



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:08 PM GMT

PDB ID : 3SXX  
Title : Hansenula polymorpha copper amine oxidase-1 in complex with Co(II)  
Authors : Klema, V.J.; Wilmot, C.M.  
Deposited on : 2011-07-15  
Resolution : 1.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

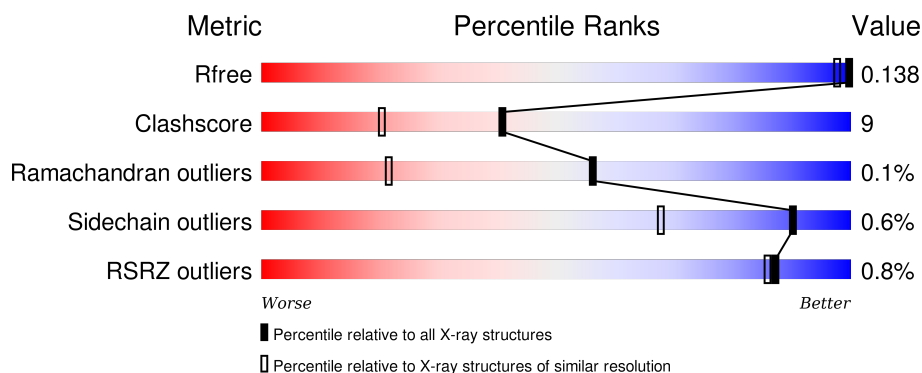
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.27 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))
$R_{free}$	91344	1194 (1.30-1.26)
Clashscore	102246	1271 (1.30-1.26)
Ramachandran outliers	100387	1217 (1.30-1.26)
Sidechain outliers	100360	1216 (1.30-1.26)
RSRZ outliers	91569	1194 (1.30-1.26)

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

Mol	Chain	Length	Quality of chain
1	A	692	<div> <div>86%</div> <div>9% • •</div> </div>
1	B	692	<div> <div>86%</div> <div>9% • •</div> </div>
1	C	692	<div> <div>85%</div> <div>11% •</div> </div>
1	D	692	<div> <div>87%</div> <div>7% • 5%</div> </div>
1	E	692	<div> <div>88%</div> <div>7% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	692	 % 86% 10%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	802[A]	-	-	-	X
3	GOL	A	802[B]	-	-	-	X
3	GOL	A	803[A]	-	-	-	X
3	GOL	A	803[B]	-	-	-	X
3	GOL	A	804	-	-	-	X
3	GOL	A	805	-	-	-	X
3	GOL	A	806	-	-	-	X
3	GOL	A	807	-	-	X	X
3	GOL	A	809	-	-	-	X
3	GOL	A	810	-	-	X	X
3	GOL	A	811	-	-	-	X
3	GOL	B	802[A]	-	-	-	X
3	GOL	B	802[B]	-	-	-	X
3	GOL	B	803	-	-	-	X
3	GOL	B	804	-	-	-	X
3	GOL	B	805[A]	-	-	X	X
3	GOL	B	805[B]	-	-	X	X
3	GOL	B	806	-	-	X	-
3	GOL	B	807	-	-	X	X
3	GOL	B	808	-	-	-	X
3	GOL	B	809	-	-	-	X
3	GOL	C	802	-	-	-	X
3	GOL	C	803	-	-	-	X
3	GOL	C	805	-	-	-	X
3	GOL	C	806	-	-	-	X
3	GOL	C	807	-	-	-	X
3	GOL	C	808	-	-	-	X
3	GOL	C	809	-	-	X	X
3	GOL	D	802	-	-	-	X
3	GOL	D	803[A]	-	-	-	X
3	GOL	D	803[B]	-	-	-	X
3	GOL	D	804	-	-	-	X
3	GOL	D	805	-	-	X	X
3	GOL	D	806	-	-	X	X
3	GOL	E	802	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	E	803	-	-	-	X
3	GOL	E	804	-	-	-	X
3	GOL	E	806	-	-	X	X
3	GOL	F	802	-	-	-	X
3	GOL	F	803	-	-	X	X
3	GOL	F	804[A]	-	-	-	X
3	GOL	F	804[B]	-	-	-	X
3	GOL	F	805	-	-	-	X
3	GOL	F	808	-	-	X	X
3	GOL	F	809	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38975 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	38	0
			5423	3465	912	1014	32			
1	B	664	Total	C	N	O	S	0	37	0
			5441	3467	926	1017	31			
1	C	666	Total	C	N	O	S	0	34	0
			5427	3467	921	1005	34			
1	D	657	Total	C	N	O	S	0	31	0
			5368	3427	916	996	29			
1	E	656	Total	C	N	O	S	3	31	0
			5355	3423	912	991	29			
1	F	665	Total	C	N	O	S	0	34	0
			5426	3469	915	1008	34			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Co	0	0
			1	1		
2	E	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		
2	C	1	Total	Co	0	0
			1	1		
2	A	1	Total	Co	0	0
			1	1		
2	F	1	Total	Co	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		

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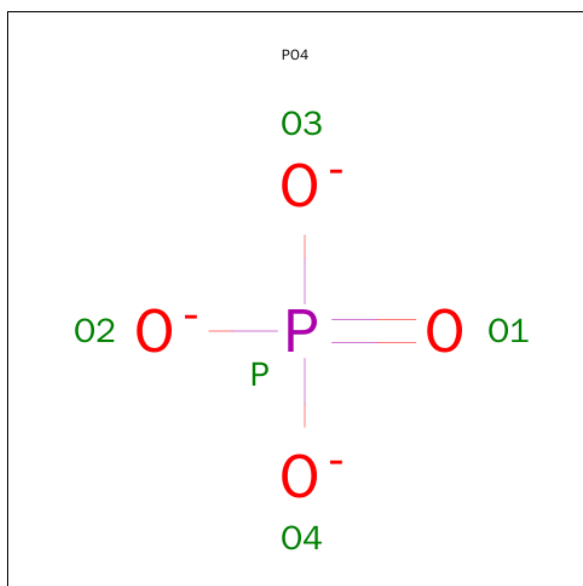
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 12	C 6	O 6	0	1
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	1
			12	6	6		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

