:ALA:O	1:F:99:SER:CB	2.37	0.72
1:G:425:LYS:HD3	1:G:492:PHE:CZ	2.25	0.72
1:F:97:ALA:O	1:F:99:SER:N	2.23	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:345:TYR:OH	11:H:808:PE5:H22	1.90	0.71
1:E:735:SER:O	1:E:736:GLU:CB	2.39	0.71
1:E:735:SER:O	1:E:736:GLU:HB3	1.90	0.71
1:B:734:LYS:H	1:B:734:LYS:HD2	1.54	0.71
1:G:1:MET:HG3	1:G:2:HIS:HB2	1.73	0.70
1:B:289:GLN:OE1	1:B:710:THR:HG22	1.92	0.70
1:D:635:GLN:HG3	9:D:808:7PE:H152	1.74	0.70
1:H:70:TRP:CZ3	4:H:804:GOL:H32	2.26	0.70
1:H:353:ASN:HB3	4:H:805:GOL:H11	1.72	0.70
1:F:759:LYS:O	1:F:760:SER:HB3	1.92	0.69
1:B:327:TYR:N	4:B:804:GOL:H32	2.06	0.69
1:G:413:GLN:NE2	1:G:475:GLN:HE22	1.90	0.69
1:D:334:ASP:OD1	2:D:801:IFM:O4	2.09	0.69
1:B:734:LYS:N	1:B:734:LYS:HD2	2.08	0.69
1:E:741:LEU:O	1:E:751:VAL:CG2	2.41	0.69
1:H:426:LYS:HE2	11:H:808:PE5:H482	1.73	0.69
1:B:27:ILE:CG2	1:B:28:THR:N	2.56	0.69
1:F:699:SER:N	1:F:700:PRO:HD3	2.07	0.69
1:B:26:ALA:O	1:B:27:ILE:CG2	2.40	0.69
1:E:370:LYS:HE3	1:E:375:GLU:OE2	1.93	0.69
1:H:2:HIS:O	1:H:3:GLU:CB	2.39	0.69
1:B:26:ALA:O	1:B:27:ILE:HG22	1.93	0.68
1:B:553:LEU:HD21	4:B:807:GOL:H11	1.76	0.68
1:A:612:GLU:OE2	4:A:805:GOL:H11	1.93	0.68
1:A:83:LEU:HD12	6:A:812:PGE:O4	1.93	0.68
1:B:733:ASN:OD1	1:B:734:LYS:O	2.11	0.68
1:C:190:LYS:HE3	4:C:806:GOL:H31	1.76	0.68
1:H:129:GLU:OE2	1:H:131:LYS:NZ	2.24	0.68
1:A:756:ARG:HH11	1:A:756:ARG:HG2	1.59	0.68
1:B:224:THR:HG23	12:B:1171:HOH:O	1.92	0.68
1:A:644:ARG:HH12	1:F:228:SER:HB3	1.58	0.67
1:A:608:GLU:OE2	4:A:805:GOL:C1	2.41	0.67
1:F:28:THR:HG21	1:F:656:ASN:HB2	1.77	0.67
11:H:808:PE5:C7	11:H:808:PE5:H42	2.21	0.67
1:D:499:GLU:O	1:D:503:THR:HB	1.94	0.66
1:A:158:ASP:CG	6:A:812:PGE:H6	2.15	0.66
3:E:802:1PE:C22	12:E:1006:HOH:O	2.41	0.66
1:G:499:GLU:O	1:G:503:THR:HB	1.93	0.66
1:A:48:GLU:HB2	1:A:83:LEU:HD23	1.77	0.66
1:C:599:PRO:HG3	10:C:805:PE4:H52	1.77	0.66
1:G:287:THR:HB	1:G:710:THR:OG1	1.95	0.66
2:A:801:IFM:C2	12:A:917:HOH:O	2.12	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:217:ASN:HB2	1:F:218:PRO:CD	2.25	0.66
1:E:44:GLY:O	1:E:102:ARG:NH2	2.29	0.66
1:G:710:THR:CG2	1:G:723:ASP:OD2	2.43	0.65
1:A:599:PRO:HB3	5:A:806:P6G:H141	1.78	0.65
1:F:604:ARG:NH2	12:F:1091:HOH:O	2.30	0.65
1:G:735:SER:O	1:G:737:ASP:N	2.25	0.65
1:H:128:HIS:HB3	12:H:997:HOH:O	1.95	0.65
1:G:742:THR:HG22	1:G:751:VAL:HG22	1.77	0.65
1:H:742:THR:HG22	1:H:751:VAL:HG22	1.79	0.65
1:B:27:ILE:HG23	1:B:28:THR:N	2.12	0.65
1:E:204:CYS:O	1:E:205:SER:HB2	1.95	0.65
1:B:27:ILE:CG2	1:B:28:THR:H	2.08	0.64
1:G:735:SER:C	1:G:737:ASP:N	2.50	0.64
1:F:1:MET:HA	1:F:292:ILE:HG21	1.79	0.64
1:H:582:ARG:HH21	1:H:582:ARG:CG	2.10	0.64
1:F:734:LYS:O	1:F:735:SER:HB2	1.96	0.64
1:E:680:GLN:OE1	5:E:803:P6G:H141	1.98	0.64
1:A:108:GLN:HG3	1:A:110:VAL:HG23	1.79	0.63
1:E:8:LEU:HD22	1:E:16:ILE:HD12	1.81	0.63
1:H:582:ARG:NH2	1:H:582:ARG:HG2	2.11	0.63
1:C:213:GLU:OE2	1:G:617:ARG:NH2	2.26	0.63
1:G:108:GLN:HG3	1:G:110:VAL:CG2	2.29	0.63
1:H:599:PRO:HB3	11:H:808:PE5:C14	2.24	0.63
1:A:217:ASN:HB2	1:A:218:PRO:CD	2.24	0.63
1:H:428:HIS:HB2	1:H:437:ILE:HD11	1.81	0.62
1:G:116:SER:HA	1:G:125:ILE:O	2.00	0.62
1:H:734:LYS:O	1:H:735:SER:CB	2.47	0.62
1:F:558:PRO:HD2	1:F:561:LYS:HE2	1.82	0.61
1:B:110:VAL:HG22	1:B:132:PHE:HB3	1.81	0.61
1:D:217:ASN:HB2	1:D:218:PRO:CD	2.31	0.61
1:F:742:THR:HA	1:F:751:VAL:HA	1.82	0.61
1:H:506:GLU:O	1:H:510:SER:HB2	2.00	0.61
1:D:352:ARG:HD3	12:D:1010:HOH:O	2.00	0.61
1:F:743:LEU:O	1:F:744:HIS:HB2	2.00	0.61
1:C:700:PRO:HD2	1:C:746:PHE:CZ	2.35	0.61
1:B:635:GLN:HG3	9:B:802:7PE:H152	1.83	0.61
1:E:31:SER:HB3	1:E:670:ILE:HG12	1.83	0.60
1:A:659:GLU:O	1:A:660:ALA:CB	2.49	0.60
1:F:26:ALA:O	1:F:27:ILE:HG22	2.02	0.60
1:B:347:ASN:HD21	4:B:805:GOL:H2	1.67	0.60
1:C:700:PRO:HG3	1:C:729:ILE:HD12	1.84	0.60
4:A:811:GOL:H32	1:F:158:ASP:OD1	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:577:ASN:OD1	1:E:582:ARG:NH2	2.33	0.60
1:H:219:ASP:OD1	4:H:807:GOL:C1	2.49	0.60
1:C:659:GLU:O	1:C:660:ALA:HB3	2.01	0.60
1:E:748:GLU:O	1:E:749:LYS:HD2	2.02	0.60
1:F:217:ASN:HB2	1:F:218:PRO:HD2	1.83	0.60
1:F:740:PRO:HA	1:F:752:LEU:O	2.02	0.60
1:E:751:VAL:O	1:E:752:LEU:HB2	2.02	0.59
1:F:457:VAL:HG11	1:F:468:MET:HE2	1.84	0.59
1:C:31:SER:HB3	1:C:670:ILE:HG12	1.84	0.59
1:E:116:SER:HA	1:E:125:ILE:O	2.02	0.59
1:G:79:ALA:HB1	1:G:202:GLU:HB2	1.84	0.59
1:G:58:ILE:HD12	1:G:58:ILE:N	2.18	0.59
1:B:27:ILE:HG22	1:B:28:THR:H	1.68	0.59
1:B:726:LYS:H	1:B:726:LYS:CD	2.16	0.59
1:C:99:SER:HB3	1:C:116:SER:HB2	1.84	0.59
1:F:26:ALA:C	1:F:27:ILE:HG22	2.23	0.59
1:B:753:ASP:O	1:B:754:SER:HB3	2.03	0.58
2:H:801:IFM:H2C1	4:H:802:GOL:O1	2.02	0.58
1:E:84:LEU:HD23	1:E:91:PHE:HB2	1.85	0.58
1:F:129:GLU:OE2	1:F:131:LYS:NZ	2.32	0.58
1:C:209:ASP:OD1	4:G:803:GOL:H32	2.02	0.58
1:C:752:LEU:HD13	1:C:757:ILE:CG1	2.33	0.58
1:E:696:ILE:HG12	1:E:743:LEU:HD12	1.84	0.58
1:F:352:ARG:CD	12:F:1034:HOH:O	2.50	0.58
1:C:696:ILE:N	1:C:696:ILE:HD12	2.18	0.58
1:D:450:ARG:NH1	4:D:804:GOL:H11	2.18	0.58
1:E:659:GLU:O	1:E:660:ALA:HB3	2.03	0.58
1:E:635:GLN:HG3	5:E:803:P6G:H61	1.86	0.58
1:E:641:GLU:HG3	12:E:965:HOH:O	2.03	0.58
1:F:1:MET:O	1:F:2:HIS:ND1	2.36	0.58
1:A:658:ASN:HB3	4:A:803:GOL:H31	1.86	0.58
1:E:58:ILE:N	1:E:58:ILE:HD12	2.19	0.58
1:C:573:TYR:HE2	1:C:621:PHE:HE1	1.50	0.57
1:G:396:PHE:HZ	4:G:802:GOL:HO3	1.51	0.57
1:B:79:ALA:HB1	1:B:202:GLU:HB2	1.86	0.57
1:B:43:ARG:HD3	1:B:56:ALA:HB3	1.85	0.57
1:C:142:LEU:HD21	1:C:263:MET:CE	2.34	0.57
1:D:97:ALA:O	1:D:99:SER:N	2.38	0.57
1:E:738:ARG:CG	1:E:738:ARG:O	2.51	0.57
1:B:417:SER:HB3	1:B:448:ILE:HG23	1.86	0.57
1:H:735:SER:HA	12:H:984:HOH:O	2.04	0.57
1:B:217:ASN:HB2	1:B:218:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:728:GLN:HG2	1:C:729:ILE:N	2.18	0.57
1:G:600:HIS:CD2	1:G:692:HIS:HB2	2.39	0.57
1:H:742:THR:HA	1:H:751:VAL:HA	1.85	0.57
1:D:742:THR:HA	1:D:750:SER:O	2.04	0.57
1:E:64:ASP:OD1	1:E:191:THR:HG23	2.04	0.57
1:G:601:LEU:HD23	1:G:602:TYR:CE2	2.40	0.57
1:B:16:ILE:HD12	1:B:106:LEU:HD11	1.86	0.57
1:F:213:GLU:HB3	1:F:224:THR:HG22	1.86	0.57
1:H:217:ASN:HB2	1:H:218:PRO:CD	2.35	0.57
1:C:97:ALA:O	1:C:99:SER:N	2.39	0.56
1:F:656:ASN:HA	12:F:1054:HOH:O	2.03	0.56
1:B:428:HIS:CD2	1:B:437:ILE:HG13	2.39	0.56
1:F:491:MET:HE1	1:F:494:LEU:HD12	1.88	0.56
1:F:745:ILE:HG22	1:F:745:ILE:O	2.04	0.56
1:H:656:ASN:O	1:H:656:ASN:CG	2.42	0.56
1:C:591:VAL:O	1:C:594:LEU:HB3	2.06	0.56
1:H:251:ASN:HB3	12:H:969:HOH:O	2.06	0.56
1:F:656:ASN:ND2	12:F:1054:HOH:O	2.36	0.56
1:B:228:SER:HB3	1:E:644:ARG:NH2	2.16	0.56
1:H:310:PRO:O	4:H:805:GOL:H2	2.06	0.56
1:B:85:HIS:ND1	12:B:1055:HOH:O	2.33	0.56
1:D:418:PRO:HB2	1:D:489:GLN:HB3	1.88	0.56
1:F:97:ALA:C	1:F:99:SER:H	2.08	0.56
1:B:656:ASN:CG	1:B:656:ASN:O	2.42	0.56
1:C:491:MET:HG3	1:C:535:VAL:HG21	1.87	0.56
1:H:395:PHE:CE1	4:H:802:GOL:H31	2.41	0.56
1:C:264:GLN:HB3	1:C:268:GLU:HB2	1.88	0.55
1:D:217:ASN:HB2	1:D:218:PRO:HD2	1.88	0.55
1:H:759:LYS:HG3	1:H:760:SER:H	1.72	0.55
1:A:749:LYS:O	1:A:750:SER:O	2.23	0.55
1:B:604:ARG:CG	9:B:802:7PE:H211	2.34	0.55
1:A:191:THR:HG22	1:A:196:ASP:H	1.70	0.55
1:E:737:ASP:CA	1:E:738:ARG:HB3	2.27	0.55
1:F:168:ILE:HD12	1:F:325:GLN:HB2	1.89	0.55
1:B:644:ARG:CD	12:D:1128:HOH:O	2.38	0.55
1:A:742:THR:O	1:A:743:LEU:CB	2.52	0.55
1:E:2:HIS:O	1:E:9:THR:HA	2.07	0.55
1:G:731:ILE:HD13	1:G:743:LEU:CD2	2.35	0.55
1:E:394:PHE:CZ	1:F:582:ARG:HG2	2.42	0.55
1:G:413:GLN:HG3	1:G:471:GLN:O	2.07	0.55
1:G:731:ILE:HG21	1:G:743:LEU:HD21	1.89	0.55
1:B:114:LYS:NZ	12:B:1091:HOH:O	2.39	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:693:GLY:C	1:E:695:ASP:H	2.11	0.54
1:E:737:ASP:CA	1:E:738:ARG:CB	2.70	0.54
1:H:587:LYS:NZ	12:H:1094:HOH:O	2.40	0.54
1:D:504:LEU:HB2	1:D:509:LEU:HD22	1.88	0.54
1:B:86:VAL:HG21	1:B:125:ILE:HG13	1.90	0.54
1:C:110:VAL:HG22	1:C:132:PHE:HB3	1.89	0.54
1:F:287:THR:OG1	1:F:710:THR:HG23	2.07	0.54
1:H:426:LYS:HG2	11:H:808:PE5:H41	1.89	0.54
1:E:714:ILE:N	1:E:714:ILE:HD13	2.23	0.54
1:B:2:HIS:HB3	1:B:10:THR:O	2.08	0.54
1:F:199:THR:HG21	1:F:253:GLN:HA	1.89	0.54
1:H:733:ASN:ND2	1:H:741:LEU:HD11	2.22	0.54
1:H:758:THR:HG22	1:H:759:LYS:N	2.23	0.54
1:C:537:LYS:HG2	12:C:1072:HOH:O	2.07	0.54
4:D:812:GOL:H12	12:D:1114:HOH:O	2.08	0.54
1:F:742:THR:HG22	1:F:751:VAL:HG13	1.89	0.54
1:D:464:ARG:HD2	1:D:534:TYR:HB2	1.90	0.53
1:G:86:VAL:HG21	1:G:125:ILE:HG13	1.89	0.53
1:A:671:HIS:CD2	4:A:803:GOL:H12	2.43	0.53
1:B:2:HIS:CB	1:B:10:THR:O	2.57	0.53
1:A:658:ASN:HB3	4:A:803:GOL:C3	2.38	0.53
1:G:475:GLN:HG3	2:G:801:IFM:H2C1	1.90	0.53
1:E:394:PHE:HZ	1:F:582:ARG:HG2	1.73	0.53
1:D:448:ILE:HG22	1:D:493:THR:HG21	1.90	0.53
1:E:741:LEU:O	1:E:751:VAL:HG22	2.08	0.53
1:F:697:HIS:O	1:F:698:LEU:HG	2.09	0.53
1:F:81:LEU:HD22	1:F:162:ASP:HB2	1.91	0.53
1:B:754:SER:OG	1:B:755:GLU:N	2.36	0.53
1:E:341:PRO:HG3	5:E:803:P6G:H172	1.91	0.53
1:E:86:VAL:HG21	1:E:125:ILE:HD11	1.90	0.53
1:B:45:THR:HG21	1:B:55:ALA:HA	1.90	0.53
1:C:293:ILE:H	1:C:293:ILE:HD12	1.74	0.53
1:G:191:THR:HG22	1:G:195:GLU:H	1.73	0.53
1:D:43:ARG:HD3	1:D:56:ALA:HB3	1.91	0.52
1:F:16:ILE:CD1	1:F:106:LEU:HD11	2.39	0.52
1:A:251:ASN:HB3	1:A:254:ASP:OD2	2.08	0.52
1:F:179:PHE:CZ	1:F:186:GLY:HA3	2.44	0.52
1:F:294:ASP:OD1	1:F:647:ARG:NH1	2.33	0.52
1:H:745:ILE:O	1:H:748:GLU:HG2	2.08	0.52
1:G:425:LYS:HD3	1:G:492:PHE:HZ	1.75	0.52
1:H:426:LYS:HD3	11:H:808:PE5:H12	1.90	0.52
1:C:718:GLN:CG	1:C:733:ASN:HD21	2.22	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:710:THR:HB	1:D:723:ASP:HA	1.91	0.52
1:A:696:ILE:HD13	1:A:696:ILE:N	2.25	0.52
1:B:27:ILE:HA	1:B:43:ARG:NH1	2.24	0.52
1:D:152:ASP:OD2	4:D:805:GOL:H12	2.09	0.52
1:B:504:LEU:HB2	1:B:509:LEU:HD22	1.91	0.52
1:C:191:THR:HG22	1:C:196:ASP:H	1.74	0.52
1:G:16:ILE:HD13	1:G:654:LEU:CD2	2.39	0.52
1:A:217:ASN:CB	1:A:218:PRO:HD2	2.36	0.52
1:H:734:LYS:O	1:H:735:SER:HB3	2.10	0.52
1:D:81:LEU:HD22	1:D:162:ASP:HB2	1.92	0.52
1:F:334:ASP:OD1	2:F:801:IFM:O4	2.14	0.52
1:F:418:PRO:HB2	1:F:489:GLN:HB3	1.92	0.52
1:A:142:LEU:HD21	1:A:263:MET:CE	2.40	0.52
1:A:413:GLN:HG3	1:A:471:GLN:O	2.10	0.52
1:C:573:TYR:HE2	1:C:621:PHE:CE1	2.28	0.51
1:B:327:TYR:HA	4:B:804:GOL:H32	1.91	0.51
1:D:450:ARG:HH11	4:D:804:GOL:H11	1.73	0.51
1:E:230:GLU:CB	1:E:233:LYS:HE3	2.39	0.51
1:E:744:HIS:HA	1:E:748:GLU:O	2.10	0.51
1:F:733:ASN:HD22	1:F:752:LEU:HD21	1.75	0.51
10:C:805:PE4:C13	10:C:805:PE4:O6	2.57	0.51
1:H:58:ILE:HD12	1:H:58:ILE:N	2.25	0.51
1:A:197:THR:O	1:A:245:SER:HA	2.11	0.51
2:D:801:IFM:C2	12:D:1243:HOH:O	2.17	0.51
1:E:110:VAL:HG22	1:E:132:PHE:HB3	1.91	0.51
1:G:653:ASP:CG	1:G:670:ILE:HD13	2.31	0.51
1:A:164:ASP:OD1	4:A:809:GOL:O1	2.10	0.51
1:C:28:THR:HG21	1:C:656:ASN:HB2	1.92	0.51
1:F:575:TYR:CG	1:F:576:PRO:HA	2.46	0.51
1:H:181:HIS:HB2	1:H:182:PRO:CD	2.40	0.51
1:H:741:LEU:HD13	1:H:752:LEU:HD23	1.90	0.51
1:A:191:THR:HG22	1:A:195:GLU:N	2.26	0.51
1:D:382:ILE:HG13	1:D:391:CYS:HB2	1.92	0.51
1:A:573:TYR:HE2	1:A:621:PHE:HE1	1.59	0.51
1:E:714:ILE:CD1	1:E:714:ILE:N	2.74	0.51
1:H:1:MET:HA	1:H:292:ILE:CG2	2.39	0.51
1:E:560:LYS:HE3	1:E:563:THR:HG21	1.92	0.51
1:G:475:GLN:CG	2:G:801:IFM:H2C1	2.41	0.51
1:E:400:LEU:HD13	1:F:401:SER:HB2	1.93	0.51
1:E:749:LYS:O	1:E:750:SER:HB2	2.11	0.50
1:E:77:PRO:HD3	1:E:173:LEU:HD12	1.92	0.50
1:F:635:GLN:HA	1:F:635:GLN:NE2	2.24	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:172:HIS:O	1:H:191:THR:HA	2.11	0.50
11:H:808:PE5:C4	11:H:808:PE5:H72	2.32	0.50
1:H:181:HIS:HB2	1:H:182:PRO:HD2	1.92	0.50
1:A:274:ARG:NH2	4:A:808:GOL:H2	2.25	0.50
1:B:710:THR:HB	1:B:723:ASP:HA	1.93	0.50
1:E:659:GLU:O	1:E:660:ALA:CB	2.60	0.50
1:G:361:THR:HB	1:G:387:GLY:HA3	1.93	0.50
1:G:731:ILE:CD1	1:G:745:ILE:HD11	2.41	0.50
1:F:224:THR:HG23	12:F:984:HOH:O	2.12	0.50
1:B:116:SER:HA	1:B:125:ILE:O	2.12	0.50
1:D:615:GLU:N	1:D:616:PRO:CD	2.75	0.50
1:H:25:GLN:C	1:H:26:ALA:O	2.47	0.50
1:E:135:TYR:O	1:E:138:LYS:HE3	2.12	0.50
1:F:699:SER:N	1:F:700:PRO:CD	2.73	0.50
1:F:745:ILE:O	1:F:746:PHE:CB	2.58	0.50
1:F:425:LYS:NZ	1:F:499:GLU:OE1	2.32	0.50
1:D:212:GLU:OE1	4:D:806:GOL:O2	2.30	0.49
1:H:1:MET:CA	1:H:292:ILE:HG21	2.39	0.49
1:A:217:ASN:CB	1:A:218:PRO:CD	2.89	0.49
1:B:28:THR:HG21	1:B:656:ASN:HB2	1.94	0.49
1:G:418:PRO:HB2	1:G:489:GLN:HB3	1.95	0.49
1:H:591:VAL:O	1:H:594:LEU:HB3	2.12	0.49
1:B:5:GLY:O	1:B:6:GLU:C	2.51	0.49
1:D:130:GLU:HG3	1:D:266:TYR:OH	2.12	0.49
1:D:79:ALA:HB1	1:D:202:GLU:HB2	1.94	0.49
1:G:1:MET:HG3	1:G:2:HIS:CB	2.39	0.49
1:A:696:ILE:CD1	1:A:715:VAL:HG11	2.43	0.49
1:C:114:LYS:HG2	1:C:128:HIS:HD2	1.78	0.49
1:C:333:TRP:HB3	1:C:416:ILE:HD13	1.93	0.49
1:F:689:LEU:HG	1:F:690:SER:N	2.25	0.49
1:B:641:GLU:HB2	12:B:1151:HOH:O	2.13	0.49
1:H:197:THR:O	1:H:245:SER:HA	2.13	0.49
1:A:249:VAL:HG11	1:A:255:GLU:HG2	1.94	0.49
1:C:635:GLN:HB2	10:C:805:PE4:H22	1.93	0.49
1:E:5:GLY:O	1:E:6:GLU:C	2.51	0.49
1:F:274:ARG:HD3	12:F:1062:HOH:O	2.12	0.49
1:A:475:GLN:CG	2:A:801:IFM:H2C1	2.42	0.49
1:B:19:ASN:O	1:B:20:ARG:HD3	2.13	0.49
1:C:160:GLY:HA2	1:C:202:GLU:OE2	2.13	0.49
1:F:86:VAL:HG21	1:F:125:ILE:HG13	1.95	0.49
1:F:179:PHE:CE1	1:F:186:GLY:HA3	2.48	0.49
1:C:142:LEU:HD21	1:C:263:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:79:ALA:HB1	1:C:202:GLU:HB2	1.94	0.49
1:D:707:ASP:OD1	1:D:726:LYS:HE2	2.13	0.49
1:E:84:LEU:HD23	1:E:91:PHE:CD2	2.48	0.49
1:D:560:LYS:HG3	1:D:560:LYS:O	2.13	0.48
1:G:81:LEU:HD22	1:G:162:ASP:HB2	1.95	0.48
1:E:81:LEU:HD22	1:E:162:ASP:HB2	1.94	0.48
1:G:130:GLU:HG3	1:G:266:TYR:OH	2.14	0.48
1:D:608:GLU:HA	1:D:636:ILE:HD12	1.94	0.48
1:E:684:ASN:HB3	5:E:803:P6G:C9	2.39	0.48
1:H:43:ARG:HD3	1:H:56:ALA:HB3	1.94	0.48
1:A:86:VAL:HG21	1:A:125:ILE:HG13	1.95	0.48
1:G:370:LYS:HD3	12:G:1093:HOH:O	2.13	0.48
1:C:144:LYS:HG2	12:C:1167:HOH:O	2.13	0.48
1:C:371:ARG:NH1	3:C:801:1PE:H222	2.28	0.48
1:D:413:GLN:HG3	1:D:471:GLN:O	2.13	0.48
1:G:412:TRP:CZ3	1:G:479:ASN:HB2	2.49	0.48
1:C:684:ASN:O	1:C:688:GLY:HA2	2.13	0.48
1:E:141:VAL:HG13	1:E:241:MET:HB3	1.95	0.48
1:E:727:GLU:OE1	1:E:727:GLU:N	2.42	0.48
1:G:457:VAL:HB	1:H:457:VAL:HB	1.94	0.48
1:G:327:TYR:CE1	2:G:801:IFM:H6C1	2.49	0.48
1:C:604:ARG:NH1	1:C:637:ASP:OD1	2.46	0.48
1:F:604:ARG:CZ	12:F:1091:HOH:O	2.62	0.48
1:H:26:ALA:O	1:H:27:ILE:HG22	2.13	0.48
1:A:656:ASN:O	1:A:656:ASN:CG	2.51	0.48
1:B:114:LYS:HG2	1:B:128:HIS:CD2	2.49	0.48
1:B:310:PRO:O	4:B:803:GOL:H31	2.14	0.48
1:D:742:THR:HA	1:D:751:VAL:HA	1.94	0.48
1:G:413:GLN:NE2	1:G:475:GLN:NE2	2.56	0.48
1:F:708:GLY:HA2	1:F:724:VAL:O	2.14	0.48
1:D:600:HIS:CD2	1:D:692:HIS:HB2	2.49	0.47
1:E:191:THR:HB	1:E:196:ASP:H	1.78	0.47
1:H:368:LYS:HD3	1:H:378:TYR:O	2.13	0.47
1:G:459:LYS:HB3	1:G:459:LYS:HE3	1.70	0.47
1:G:615:GLU:HB3	1:G:616:PRO:HD3	1.95	0.47
1:G:678:SER:HA	1:G:681:MET:CE	2.44	0.47
1:A:263:MET:CE	1:A:269:GLU:HG3	2.45	0.47
1:D:575:TYR:HB2	12:D:1074:HOH:O	2.15	0.47
1:E:136:ARG:HG3	1:E:137:LYS:HG3	1.97	0.47
1:G:136:ARG:HG3	1:G:137:LYS:HG3	1.97	0.47
1:H:179:PHE:CZ	1:H:186:GLY:HA3	2.48	0.47
1:C:575:TYR:HB2	12:C:1035:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:71:GLU:O	1:E:328:GLN:HG2	2.14	0.47
1:G:44:GLY:O	1:G:102:ARG:NH2	2.38	0.47
1:G:16:ILE:CD1	1:G:654:LEU:HD22	2.44	0.47
1:A:34:MET:HG2	1:A:304:HIS:HE1	1.80	0.47
1:B:724:VAL:HG22	1:B:729:ILE:HG23	1.96	0.47
1:F:457:VAL:HG11	1:F:468:MET:CE	2.43	0.47
1:C:86:VAL:HG21	1:C:125:ILE:HG13	1.97	0.47
1:C:302:ILE:O	1:C:306:ILE:HG13	2.14	0.47
1:H:98:ALA:O	1:H:99:SER:CB	2.63	0.47
1:C:113:ARG:NH2	1:C:129:GLU:OE1	2.45	0.47
1:C:752:LEU:HD13	1:C:757:ILE:HG12	1.96	0.47
1:G:712:LYS:NZ	12:G:1058:HOH:O	2.32	0.47
1:B:738:ARG:CZ	1:B:755:GLU:HG3	2.45	0.47
1:B:729:ILE:CD1	1:B:745:ILE:HG21	2.45	0.47
1:B:745:ILE:O	1:B:748:GLU:HG2	2.14	0.47
1:C:448:ILE:HG22	1:C:493:THR:HG21	1.97	0.47
1:D:80:LEU:HD23	1:D:131:LYS:HD3	1.96	0.47
1:F:26:ALA:HA	1:F:29:GLU:HB2	1.97	0.47
1:G:191:THR:HG22	1:G:195:GLU:N	2.29	0.47
1:D:738:ARG:HE	1:D:755:GLU:HA	1.80	0.47
1:E:624:LEU:N	1:E:624:LEU:HD12	2.30	0.47
1:G:370:LYS:HE3	1:G:375:GLU:OE2	2.15	0.47
1:C:191:THR:CG2	12:C:954:HOH:O	2.53	0.47
1:F:731:ILE:HB	1:F:757:ILE:HG21	1.97	0.47
1:H:715:VAL:CG2	1:H:720:LEU:HD22	2.45	0.47
1:A:475:GLN:HG3	2:A:801:IFM:H2C1	1.95	0.46
1:D:741:LEU:O	1:D:742:THR:HG23	2.15	0.46
1:F:422:TYR:HE2	6:F:806:PGE:H42	1.79	0.46
1:F:98:ALA:HB2	12:F:1136:HOH:O	2.15	0.46
1:A:491:MET:HA	1:A:491:MET:HE2	1.97	0.46
1:B:100:PHE:CZ	1:B:102:ARG:HB2	2.50	0.46
1:E:55:ALA:O	1:E:56:ALA:HB2	2.15	0.46
1:F:13:GLY:O	1:F:296:VAL:HG23	2.15	0.46
1:C:99:SER:O	1:C:115:VAL:HA	2.15	0.46
1:D:692:HIS:O	1:D:695:ASP:HB2	2.16	0.46
1:F:756:ARG:O	1:F:757:ILE:CB	2.59	0.46
1:E:670:ILE:HD12	1:E:670:ILE:HG23	1.68	0.46
1:E:96:GLU:O	1:E:96:GLU:HG3	2.15	0.46
1:F:743:LEU:O	1:F:744:HIS:CB	2.64	0.46
1:G:141:VAL:HG13	1:G:241:MET:HB3	1.96	0.46
1:G:287:THR:HB	1:G:710:THR:HG1	1.80	0.46
1:B:327:TYR:CA	4:B:804:GOL:H32	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:728:GLN:HG3	1:C:758:THR:HG23	1.98	0.46
1:E:359:HIS:HB2	1:E:444:MET:SD	2.56	0.46
1:F:733:ASN:HD22	1:F:752:LEU:CD2	2.28	0.46
1:A:692:HIS:O	1:A:695:ASP:HB2	2.15	0.46
1:B:575:TYR:CG	1:B:576:PRO:HA	2.50	0.46
1:B:726:LYS:H	1:B:726:LYS:HD2	1.80	0.46
1:G:301:ASN:O	1:G:675:ASN:HB3	2.16	0.46
1:E:230:GLU:HB3	1:E:233:LYS:HE3	1.97	0.46
1:E:332:PHE:CZ	1:E:382:ILE:HG12	2.50	0.46
1:G:729:ILE:HD11	1:G:761:ARG:HG3	1.98	0.46
1:H:618:THR:HG22	1:H:620:HIS:H	1.80	0.46
1:E:197:THR:O	1:E:245:SER:HA	2.16	0.46
1:C:718:GLN:OE1	1:C:738:ARG:HA	2.16	0.46
1:H:362:LEU:HD13	1:H:366:ARG:NH2	2.30	0.46
1:C:382:ILE:O	1:C:390:LEU:HB2	2.16	0.45
1:C:738:ARG:CZ	1:C:755:GLU:HG3	2.46	0.45
1:D:1:MET:N	1:D:1:MET:SD	2.83	0.45
1:D:731:ILE:HB	1:D:757:ILE:CG2	2.45	0.45
1:F:656:ASN:O	1:F:656:ASN:CG	2.55	0.45
1:A:671:HIS:HB3	12:A:957:HOH:O	2.16	0.45
1:A:98:ALA:O	1:A:99:SER:HB3	2.15	0.45
1:C:315:LEU:O	4:C:809:GOL:H32	2.16	0.45
1:E:545:GLU:HG2	1:E:547:PHE:O	2.16	0.45
1:E:6:GLU:HB3	1:E:7:HIS:H	1.49	0.45
1:A:615:GLU:HB3	1:A:616:PRO:HD3	1.99	0.45
1:B:504:LEU:HD12	1:B:509:LEU:HD13	1.98	0.45
1:B:700:PRO:HG3	1:B:729:ILE:HG12	1.97	0.45
1:C:575:TYR:CG	1:C:576:PRO:HA	2.51	0.45
1:D:584:GLN:O	1:D:586:ILE:HG23	2.16	0.45
1:F:655:LEU:O	1:F:656:ASN:C	2.55	0.45
1:F:214:ASP:OD1	4:F:805:GOL:O2	2.34	0.45
1:G:94:SER:O	1:G:97:ALA:CB	2.64	0.45
1:H:86:VAL:HG21	1:H:125:ILE:HG13	1.98	0.45
1:C:191:THR:HG22	1:C:195:GLU:N	2.31	0.45
1:C:375:GLU:O	1:C:451:PHE:HA	2.15	0.45
1:D:582:ARG:HD3	12:D:985:HOH:O	2.16	0.45
1:D:696:ILE:HG12	1:D:715:VAL:HG11	1.97	0.45
1:D:684:ASN:HB3	9:D:808:7PE:H112	1.97	0.45
1:E:84:LEU:HD13	1:E:147:VAL:HG21	1.96	0.45
1:F:224:THR:CG2	12:F:984:HOH:O	2.65	0.45
1:F:710:THR:HB	1:F:723:ASP:HA	1.98	0.45
1:G:8:LEU:HA	1:G:17:ILE:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:697:HIS:HD2	12:C:1087:HOH:O	1.98	0.45
1:F:197:THR:O	1:F:245:SER:HA	2.16	0.45
1:H:427:TYR:CE1	1:H:431:THR:HG21	2.51	0.45
1:G:115:VAL:O	1:G:126:THR:HA	2.17	0.45
1:H:1:MET:O	1:H:1:MET:HG3	2.17	0.45
1:C:172:HIS:HE1	12:C:923:HOH:O	1.99	0.45
1:C:599:PRO:HB3	10:C:805:PE4:H42	1.99	0.45
1:E:119:MET:HG2	1:E:123:ALA:O	2.16	0.45
1:E:47:ALA:HB1	1:E:82:THR:HB	1.99	0.45
1:G:382:ILE:HD12	1:G:391:CYS:HB2	1.99	0.45
1:G:761:ARG:O	1:G:762:LEU:HD13	2.16	0.45
1:H:164:ASP:CG	4:H:807:GOL:H2	2.35	0.45
1:C:587:LYS:HE2	1:C:622:SER:HB2	1.99	0.45
1:D:327:TYR:OH	4:D:802:GOL:C3	2.65	0.45
1:A:394:PHE:HZ	1:B:582:ARG:HG2	1.82	0.45
1:F:27:ILE:HG23	1:F:28:THR:H	1.82	0.45
1:E:468:MET:SD	1:F:468:MET:HE3	2.57	0.45
1:B:197:THR:O	1:B:245:SER:HA	2.17	0.45
1:D:508:THR:O	1:D:512:VAL:HG23	2.17	0.44
1:F:491:MET:CE	1:F:491:MET:HA	2.47	0.44
1:D:18:LYS:NZ	1:D:29:GLU:OE1	2.35	0.44
1:D:756:ARG:CG	1:D:757:ILE:N	2.81	0.44
1:E:727:GLU:H	1:E:727:GLU:CD	2.19	0.44
1:H:345:TYR:OH	11:H:808:PE5:H11	2.17	0.44
1:A:604:ARG:NH1	1:A:608:GLU:OE1	2.50	0.44
9:B:802:7PE:H201	12:B:1039:HOH:O	2.16	0.44
1:C:229:LEU:HD12	1:C:229:LEU:N	2.33	0.44
1:C:18:LYS:NZ	1:C:29:GLU:OE1	2.50	0.44
1:B:129:GLU:OE2	1:B:131:LYS:NZ	2.47	0.44
1:D:501:LEU:HD23	1:D:509:LEU:HD11	2.00	0.44
1:D:98:ALA:O	1:D:99:SER:CB	2.64	0.44
1:E:594:LEU:HD12	1:E:598:HIS:HD2	1.81	0.44
1:H:2:HIS:ND1	1:H:9:THR:HB	2.32	0.44
1:H:478:GLU:HB2	1:H:575:TYR:CD2	2.52	0.44
1:H:323:SER:HB3	1:H:670:ILE:HG22	2.00	0.44
1:A:181:HIS:HB2	1:A:182:PRO:CD	2.47	0.44
1:E:13:GLY:N	1:E:292:ILE:HD11	2.33	0.44
1:F:731:ILE:HB	1:F:757:ILE:CG2	2.47	0.44
1:H:566:LEU:HD11	1:H:573:TYR:OH	2.17	0.44
1:C:659:GLU:O	1:C:660:ALA:CB	2.65	0.44
1:E:577:ASN:N	4:E:805:GOL:O3	2.37	0.44
1:G:659:GLU:O	1:G:660:ALA:HB3	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:643:TYR:O	1:C:646:PHE:HB3	2.18	0.44
1:E:718:GLN:HA	1:E:735:SER:OG	2.18	0.44
1:F:422:TYR:CE2	6:F:806:PGE:H42	2.53	0.44
1:A:215:TYR:HE1	6:A:812:PGE:H22	1.83	0.44
1:A:301:ASN:O	1:A:675:ASN:HB3	2.18	0.44
1:A:753:ASP:O	1:A:754:SER:CB	2.66	0.44
1:B:327:TYR:CE2	4:B:808:GOL:H32	2.53	0.44
1:C:320:ARG:HA	1:C:670:ILE:O	2.18	0.44
1:C:754:SER:O	1:C:755:GLU:HB2	2.17	0.44
1:E:203:THR:O	1:E:239:LYS:HA	2.17	0.44
1:E:693:GLY:C	1:E:695:ASP:N	2.71	0.44
1:G:577:ASN:OD1	1:G:582:ARG:NH2	2.46	0.44
1:H:639:VAL:O	1:H:642:ALA:HB3	2.17	0.44
1:H:715:VAL:HG22	1:H:720:LEU:HD22	2.00	0.44
1:C:501:LEU:HD23	1:C:509:LEU:HD11	2.00	0.43
4:A:811:GOL:C3	1:F:158:ASP:OD1	2.66	0.43
1:H:508:THR:O	1:H:512:VAL:HG23	2.18	0.43
1:A:47:ALA:O	1:A:81:LEU:HD12	2.18	0.43
1:B:99:SER:HB3	1:B:116:SER:HB2	1.99	0.43
1:C:233:LYS:HA	1:C:234:PRO:HD3	1.82	0.43
1:E:693:GLY:O	1:E:694:ASP:HB2	2.18	0.43
1:A:108:GLN:HG3	1:A:110:VAL:CG2	2.46	0.43
1:C:459:LYS:HZ1	4:D:809:GOL:H32	1.83	0.43
1:G:179:PHE:CE1	1:G:186:GLY:HA3	2.53	0.43
1:H:749:LYS:O	1:H:750:SER:HB3	2.18	0.43
1:A:732:THR:HG23	12:A:980:HOH:O	2.17	0.43
1:B:391:CYS:HB3	1:B:410:ASN:HB3	1.99	0.43
1:G:731:ILE:HD12	1:G:745:ILE:HD11	1.99	0.43
1:E:199:THR:HG21	1:E:253:GLN:HA	2.00	0.43
1:B:428:HIS:CG	1:B:437:ILE:HG13	2.53	0.43
1:C:573:TYR:CE2	1:C:621:PHE:CE1	3.07	0.43
1:E:630:ALA:HB2	1:E:645:ASN:HB3	2.01	0.43
1:G:382:ILE:HD12	1:G:391:CYS:CB	2.49	0.43
1:G:568:LYS:HB3	1:G:568:LYS:HE2	1.76	0.43
1:G:7:HIS:CE1	1:G:20:ARG:HD3	2.54	0.43
1:H:18:LYS:NZ	1:H:29:GLU:OE1	2.47	0.43
1:H:345:TYR:OH	11:H:808:PE5:C2	2.64	0.43
1:C:154:ASP:CG	1:G:644:ARG:NH1	2.72	0.43
1:H:277:TRP:HA	1:H:280:LEU:HD12	2.01	0.43
1:A:43:ARG:HD3	1:A:56:ALA:HB3	2.01	0.43
1:B:342:MET:HE2	12:B:970:HOH:O	2.17	0.43
1:B:725:THR:OG1	1:B:728:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:172:HIS:O	1:D:191:THR:HA	2.17	0.43
1:E:95:GLU:HG2	1:E:95:GLU:H	1.68	0.43
1:F:689:LEU:O	1:F:690:SER:HB3	2.18	0.43
1:F:731:ILE:O	1:F:757:ILE:CG2	2.59	0.43
1:H:144:LYS:HE3	1:H:266:TYR:CD2	2.53	0.43
1:A:191:THR:CG2	1:A:196:ASP:H	2.32	0.43
1:D:727:GLU:O	1:D:761:ARG:N	2.45	0.43
1:G:575:TYR:CG	1:G:576:PRO:HA	2.54	0.43
1:H:741:LEU:O	1:H:742:THR:HG23	2.18	0.43
1:H:758:THR:CG2	1:H:759:LYS:N	2.82	0.43
1:B:16:ILE:HD13	1:B:300:PHE:CD2	2.54	0.43
1:H:139:HIS:O	1:H:242:ILE:HA	2.19	0.43
1:B:249:VAL:HG11	1:B:255:GLU:HG2	2.01	0.42
12:A:1080:HOH:O	1:C:644:ARG:HD2	2.19	0.42
1:E:287:THR:HB	1:E:710:THR:HG23	2.01	0.42
1:D:733:ASN:OD1	1:D:733:ASN:C	2.57	0.42
1:D:756:ARG:CG	1:D:757:ILE:H	2.32	0.42
1:F:557:ILE:HA	1:F:558:PRO:C	2.39	0.42
1:H:49:ASP:HB3	1:H:53:ALA:HB3	2.01	0.42
1:H:667:ILE:HA	1:H:667:ILE:HD12	1.75	0.42
1:A:116:SER:HA	1:A:125:ILE:O	2.19	0.42
1:C:6:GLU:H	1:C:6:GLU:HG2	1.51	0.42
1:D:327:TYR:HD1	1:D:327:TYR:HA	1.71	0.42
1:E:319:ALA:HB2	1:E:332:PHE:CD1	2.55	0.42
1:G:97:ALA:O	1:G:99:SER:N	2.53	0.42
1:H:114:LYS:HG3	1:H:128:HIS:HD2	1.78	0.42
1:H:384:GLY:HA3	1:H:390:LEU:HD11	2.01	0.42
1:H:731:ILE:HD13	1:H:743:LEU:HD23	2.01	0.42
1:H:761:ARG:HH21	1:H:761:ARG:HB3	1.84	0.42
1:B:18:LYS:HG2	1:B:29:GLU:OE1	2.19	0.42
1:E:139:HIS:O	1:E:242:ILE:HA	2.18	0.42
1:F:729:ILE:HD12	1:F:760:SER:HA	2.01	0.42
1:A:702:LEU:HD23	1:A:709:TYR:CE2	2.55	0.42
1:C:229:LEU:N	1:C:229:LEU:CD1	2.82	0.42
1:E:468:MET:SD	1:F:468:MET:CE	3.08	0.42
1:E:491:MET:HG3	1:E:535:VAL:HG21	2.02	0.42
1:F:338:TYR:HA	1:F:680:GLN:HE22	1.84	0.42
1:F:514:GLU:HG2	1:F:514:GLU:H	1.73	0.42
1:A:760:SER:OG	1:A:762:LEU:HD12	2.19	0.42
1:C:116:SER:HA	1:C:125:ILE:O	2.20	0.42
1:F:512:VAL:O	1:F:516:ILE:HG12	2.20	0.42
1:G:142:LEU:HD21	1:G:263:MET:CE	2.42	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:681:MET:HE3	1:B:681:MET:HB2	1.91	0.42
1:D:615:GLU:HB3	1:D:616:PRO:HD3	2.02	0.42
1:E:287:THR:O	1:E:709:TYR:HA	2.20	0.42
1:G:17:ILE:HA	1:G:102:ARG:O	2.20	0.42
1:G:360:ARG:HH11	1:G:360:ARG:HG2	1.85	0.42
1:A:599:PRO:CB	5:A:806:P6G:H141	2.46	0.42
1:C:508:THR:O	1:C:512:VAL:HG23	2.19	0.42
1:H:637:ASP:OD2	1:H:701:ARG:NH1	2.53	0.42
1:A:464:ARG:HD2	1:A:534:TYR:HB2	2.02	0.42
1:B:361:THR:HB	1:B:387:GLY:HA3	2.02	0.42
1:D:686:PHE:CE1	1:D:703:PRO:HG3	2.55	0.42
1:D:459:LYS:HB3	1:D:459:LYS:HE3	1.84	0.41
1:D:336:GLU:O	9:D:808:7PE:H32	2.20	0.41
1:E:233:LYS:HA	1:E:234:PRO:HD3	1.90	0.41
1:E:412:TRP:CZ3	1:E:479:ASN:HB2	2.55	0.41
1:G:644:ARG:HD3	12:G:1020:HOH:O	2.19	0.41
1:A:263:MET:HE3	1:A:269:GLU:HG3	2.03	0.41
1:A:696:ILE:HD12	1:A:715:VAL:HG11	2.02	0.41
1:C:165:VAL:HB	12:C:1184:HOH:O	2.20	0.41
1:A:368:LYS:HD3	1:A:378:TYR:O	2.20	0.41
1:A:582:ARG:HD2	1:B:394:PHE:HZ	1.84	0.41
1:A:618:THR:HG22	1:A:620:HIS:H	1.85	0.41
5:A:806:P6G:H52	5:A:806:P6G:H22	1.90	0.41
1:D:178:TYR:OH	1:D:180:SER:HB3	2.20	0.41
1:D:181:HIS:HB2	1:D:182:PRO:CD	2.50	0.41
1:D:6:GLU:O	1:D:7:HIS:HB2	2.19	0.41
1:F:734:LYS:H	1:F:734:LYS:HG2	1.76	0.41
1:G:678:SER:HA	1:G:681:MET:HE3	2.01	0.41
1:D:551:TYR:CZ	4:D:807:GOL:H11	2.55	0.41
1:E:637:ASP:O	1:E:637:ASP:CG	2.58	0.41
1:F:381:TRP:CH2	1:F:413:GLN:NE2	2.88	0.41
1:F:448:ILE:HG22	1:F:493:THR:HG21	2.03	0.41
1:H:375:GLU:O	1:H:451:PHE:HA	2.19	0.41
1:A:274:ARG:NE	4:A:808:GOL:O1	2.52	0.41
1:B:20:ARG:HD2	1:B:20:ARG:HA	1.76	0.41
12:A:1080:HOH:O	1:C:644:ARG:CD	2.68	0.41
1:D:361:THR:HB	1:D:387:GLY:HA3	2.03	0.41
1:G:327:TYR:OH	4:G:802:GOL:H31	2.20	0.41
1:B:315:LEU:H	4:B:803:GOL:H12	1.86	0.41
1:B:85:HIS:HA	1:B:89:GLU:O	2.20	0.41
1:C:293:ILE:HD12	1:C:293:ILE:N	2.35	0.41
1:D:131:LYS:HA	1:D:142:LEU:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:734:LYS:HB2	1:F:735:SER:H	1.70	0.41
1:G:179:PHE:CZ	1:G:186:GLY:HA3	2.55	0.41
1:G:58:ILE:H	1:G:58:ILE:HD12	1.84	0.41
1:G:646:PHE:O	1:G:650:VAL:HG22	2.21	0.41
1:H:79:ALA:HB3	1:H:241:MET:HB2	2.01	0.41
1:H:356:LYS:HB3	1:H:356:LYS:HE2	1.90	0.41
1:H:414:ILE:O	1:H:418:PRO:HD2	2.21	0.41
1:B:179:PHE:CE1	1:B:186:GLY:HA3	2.56	0.41
1:C:47:ALA:HB1	1:C:82:THR:HB	2.02	0.41
1:D:477:HIS:HE1	1:D:585:CYS:O	2.04	0.41
1:E:301:ASN:O	1:E:675:ASN:HB3	2.20	0.41
1:F:60:THR:HB	1:F:315:LEU:HD13	2.02	0.41
1:G:546:GLN:OE1	1:G:586:ILE:HG21	2.21	0.41
1:G:692:HIS:O	1:G:695:ASP:HB2	2.21	0.41
1:H:246:SER:HA	1:H:249:VAL:O	2.20	0.41
1:A:7:HIS:HB3	1:A:19:ASN:OD1	2.21	0.41
1:B:190:LYS:HA	1:B:196:ASP:O	2.21	0.41
1:B:704:ASP:OD2	4:D:805:GOL:O3	2.38	0.41
1:C:696:ILE:CD1	1:C:696:ILE:N	2.84	0.41
1:E:341:PRO:HG2	1:E:680:GLN:NE2	2.35	0.41
1:F:133:ALA:HA	1:F:141:VAL:HA	2.02	0.41
1:F:570:ASP:N	1:F:570:ASP:OD1	2.51	0.41
1:G:31:SER:HB3	1:G:670:ILE:HG12	2.02	0.41
1:G:415:HIS:ND1	1:G:419:ASP:OD2	2.44	0.41
1:H:458:TYR:CE2	1:H:460:PRO:HA	2.55	0.41
1:H:69:LYS:HA	8:H:803:PG4:H72	2.02	0.41
1:C:16:ILE:CG1	1:C:104:LEU:HB3	2.50	0.41
1:C:491:MET:HA	1:C:491:MET:CE	2.51	0.41
1:D:45:THR:HG21	1:D:55:ALA:HA	2.01	0.41
1:E:28:THR:HG21	1:E:656:ASN:HB2	2.02	0.41
1:F:573:TYR:CE2	1:F:621:PHE:HE1	2.38	0.41
1:F:751:VAL:HG12	1:F:752:LEU:N	2.35	0.41
1:G:737:ASP:CA	1:G:738:ARG:CB	2.92	0.41
1:A:432:GLY:O	1:A:434:ASP:N	2.54	0.41
10:C:805:PE4:C8	10:C:805:PE4:H142	2.50	0.41
1:D:573:TYR:HE2	1:D:621:PHE:HE1	1.68	0.41
1:D:605:LYS:HA	1:D:605:LYS:HD3	1.92	0.41
8:D:803:PG4:H11	8:D:803:PG4:H32	1.76	0.41
1:A:644:ARG:NH1	1:F:228:SER:HB3	2.33	0.41
1:F:49:ASP:HB3	1:F:53:ALA:HB3	2.02	0.41
1:H:356:LYS:HE3	1:H:440:TYR:CZ	2.56	0.41
1:G:129:GLU:OE2	1:G:131:LYS:NZ	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:422:TYR:HE2	11:H:808:PE5:H62	1.86	0.41
1:A:44:GLY:O	1:A:102:ARG:NH2	2.38	0.40
1:F:43:ARG:HD3	1:F:56:ALA:HB3	2.02	0.40
1:A:58:ILE:HD12	1:A:58:ILE:N	2.36	0.40
1:B:733:ASN:C	1:B:734:LYS:O	2.58	0.40
1:E:15:ASP:OD2	1:E:17:ILE:HD11	2.22	0.40
1:G:619:LEU:O	1:G:620:HIS:HB2	2.21	0.40
1:G:97:ALA:O	1:G:98:ALA:C	2.58	0.40
1:A:31:SER:HB3	1:A:670:ILE:HG12	2.02	0.40
1:B:726:LYS:N	1:B:726:LYS:HD2	2.37	0.40
1:B:729:ILE:HD11	1:B:745:ILE:HG21	2.02	0.40
1:D:612:GLU:OE2	1:D:638:LYS:NZ	2.54	0.40
1:E:230:GLU:CD	1:E:233:LYS:HE3	2.42	0.40
1:G:612:GLU:OE2	4:G:803:GOL:H31	2.21	0.40
1:A:573:TYR:CE2	1:A:621:PHE:HE1	2.39	0.40
1:B:316:PRO:CB	1:B:331:ALA:HB2	2.52	0.40
1:B:604:ARG:HG2	9:B:802:7PE:C21	2.42	0.40
1:D:741:LEU:C	1:D:742:THR:HG23	2.42	0.40
1:E:29:GLU:HG2	1:E:102:ARG:NH1	2.37	0.40
1:E:466:GLU:OE1	1:E:468:MET:CE	2.70	0.40
1:F:491:MET:HE1	1:F:491:MET:HA	2.01	0.40
1:F:594:LEU:HD12	1:F:598:HIS:HD2	1.86	0.40
1:H:381:TRP:CH2	1:H:413:GLN:CD	2.95	0.40
1:B:604:ARG:HB3	1:B:604:ARG:HE	1.47	0.40
1:D:201:VAL:HG11	1:D:260:ALA:HB2	2.03	0.40
1:D:412:TRP:CZ3	1:D:479:ASN:HB2	2.57	0.40
1:D:79:ALA:HB3	1:D:241:MET:HB2	2.04	0.40
1:E:117:GLN:O	1:E:124:THR:HA	2.21	0.40
1:F:361:THR:HB	1:F:387:GLY:HA3	2.04	0.40
1:G:381:TRP:CH2	1:G:413:GLN:NE2	2.90	0.40
1:G:615:GLU:HB3	1:G:616:PRO:CD	2.51	0.40
1:H:624:LEU:HD12	1:H:624:LEU:N	2.36	0.40
1:H:719:THR:H	1:H:735:SER:HB3	1.86	0.40
1:H:754:SER:O	1:H:755:GLU:C	2.59	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	760/769 (99%)	721 (95%)	29 (4%)	10 (1%)	18	17
1	B	759/769 (99%)	720 (95%)	33 (4%)	6 (1%)	27	30
1	C	759/769 (99%)	728 (96%)	25 (3%)	6 (1%)	27	30
1	D	759/769 (99%)	723 (95%)	34 (4%)	2 (0%)	50	60
1	E	759/769 (99%)	696 (92%)	48 (6%)	15 (2%)	11	8
1	F	759/769 (99%)	701 (92%)	44 (6%)	14 (2%)	13	10
1	G	760/769 (99%)	718 (94%)	31 (4%)	11 (1%)	16	15
1	H	759/769 (99%)	715 (94%)	35 (5%)	9 (1%)	19	19
All	All	6074/6152 (99%)	5722 (94%)	279 (5%)	73 (1%)	19	19

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	THR
1	A	750	SER
1	A	754	SER
1	B	6	GLU
1	B	27	ILE
1	B	735	SER
1	C	6	GLU
1	C	98	ALA
1	C	694	ASP
1	D	98	ALA
1	E	736	GLU
1	E	738	ARG
1	E	750	SER
1	E	751	VAL
1	F	27	ILE
1	F	98	ALA
1	F	99	SER
1	F	744	HIS
1	F	746	PHE

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Mol	Chain	Res	Type
1	F	757	ILE
1	G	209	ASP
1	G	660	ALA
1	G	736	GLU
1	G	738	ARG
1	H	3	GLU
1	H	735	SER
1	A	6	GLU
1	A	98	ALA
1	A	743	LEU
1	A	749	LYS
1	A	753	ASP
1	E	660	ALA
1	F	738	ARG
1	F	754	SER
1	F	760	SER
1	G	2	HIS
1	G	98	ALA
1	H	2	HIS
1	H	6	GLU
1	H	98	ALA
1	H	99	SER
1	A	2	HIS
1	A	660	ALA
1	C	660	ALA
1	D	99	SER
1	E	6	GLU
1	E	98	ALA
1	E	205	SER
1	E	209	ASP
1	F	2	HIS
1	F	690	SER
1	F	700	PRO
1	G	210	ALA
1	H	750	SER
1	B	37	ASN
1	B	98	ALA
1	B	754	SER
1	C	2	HIS
1	C	37	ASN
1	E	26	ALA
1	E	474	ASP

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Mol	Chain	Res	Type
1	E	746	PHE
1	F	735	SER
1	F	758	THR
1	G	314	SER
1	G	737	ASP
1	H	314	SER
1	G	474	ASP
1	E	87	ASP
1	G	37	ASN
1	E	182	PRO
1	H	27	ILE
1	E	757	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/658 (99%)	616 (95%)	35 (5%)	31	40
1	B	650/658 (99%)	615 (95%)	35 (5%)	31	40
1	C	650/658 (99%)	609 (94%)	41 (6%)	25	32
1	D	650/658 (99%)	615 (95%)	35 (5%)	31	40
1	E	650/658 (99%)	598 (92%)	52 (8%)	17	20
1	F	650/658 (99%)	609 (94%)	41 (6%)	25	32
1	G	651/658 (99%)	600 (92%)	51 (8%)	18	22
1	H	650/658 (99%)	616 (95%)	34 (5%)	32	42
All	All	5202/5264 (99%)	4878 (94%)	324 (6%)	26	33

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	83	LEU
1	A	94	SER
1	A	96	GLU
1	A	129	GLU

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Mol	Chain	Res	Type
1	A	191	THR
1	A	217	ASN
1	A	229	LEU
1	A	257	LEU
1	A	258	LEU
1	A	261	LYS
1	A	275	LEU
1	A	280	LEU
1	A	289	GLN
1	A	298	LEU
1	A	378	TYR
1	A	390	LEU
1	A	417	SER
1	A	506	GLU
1	A	509	LEU
1	A	537	LYS
1	A	604	ARG
1	A	647	ARG
1	A	655	LEU
1	A	670	ILE
1	A	698	LEU
1	A	701	ARG
1	A	702	LEU
1	A	727	GLU
1	A	732	THR
1	A	739	LYS
1	A	741	LEU
1	A	750	SER
1	A	752	LEU
1	A	757	ILE
1	B	2	HIS
1	B	20	ARG
1	B	80	LEU
1	B	96	GLU
1	B	102	ARG
1	B	144	LYS
1	B	224	THR
1	B	228	SER
1	B	230	GLU
1	B	233	LYS
1	B	289	GLN
1	B	370	LYS

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Mol	Chain	Res	Type
1	B	378	TYR
1	B	425	LYS
1	B	503	THR
1	B	506	GLU
1	B	507	LYS
1	B	509	LEU
1	B	524	SER
1	B	582	ARG
1	B	604	ARG
1	B	659	GLU
1	B	710	THR
1	B	720	LEU
1	B	726	LYS
1	B	729	ILE
1	B	734	LYS
1	B	735	SER
1	B	736	GLU
1	B	741	LEU
1	B	742	THR
1	B	743	LEU
1	B	748	GLU
1	B	750	SER
1	B	760	SER
1	C	1	MET
1	C	2	HIS
1	C	6	GLU
1	C	18	LYS
1	C	94	SER
1	C	118	ARG
1	C	147	VAL
1	C	191	THR
1	C	227	LEU
1	C	228	SER
1	C	230	GLU
1	C	257	LEU
1	C	258	LEU
1	C	261	LYS
1	C	275	LEU
1	C	280	LEU
1	C	289	GLN
1	C	298	LEU
1	C	349	GLU

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Mol	Chain	Res	Type
1	C	352	ARG
1	C	370	LYS
1	C	378	TYR
1	C	495	GLN
1	C	503	THR
1	C	509	LEU
1	C	510	SER
1	C	537	LYS
1	C	569	GLU
1	C	582	ARG
1	C	604	ARG
1	C	655	LEU
1	C	698	LEU
1	C	702	LEU
1	C	710	THR
1	C	718	GLN
1	C	728	GLN
1	C	735	SER
1	C	750	SER
1	C	754	SER
1	C	757	ILE
1	C	760	SER
1	D	1	MET
1	D	27	ILE
1	D	80	LEU
1	D	94	SER
1	D	99	SER
1	D	101	GLU
1	D	102	ARG
1	D	147	VAL
1	D	205	SER
1	D	228	SER
1	D	233	LYS
1	D	275	LEU
1	D	289	GLN
1	D	349	GLU
1	D	370	LYS
1	D	378	TYR
1	D	397	LYS
1	D	417	SER
1	D	426	LYS
1	D	503	THR

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Mol	Chain	Res	Type
1	D	509	LEU
1	D	524	SER
1	D	582	ARG
1	D	605	LYS
1	D	667	ILE
1	D	699	SER
1	D	710	THR
1	D	726	LYS
1	D	735	SER
1	D	736	GLU
1	D	741	LEU
1	D	742	THR
1	D	748	GLU
1	D	750	SER
1	D	761	ARG
1	E	2	HIS
1	E	16	ILE
1	E	22	GLU
1	E	29	GLU
1	E	89	GLU
1	E	96	GLU
1	E	99	SER
1	E	114	LYS
1	E	171	ASP
1	E	174	GLN
1	E	193	SER
1	E	217	ASN
1	E	226	SER
1	E	228	SER
1	E	243	ILE
1	E	257	LEU
1	E	258	LEU
1	E	259	GLU
1	E	261	LYS
1	E	262	HIS
1	E	275	LEU
1	E	280	LEU
1	E	289	GLN
1	E	298	LEU
1	E	370	LYS
1	E	378	TYR
1	E	390	LEU

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Mol	Chain	Res	Type
1	E	503	THR
1	E	506	GLU
1	E	509	LEU
1	E	540	LYS
1	E	560	LYS
1	E	604	ARG
1	E	655	LEU
1	E	659	GLU
1	E	661	VAL
1	E	696	ILE
1	E	698	LEU
1	E	702	LEU
1	E	710	THR
1	E	714	ILE
1	E	726	LYS
1	E	732	THR
1	E	734	LYS
1	E	741	LEU
1	E	742	THR
1	E	743	LEU
1	E	749	LYS
1	E	751	VAL
1	E	753	ASP
1	E	755	GLU
1	E	757	ILE
1	F	2	HIS
1	F	20	ARG
1	F	22	GLU
1	F	80	LEU
1	F	94	SER
1	F	102	ARG
1	F	128	HIS
1	F	171	ASP
1	F	224	THR
1	F	228	SER
1	F	233	LYS
1	F	275	LEU
1	F	295	GLN
1	F	296	VAL
1	F	349	GLU
1	F	352	ARG
1	F	378	TYR

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Mol	Chain	Res	Type
1	F	417	SER
1	F	506	GLU
1	F	509	LEU
1	F	514	GLU
1	F	582	ARG
1	F	603	ASP
1	F	604	ARG
1	F	637	ASP
1	F	641	GLU
1	F	659	GLU
1	F	667	ILE
1	F	710	THR
1	F	716	LYS
1	F	728	GLN
1	F	734	LYS
1	F	735	SER
1	F	736	GLU
1	F	738	ARG
1	F	742	THR
1	F	743	LEU
1	F	749	LYS
1	F	750	SER
1	F	756	ARG
1	F	759	LYS
1	G	2	HIS
1	G	3	GLU
1	G	16	ILE
1	G	20	ARG
1	G	52	ASP
1	G	83	LEU
1	G	92	ILE
1	G	99	SER
1	G	118	ARG
1	G	147	VAL
1	G	190	LYS
1	G	191	THR
1	G	193	SER
1	G	213	GLU
1	G	227	LEU
1	G	229	LEU
1	G	233	LYS
1	G	255	GLU

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Mol	Chain	Res	Type
1	G	257	LEU
1	G	258	LEU
1	G	261	LYS
1	G	275	LEU
1	G	280	LEU
1	G	282	SER
1	G	292	ILE
1	G	298	LEU
1	G	334	ASP
1	G	370	LYS
1	G	378	TYR
1	G	390	LEU
1	G	417	SER
1	G	426	LYS
1	G	495	GLN
1	G	503	THR
1	G	506	GLU
1	G	568	LYS
1	G	604	ARG
1	G	644	ARG
1	G	655	LEU
1	G	661	VAL
1	G	696	ILE
1	G	702	LEU
1	G	726	LYS
1	G	736	GLU
1	G	739	LYS
1	G	743	LEU
1	G	749	LYS
1	G	750	SER
1	G	754	SER
1	G	756	ARG
1	G	760	SER
1	H	2	HIS
1	H	27	ILE
1	H	80	LEU
1	H	83	LEU
1	H	99	SER
1	H	102	ARG
1	H	224	THR
1	H	258	LEU
1	H	261	LYS

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Mol	Chain	Res	Type
1	H	274	ARG
1	H	275	LEU
1	H	346	SER
1	H	370	LYS
1	H	378	TYR
1	H	400	LEU
1	H	417	SER
1	H	495	GLN
1	H	503	THR
1	H	507	LYS
1	H	519	SER
1	H	537	LYS
1	H	560	LYS
1	H	582	ARG
1	H	641	GLU
1	H	667	ILE
1	H	699	SER
1	H	720	LEU
1	H	726	LYS
1	H	734	LYS
1	H	742	THR
1	H	743	LEU
1	H	754	SER
1	H	756	ARG
1	H	761	ARG

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	495	GLN
1	A	680	GLN
1	B	128	HIS
1	B	347	ASN
1	C	128	HIS
1	C	217	ASN
1	C	429	GLN
1	C	680	GLN
1	D	429	GLN
1	E	289	GLN
1	E	697	HIS
1	F	429	GLN
1	F	455	HIS

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Mol	Chain	Res	Type
1	F	680	GLN
1	G	7	HIS
1	G	264	GLN
1	G	429	GLN
1	G	475	GLN
1	H	7	HIS
1	H	680	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 74 ligands modelled in this entry, 7 are monoatomic - leaving 67 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	$\# Z  > 2$
2	IFM	A	801	-	10,10,10	1.63	2 (20%)	13,13,13	3.14	5 (38%)
3	1PE	A	802	-	15,15,15	0.74	0	14,14,14	0.70	0
4	GOL	A	803	-	5,5,5	0.55	0	5,5,5	1.15	0
4	GOL	A	804	-	5,5,5	0.78	0	5,5,5	2.11	2 (40%)
4	GOL	A	805	-	5,5,5	0.23	0	5,5,5	0.62	0
5	P6G	A	806	-	18,18,18	0.61	0	17,17,17	0.82	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	807	-	5,5,5	0.51	0	5,5,5	1.14	1 (20%)
4	GOL	A	808	-	5,5,5	0.45	0	5,5,5	0.69	0
4	GOL	A	809	-	5,5,5	0.46	0	5,5,5	0.48	0
4	GOL	A	810	-	5,5,5	0.52	0	5,5,5	0.95	0
4	GOL	A	811	-	5,5,5	0.49	0	5,5,5	1.26	0
6	PGE	A	812	-	9,9,9	0.57	0	8,8,8	0.43	0
8	PG4	B	801	-	12,12,12	0.58	0	11,11,11	0.45	0
9	7PE	B	802	-	20,20,20	0.63	0	19,19,19	0.99	1 (5%)
4	GOL	B	803	-	5,5,5	0.53	0	5,5,5	1.69	1 (20%)
4	GOL	B	804	-	5,5,5	0.68	0	5,5,5	1.39	1 (20%)
4	GOL	B	805	-	5,5,5	0.45	0	5,5,5	0.97	0
4	GOL	B	806	-	5,5,5	0.26	0	5,5,5	0.52	0
4	GOL	B	807	-	5,5,5	0.52	0	5,5,5	0.89	0
4	GOL	B	808	-	5,5,5	0.61	0	5,5,5	2.10	1 (20%)
3	1PE	C	801	-	15,15,15	0.67	0	14,14,14	0.97	0
4	GOL	C	802	-	5,5,5	0.47	0	5,5,5	0.41	0
4	GOL	C	803	-	5,5,5	0.27	0	5,5,5	1.34	1 (20%)
4	GOL	C	804	-	5,5,5	0.41	0	5,5,5	1.39	1 (20%)
10	PE4	C	805	-	23,23,23	0.93	0	22,22,22	1.32	2 (9%)
4	GOL	C	806	-	5,5,5	0.59	0	5,5,5	0.76	0
6	PGE	C	807	-	9,9,9	0.46	0	8,8,8	0.84	0
4	GOL	C	808	-	5,5,5	0.40	0	5,5,5	0.71	0
4	GOL	C	809	-	5,5,5	0.60	0	5,5,5	2.23	1 (20%)
2	IFM	D	801	-	10,10,10	2.16	5 (50%)	13,13,13	3.25	8 (61%)
4	GOL	D	802	-	5,5,5	0.47	0	5,5,5	0.71	0
8	PG4	D	803	-	12,12,12	0.61	0	11,11,11	0.61	0
4	GOL	D	804	-	5,5,5	0.35	0	5,5,5	0.35	0
4	GOL	D	805	-	5,5,5	0.15	0	5,5,5	0.97	0
4	GOL	D	806	-	5,5,5	0.67	0	5,5,5	1.08	0
4	GOL	D	807	-	5,5,5	0.32	0	5,5,5	0.52	0
9	7PE	D	808	-	20,20,20	0.74	0	19,19,19	1.44	3 (15%)
4	GOL	D	809	-	5,5,5	0.37	0	5,5,5	1.35	1 (20%)
4	GOL	D	810	-	5,5,5	0.35	0	5,5,5	1.93	1 (20%)
4	GOL	D	811	-	5,5,5	0.37	0	5,5,5	0.32	0
4	GOL	D	812	-	5,5,5	1.30	0	5,5,5	1.85	2 (40%)
2	IFM	E	801	-	10,10,10	1.45	2 (20%)	13,13,13	2.69	5 (38%)
3	1PE	E	802	-	15,15,15	0.72	0	14,14,14	0.38	0
5	P6G	E	803	-	18,18,18	0.67	0	17,17,17	0.78	0
4	GOL	E	804	-	5,5,5	0.23	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	E	805	-	5,5,5	0.35	0	5,5,5	0.24	0
4	GOL	E	806	-	5,5,5	0.45	0	5,5,5	0.85	0
4	GOL	E	807	-	5,5,5	0.23	0	5,5,5	0.96	0
2	IFM	F	801	-	10,10,10	1.29	1 (10%)	13,13,13	2.41	3 (23%)
4	GOL	F	802	-	5,5,5	0.29	0	5,5,5	0.76	0
8	PG4	F	803	-	12,12,12	0.56	0	11,11,11	0.48	0
4	GOL	F	804	-	5,5,5	0.49	0	5,5,5	0.49	0
4	GOL	F	805	-	5,5,5	0.60	0	5,5,5	0.63	0
6	PGE	F	806	-	9,9,9	0.52	0	8,8,8	0.46	0
2	IFM	G	801	-	10,10,10	1.17	1 (10%)	13,13,13	2.62	7 (53%)
4	GOL	G	802	-	5,5,5	0.19	0	5,5,5	0.73	0
4	GOL	G	803	-	5,5,5	0.16	0	5,5,5	0.82	0
4	GOL	G	804	-	5,5,5	0.31	0	5,5,5	0.59	0
6	PGE	G	805	-	9,9,9	0.72	0	8,8,8	0.55	0
2	IFM	H	801	-	10,10,10	1.18	2 (20%)	13,13,13	2.91	5 (38%)
4	GOL	H	802	-	5,5,5	0.31	0	5,5,5	0.53	0
8	PG4	H	803	-	12,12,12	0.70	0	11,11,11	0.48	0
4	GOL	H	804	-	5,5,5	0.35	0	5,5,5	0.61	0
4	GOL	H	805	-	5,5,5	0.46	0	5,5,5	1.09	1 (20%)
4	GOL	H	806	-	5,5,5	0.42	0	5,5,5	1.06	0
4	GOL	H	807	-	5,5,5	0.36	0	5,5,5	0.72	0
11	PE5	H	808	-	26,26,26	0.79	0	25,25,25	0.90	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	IFM	A	801	-	-	0/2/16/16	0/1/1/1
3	1PE	A	802	-	-	0/13/13/13	0/0/0/0
4	GOL	A	803	-	-	0/4/4/4	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	805	-	-	0/4/4/4	0/0/0/0
5	P6G	A	806	-	-	0/16/16/16	0/0/0/0
4	GOL	A	807	-	-	0/4/4/4	0/0/0/0
4	GOL	A	808	-	-	0/4/4/4	0/0/0/0
4	GOL	A	809	-	-	0/4/4/4	0/0/0/0
4	GOL	A	810	-	-	0/4/4/4	0/0/0/0
4	GOL	A	811	-	-	0/4/4/4	0/0/0/0
6	PGE	A	812	-	-	0/7/7/7	0/0/0/0
8	PG4	B	801	-	-	0/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	7PE	B	802	-	-	0/18/18/18	0/0/0/0
4	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	GOL	B	804	-	-	0/4/4/4	0/0/0/0
4	GOL	B	805	-	-	0/4/4/4	0/0/0/0
4	GOL	B	806	-	-	0/4/4/4	0/0/0/0
4	GOL	B	807	-	-	0/4/4/4	0/0/0/0
4	GOL	B	808	-	-	0/4/4/4	0/0/0/0
3	1PE	C	801	-	-	0/13/13/13	0/0/0/0
4	GOL	C	802	-	-	0/4/4/4	0/0/0/0
4	GOL	C	803	-	-	0/4/4/4	0/0/0/0
4	GOL	C	804	-	-	0/4/4/4	0/0/0/0
10	PE4	C	805	-	-	0/21/21/21	0/0/0/0
4	GOL	C	806	-	-	0/4/4/4	0/0/0/0
6	PGE	C	807	-	-	0/7/7/7	0/0/0/0
4	GOL	C	808	-	-	0/4/4/4	0/0/0/0
4	GOL	C	809	-	-	0/4/4/4	0/0/0/0
2	IFM	D	801	-	-	0/2/16/16	0/1/1/1
4	GOL	D	802	-	-	0/4/4/4	0/0/0/0
8	PG4	D	803	-	-	0/10/10/10	0/0/0/0
4	GOL	D	804	-	-	0/4/4/4	0/0/0/0
4	GOL	D	805	-	-	0/4/4/4	0/0/0/0
4	GOL	D	806	-	-	0/4/4/4	0/0/0/0
4	GOL	D	807	-	-	0/4/4/4	0/0/0/0
9	7PE	D	808	-	-	0/18/18/18	0/0/0/0
4	GOL	D	809	-	-	0/4/4/4	0/0/0/0
4	GOL	D	810	-	-	0/4/4/4	0/0/0/0
4	GOL	D	811	-	-	0/4/4/4	0/0/0/0
4	GOL	D	812	-	-	0/4/4/4	0/0/0/0
2	IFM	E	801	-	-	0/2/16/16	0/1/1/1
3	1PE	E	802	-	-	0/13/13/13	0/0/0/0
5	P6G	E	803	-	-	0/16/16/16	0/0/0/0
4	GOL	E	804	-	-	0/4/4/4	0/0/0/0
4	GOL	E	805	-	-	0/4/4/4	0/0/0/0
4	GOL	E	806	-	-	0/4/4/4	0/0/0/0
4	GOL	E	807	-	-	0/4/4/4	0/0/0/0
2	IFM	F	801	-	-	0/2/16/16	1/1/1/1
4	GOL	F	802	-	-	0/4/4/4	0/0/0/0
8	PG4	F	803	-	-	0/10/10/10	0/0/0/0
4	GOL	F	804	-	-	0/4/4/4	0/0/0/0
4	GOL	F	805	-	-	0/4/4/4	0/0/0/0
6	PGE	F	806	-	-	0/7/7/7	0/0/0/0
2	IFM	G	801	-	-	0/2/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	802	-	-	0/4/4/4	0/0/0/0
4	GOL	G	803	-	-	0/4/4/4	0/0/0/0
4	GOL	G	804	-	-	0/4/4/4	0/0/0/0
6	PGE	G	805	-	-	0/7/7/7	0/0/0/0
2	IFM	H	801	-	-	0/2/16/16	1/1/1/1
4	GOL	H	802	-	-	0/4/4/4	0/0/0/0
8	PG4	H	803	-	-	0/10/10/10	0/0/0/0
4	GOL	H	804	-	-	0/4/4/4	0/0/0/0
4	GOL	H	805	-	-	0/4/4/4	0/0/0/0
4	GOL	H	806	-	-	0/4/4/4	0/0/0/0
4	GOL	H	807	-	-	0/4/4/4	0/0/0/0
11	PE5	H	808	-	-	0/24/24/24	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	IFM	C5-C4	-3.25	1.49	1.53
2	D	801	IFM	C5-C4	-3.14	1.49	1.53
2	D	801	IFM	C2-N	-3.08	1.41	1.46
2	E	801	IFM	C3-C4	2.97	1.56	1.52
2	D	801	IFM	O4-C4	-2.95	1.35	1.43
2	F	801	IFM	C3-C4	2.87	1.56	1.52
2	D	801	IFM	C3-C4	2.78	1.56	1.52
2	G	801	IFM	C3-C4	2.53	1.56	1.52
2	A	801	IFM	C3-C4	2.23	1.55	1.52
2	H	801	IFM	C3-C4	2.22	1.55	1.52
2	D	801	IFM	O3-C3	2.20	1.48	1.43
2	E	801	IFM	O3-C3	2.03	1.48	1.43
2	H	801	IFM	O3-C3	2.00	1.47	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	IFM	O4-C4-C5	-7.84	97.27	110.14
2	H	801	IFM	C1-N-C2	7.27	121.66	111.98
2	E	801	IFM	O4-C4-C5	-6.91	98.79	110.14
2	A	801	IFM	O4-C4-C5	-6.89	98.83	110.14
2	F	801	IFM	C1-N-C2	6.74	120.96	111.98
2	A	801	IFM	C1-N-C2	6.47	120.59	111.98
2	G	801	IFM	C1-N-C2	5.84	119.75	111.98
2	H	801	IFM	O4-C4-C5	-5.77	100.67	110.14
4	B	808	GOL	O3-C3-C2	-4.19	91.73	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	IFM	O3-C3-C4	4.15	118.27	110.24
4	D	810	GOL	O1-C1-C2	-3.95	92.80	110.37
2	E	801	IFM	C1-N-C2	3.89	117.16	111.98
4	C	809	GOL	C3-C2-C1	-3.72	95.89	111.00
2	D	801	IFM	C3-C2-N	-3.53	104.15	111.31
2	D	801	IFM	O6-C6-C5	-3.49	104.27	111.42
2	F	801	IFM	O3-C3-C4	3.45	116.90	110.24
10	C	805	PE4	C15-O8-C14	3.37	125.33	112.83
4	A	804	GOL	O1-C1-C2	-3.32	95.63	110.37
2	G	801	IFM	C1-C5-C4	3.28	115.43	108.56
2	G	801	IFM	O4-C4-C5	-3.26	104.80	110.14
9	D	808	7PE	O4-C5-C6	-3.21	96.18	110.41
2	H	801	IFM	O3-C3-C4	3.19	116.40	110.24
2	E	801	IFM	O3-C3-C4	3.18	116.39	110.24
2	D	801	IFM	C1-N-C2	3.15	116.18	111.98
4	D	812	GOL	O2-C2-C3	3.04	122.50	108.44
2	G	801	IFM	C3-C2-N	-2.97	105.29	111.31
2	E	801	IFM	C3-C2-N	-2.92	105.40	111.31
9	D	808	7PE	O7-C8-C9	-2.87	97.67	110.41
2	D	801	IFM	C5-C1-N	-2.87	105.03	112.42
2	A	801	IFM	O4-C4-C3	2.86	115.22	110.00
2	F	801	IFM	O4-C4-C5	-2.66	105.78	110.14
2	H	801	IFM	C5-C1-N	-2.65	105.61	112.42
4	A	804	GOL	O2-C2-C3	2.59	120.41	108.44
4	C	804	GOL	O1-C1-C2	-2.56	99.01	110.37
2	E	801	IFM	O6-C6-C5	-2.54	106.22	111.42
2	G	801	IFM	O4-C4-C3	2.48	114.51	110.00
2	D	801	IFM	C1-C5-C4	-2.47	103.40	108.56
4	C	803	GOL	O1-C1-C2	-2.35	99.92	110.37
4	B	803	GOL	O3-C3-C2	-2.34	99.95	110.37
4	B	804	GOL	C3-C2-C1	-2.29	101.69	111.00
10	C	805	PE4	O7-C13-C14	2.29	120.58	110.41
2	G	801	IFM	O3-C3-C4	2.24	114.57	110.24
2	A	801	IFM	C3-C2-N	-2.22	106.81	111.31
4	H	805	GOL	O1-C1-C2	-2.20	100.57	110.37
9	B	802	7PE	C20-O19-C18	2.15	120.83	112.83
2	D	801	IFM	C2-C3-C4	-2.15	107.68	110.17
4	D	812	GOL	C3-C2-C1	-2.14	102.33	111.00
2	G	801	IFM	C6-C5-C4	-2.14	108.17	112.03
4	D	809	GOL	O1-C1-C2	-2.13	100.89	110.37
2	A	801	IFM	C6-C5-C4	-2.11	108.22	112.03
2	H	801	IFM	C2-C3-C4	-2.09	107.75	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	808	7PE	C20-O19-C18	2.08	120.55	112.83
4	A	807	GOL	O1-C1-C2	-2.04	101.30	110.37

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	801	IFM	C1-C2-C3-C4-C5-N
2	F	801	IFM	C1-C2-C3-C4-C5-N

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	762/769 (99%)	-0.03	10 (1%) 74 82	30, 40, 65, 98	0
1	B	761/769 (98%)	0.13	26 (3%) 43 53	28, 40, 64, 97	0
1	C	761/769 (98%)	0.12	29 (3%) 38 49	28, 40, 64, 99	0
1	D	761/769 (98%)	0.09	32 (4%) 35 45	28, 39, 68, 97	0
1	E	761/769 (98%)	0.63	103 (13%) 4 6	35, 53, 101, 142	0
1	F	761/769 (98%)	0.32	46 (6%) 21 30	32, 49, 86, 131	0
1	G	762/769 (99%)	0.49	81 (10%) 7 11	38, 52, 83, 110	0
1	H	761/769 (98%)	0.27	44 (5%) 22 31	37, 50, 85, 115	0
All	All	6090/6152 (98%)	0.25	371 (6%) 21 29	28, 46, 80, 142	0

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ALA	11.6
1	G	98	ALA	8.9
1	F	98	ALA	8.0
1	E	208	ALA	7.8
1	H	751	VAL	7.8
1	A	762	LEU	7.7
1	E	752	LEU	7.5
1	E	753	ASP	7.3
1	H	98	ALA	6.6
1	F	754	SER	6.5
1	E	125	ILE	6.5
1	F	761	ARG	6.4
1	E	229	LEU	6.4
1	E	232	GLY	6.3
1	C	1	MET	5.8
1	F	736	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	230	GLU	5.7
1	D	98	ALA	5.5
1	G	118	ARG	5.4
1	C	97	ALA	5.4
1	F	741	LEU	5.4
1	G	741	LEU	5.4
1	E	233	LYS	5.3
1	E	729	ILE	5.1
1	B	98	ALA	5.1
1	E	147	VAL	5.1
1	E	659	GLU	4.9
1	H	761	ARG	4.9
1	F	757	ILE	4.9
1	E	98	ALA	4.8
1	D	761	ARG	4.8
1	E	118	ARG	4.8
1	G	97	ALA	4.8
1	E	231	ALA	4.7
1	E	234	PRO	4.7
1	H	506	GLU	4.5
1	E	1	MET	4.5
1	E	757	ILE	4.4
1	A	98	ALA	4.4
1	G	746	PHE	4.4
1	E	149	SER	4.4
1	F	752	LEU	4.3
1	G	694	ASP	4.3
1	G	740	PRO	4.2
1	E	124	THR	4.2
1	E	206	LEU	4.2
1	G	6	GLU	4.2
1	E	227	LEU	4.2
1	F	1	MET	4.2
1	G	752	LEU	4.2
1	G	751	VAL	4.1
1	H	753	ASP	4.1
1	E	742	THR	4.1
1	F	720	LEU	4.0
1	F	739	LYS	4.0
1	H	742	THR	3.9
1	E	92	ILE	3.9
1	G	153	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	96	GLU	3.9
1	E	726	LYS	3.8
1	G	762	LEU	3.8
1	E	235	VAL	3.8
1	G	96	GLU	3.8
1	C	96	GLU	3.8
1	E	150	ASP	3.8
1	C	232	GLY	3.8
1	G	120	LYS	3.8
1	E	192	VAL	3.8
1	E	117	GLN	3.7
1	H	741	LEU	3.7
1	G	731	ILE	3.7
1	H	752	LEU	3.7
1	G	737	ASP	3.6
1	E	751	VAL	3.6
1	E	708	GLY	3.6
1	C	231	ALA	3.6
1	H	20	ARG	3.6
1	B	1	MET	3.6
1	D	751	VAL	3.5
1	G	249	VAL	3.5
1	G	750	SER	3.5
1	E	754	SER	3.5
1	E	152	ASP	3.5
1	B	737	ASP	3.5
1	D	727	GLU	3.5
1	E	151	GLN	3.5
1	F	504	LEU	3.4
1	D	744	HIS	3.4
1	E	228	SER	3.4
1	B	753	ASP	3.4
1	E	728	GLN	3.4
1	F	502	GLN	3.4
1	E	94	SER	3.4
1	H	759	LYS	3.4
1	G	149	SER	3.3
1	G	729	ILE	3.3
1	D	736	GLU	3.3
1	F	26	ALA	3.3
1	H	743	LEU	3.3
1	E	123	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	756	ARG	3.2
1	G	758	THR	3.2
1	G	760	SER	3.2
1	H	504	LEU	3.2
1	G	742	THR	3.2
1	H	740	PRO	3.2
1	F	718	GLN	3.2
1	G	124	THR	3.2
1	H	748	GLU	3.2
1	E	2	HIS	3.1
1	G	730	THR	3.1
1	F	743	LEU	3.1
1	E	207	ASP	3.1
1	E	524	SER	3.1
1	G	756	ARG	3.1
1	C	751	VAL	3.1
1	E	119	MET	3.1
1	G	206	LEU	3.1
1	G	743	LEU	3.1
1	H	747	GLY	3.1
1	E	658	ASN	3.1
1	G	728	GLN	3.1
1	E	93	MET	3.1
1	G	151	GLN	3.0
1	C	233	LYS	3.0
1	H	567	ILE	3.0
1	A	727	GLU	3.0
1	F	501	LEU	3.0
1	D	757	ILE	3.0
1	E	727	GLU	3.0
1	C	209	ASP	3.0
1	H	760	SER	3.0
1	G	258	LEU	3.0
1	H	194	TYR	3.0
1	E	177	HIS	3.0
1	F	742	THR	2.9
1	H	694	ASP	2.9
1	E	122	GLY	2.9
1	A	96	GLU	2.9
1	G	753	ASP	2.9
1	E	738	ARG	2.9
1	E	218	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	333	TRP	2.9
1	G	122	GLY	2.9
1	F	753	ASP	2.9
1	B	736	GLU	2.9
1	G	119	MET	2.9
1	D	748	GLU	2.8
1	G	121	ASN	2.8
1	E	672	THR	2.8
1	F	756	ARG	2.8
1	H	1	MET	2.8
1	E	86	VAL	2.8
1	C	21	TYR	2.8
1	D	317	ILE	2.8
1	C	118	ARG	2.8
1	D	672	THR	2.8
1	E	174	GLN	2.8
1	F	292	ILE	2.8
1	G	726	LYS	2.8
1	F	715	VAL	2.8
1	E	755	GLU	2.8
1	F	6	GLU	2.8
1	E	623	SER	2.8
1	E	750	SER	2.8
1	B	333	TRP	2.8
1	F	725	THR	2.8
1	A	1	MET	2.8
1	G	251	ASN	2.8
1	E	730	THR	2.8
1	D	96	GLU	2.8
1	G	177	HIS	2.8
1	G	150	ASP	2.8
1	G	99	SER	2.8
1	C	20	ARG	2.8
1	G	745	ILE	2.8
1	D	624	LEU	2.7
1	F	400	LEU	2.7
1	G	194	TYR	2.7
1	C	92	ILE	2.7
1	B	331	ALA	2.7
1	G	333	TRP	2.7
1	E	156	VAL	2.7
1	E	760	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	508	THR	2.7
1	G	92	ILE	2.7
1	C	23	ALA	2.7
1	H	692	HIS	2.7
1	E	724	VAL	2.7
1	F	94	SER	2.7
1	H	520	ASP	2.7
1	D	742	THR	2.7
1	E	759	LYS	2.6
1	C	676	GLY	2.6
1	D	1	MET	2.6
1	C	748	GLU	2.6
1	F	506	GLU	2.6
1	G	116	SER	2.6
1	E	91	PHE	2.6
1	E	209	ASP	2.6
1	F	735	SER	2.6
1	E	120	LYS	2.6
1	E	155	ALA	2.6
1	E	673	ALA	2.6
1	H	749	LYS	2.6
1	D	746	PHE	2.6
1	E	736	GLU	2.6
1	A	749	LYS	2.5
1	E	473	PRO	2.5
1	H	7	HIS	2.5
1	B	751	VAL	2.5
1	E	676	GLY	2.5
1	G	659	GLU	2.5
1	G	623	SER	2.5
1	B	726	LYS	2.5
1	E	338	TYR	2.5
1	G	7	HIS	2.5
1	C	672	THR	2.5
1	E	96	GLU	2.5
1	F	755	GLU	2.5
1	E	66	ALA	2.5
1	E	260	ALA	2.5
1	F	716	LYS	2.5
1	G	1	MET	2.5
1	B	659	GLU	2.5
1	A	507	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	717	GLY	2.5
1	G	23	ALA	2.5
1	B	740	PRO	2.5
1	G	698	LEU	2.5
1	H	737	ASP	2.5
1	E	597	LEU	2.5
1	H	174	GLN	2.5
1	E	674	ALA	2.5
1	D	745	ILE	2.5
1	D	759	LYS	2.4
1	E	211	SER	2.4
1	F	744	HIS	2.4
1	G	208	ALA	2.4
1	E	116	SER	2.4
1	E	761	ARG	2.4
1	B	624	LEU	2.4
1	F	540	LYS	2.4
1	B	337	ILE	2.4
1	H	696	ILE	2.4
1	E	178	TYR	2.4
1	D	509	LEU	2.4
1	B	674	ALA	2.4
1	G	761	ARG	2.4
1	H	195	GLU	2.4
1	G	209	ASP	2.4
1	C	317	ILE	2.4
1	G	739	LYS	2.4
1	H	540	LYS	2.4
1	F	738	ARG	2.4
1	G	736	GLU	2.4
1	G	250	ASP	2.3
1	D	673	ALA	2.3
1	E	337	ILE	2.3
1	G	195	GLU	2.3
1	D	333	TRP	2.3
1	F	505	ASP	2.3
1	F	737	ASP	2.3
1	E	121	ASN	2.3
1	C	95	GLU	2.3
1	D	674	ALA	2.3
1	D	677	ALA	2.3
1	G	24	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	123	ALA	2.3
1	G	732	THR	2.3
1	H	258	LEU	2.3
1	G	757	ILE	2.3
1	F	747	GLY	2.3
1	D	737	ASP	2.3
1	D	747	GLY	2.3
1	F	290	ASN	2.3
1	B	319	ALA	2.3
1	C	24	ALA	2.3
1	G	173	LEU	2.3
1	B	759	LYS	2.3
1	B	20	ARG	2.3
1	B	748	GLU	2.3
1	G	637	ASP	2.3
1	C	677	ALA	2.3
1	E	153	THR	2.3
1	E	308	ALA	2.3
1	B	318	GLY	2.2
1	G	749	LYS	2.2
1	D	743	LEU	2.2
1	H	509	LEU	2.2
1	H	569	GLU	2.2
1	H	507	LYS	2.2
1	D	382	ILE	2.2
1	G	176	HIS	2.2
1	H	94	SER	2.2
1	C	740	PRO	2.2
1	E	740	PRO	2.2
1	C	673	ALA	2.2
1	H	568	LYS	2.2
1	G	83	LEU	2.2
1	C	235	VAL	2.2
1	E	731	ILE	2.2
1	D	676	GLY	2.2
1	A	757	ILE	2.2
1	G	747	GLY	2.2
1	E	624	LEU	2.2
1	G	152	ASP	2.2
1	B	177	HIS	2.2
1	F	692	HIS	2.2
1	G	261	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	728	GLN	2.2
1	H	177	HIS	2.2
1	E	670	ILE	2.1
1	G	117	GLN	2.1
1	E	341	PRO	2.1
1	E	100	PHE	2.1
1	F	97	ALA	2.1
1	G	624	LEU	2.1
1	C	149	SER	2.1
1	F	749	LYS	2.1
1	G	727	GLU	2.1
1	B	209	ASP	2.1
1	E	171	ASP	2.1
1	B	332	PHE	2.1
1	G	256	ALA	2.1
1	H	658	ASN	2.1
1	H	750	SER	2.1
1	A	742	THR	2.1
1	F	727	GLU	2.1
1	E	225	PHE	2.1
1	B	99	SER	2.1
1	C	94	SER	2.1
1	H	754	SER	2.1
1	B	676	GLY	2.1
1	E	262	HIS	2.1
1	B	672	THR	2.1
1	H	501	LEU	2.1
1	E	115	VAL	2.1
1	F	20	ARG	2.1
1	E	289	GLN	2.1
1	F	740	PRO	2.1
1	G	290	ASN	2.1
1	E	226	SER	2.1
1	C	694	ASP	2.1
1	D	319	ALA	2.1
1	E	189	ALA	2.1
1	D	741	LEU	2.1
1	G	175	GLY	2.1
1	G	604	ARG	2.1
1	D	675	ASN	2.1
1	A	736	GLU	2.1
1	E	261	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	338	TYR	2.1
1	E	319	ALA	2.1
1	H	738	ARG	2.0
1	D	752	LEU	2.0
1	C	99	SER	2.0
1	C	750	SER	2.0
1	G	178	TYR	2.0
1	G	220	GLY	2.0
1	E	267	GLU	2.0
1	G	569	GLU	2.0
1	F	278	ASP	2.0
1	E	732	THR	2.0
1	E	758	THR	2.0
1	E	21	TYR	2.0
1	E	290	ASN	2.0
1	D	750	SER	2.0
1	H	519	SER	2.0
1	H	561	LYS	2.0
1	B	514	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	H	802	6/6	0.25	5.97	58,73,84,85	0
4	GOL	D	807	6/6	0.18	5.58	55,64,71,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1PE	E	802	16/16	0.23	5.19	62,75,101,104	0
3	1PE	A	802	16/16	0.22	5.02	50,62,83,101	0
4	GOL	D	802	6/6	0.32	4.69	50,58,60,62	0
4	GOL	B	805	6/6	0.22	4.25	59,73,75,75	0
4	GOL	H	805	6/6	0.21	4.20	51,52,59,60	0
4	GOL	D	804	6/6	0.17	4.20	47,54,57,62	0
6	PGE	G	805	10/10	0.26	4.02	54,66,73,78	0
4	GOL	G	804	6/6	0.19	4.01	68,68,70,72	0
4	GOL	B	806	6/6	0.19	3.92	57,64,70,77	0
2	IFM	H	801	10/10	0.24	3.85	56,70,75,82	0
4	GOL	G	802	6/6	0.34	3.40	52,64,71,76	0
3	1PE	C	801	16/16	0.16	3.31	44,61,79,82	0
8	PG4	D	803	13/13	0.20	3.29	48,65,75,77	0
4	GOL	A	811	6/6	0.13	3.19	45,50,51,51	0
6	PGE	A	812	10/10	0.22	3.14	40,51,58,60	0
2	IFM	E	801	10/10	0.32	2.91	44,59,71,73	0
2	IFM	G	801	10/10	0.32	2.75	55,79,87,98	0
4	GOL	A	803	6/6	0.27	2.70	46,60,72,75	0
11	PE5	H	808	27/27	0.20	2.67	53,72,84,96	0
4	GOL	D	809	6/6	0.15	2.58	45,54,57,60	0
4	GOL	F	802	6/6	0.25	2.55	52,58,61,65	0
4	GOL	B	807	6/6	0.21	2.48	59,65,74,82	0
2	IFM	F	801	10/10	0.25	2.28	49,56,65,72	0
8	PG4	B	801	13/13	0.16	2.20	46,57,87,88	0
10	PE4	C	805	24/24	0.23	2.06	39,48,59,68	0
4	GOL	E	804	6/6	0.17	2.01	54,59,62,63	0
6	PGE	C	807	10/10	0.15	1.95	42,51,57,59	0
5	P6G	E	803	19/19	0.26	1.79	52,67,71,73	0
5	P6G	A	806	19/19	0.18	1.78	41,49,64,70	0
6	PGE	F	806	10/10	0.21	1.76	62,65,71,74	0
4	GOL	H	804	6/6	0.15	1.71	46,52,57,61	0
8	PG4	H	803	13/13	0.18	1.71	57,68,83,88	0
2	IFM	A	801	10/10	0.20	1.57	38,51,60,62	0
4	GOL	C	806	6/6	0.26	1.45	64,77,87,89	0
4	GOL	E	805	6/6	0.17	1.41	63,77,85,87	0
8	PG4	F	803	13/13	0.16	1.40	56,62,75,77	0
7	CA	D	814	1/1	0.15	1.31	45,45,45,45	0
4	GOL	B	804	6/6	0.20	1.14	33,35,40,47	0
4	GOL	D	810	6/6	0.19	1.09	33,37,40,41	0
4	GOL	C	804	6/6	0.22	1.08	43,46,53,57	0
4	GOL	A	807	6/6	0.16	1.08	57,59,72,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	804	6/6	0.16	1.04	42,43,46,52	0
4	GOL	C	802	6/6	0.16	0.98	43,57,62,73	0
4	GOL	D	811	6/6	0.13	0.92	49,56,61,71	0
4	GOL	A	808	6/6	0.17	0.79	59,61,66,85	0
9	7PE	B	802	21/21	0.18	0.77	36,45,52,55	0
4	GOL	E	806	6/6	0.15	0.64	46,47,50,54	0
4	GOL	D	812	6/6	0.20	0.63	32,38,40,45	0
4	GOL	F	805	6/6	0.14	0.55	39,62,67,70	0
4	GOL	H	807	6/6	0.17	0.49	70,70,73,76	0
4	GOL	E	807	6/6	0.19	0.48	43,53,60,60	0
4	GOL	C	809	6/6	0.18	0.47	37,42,49,52	0
4	GOL	B	808	6/6	0.24	0.45	36,43,46,48	0
7	CA	C	810	1/1	0.14	0.42	36,36,36,36	0
4	GOL	F	804	6/6	0.16	0.41	47,48,50,53	0
4	GOL	C	808	6/6	0.13	0.34	35,38,39,42	0
4	GOL	H	806	6/6	0.14	0.32	48,62,65,73	0
4	GOL	C	803	6/6	0.11	0.25	45,48,52,59	0
7	CA	B	809	1/1	0.12	0.23	43,43,43,43	0
4	GOL	A	810	6/6	0.13	0.16	37,37,39,40	0
9	7PE	D	808	21/21	0.16	0.11	41,48,54,59	0
4	GOL	D	806	6/6	0.12	0.11	56,64,67,71	0
7	CA	G	806	1/1	0.12	-0.11	55,55,55,55	0
7	CA	E	808	1/1	0.11	-0.16	54,54,54,54	0
4	GOL	D	805	6/6	0.12	-0.27	63,64,69,70	0
7	CA	A	813	1/1	0.10	-0.35	44,44,44,44	0
2	IFM	D	801	10/10	0.19	-0.65	35,44,50,63	0
4	GOL	B	803	6/6	0.13	-0.69	35,41,44,46	0
4	GOL	A	809	6/6	0.13	-0.76	58,66,67,73	0
4	GOL	G	803	6/6	0.09	-1.38	65,76,86,86	0
4	GOL	A	805	6/6	0.07	-1.59	57,64,74,75	0
7	CA	D	813	1/1	0.04	-41.00	54,54,54,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.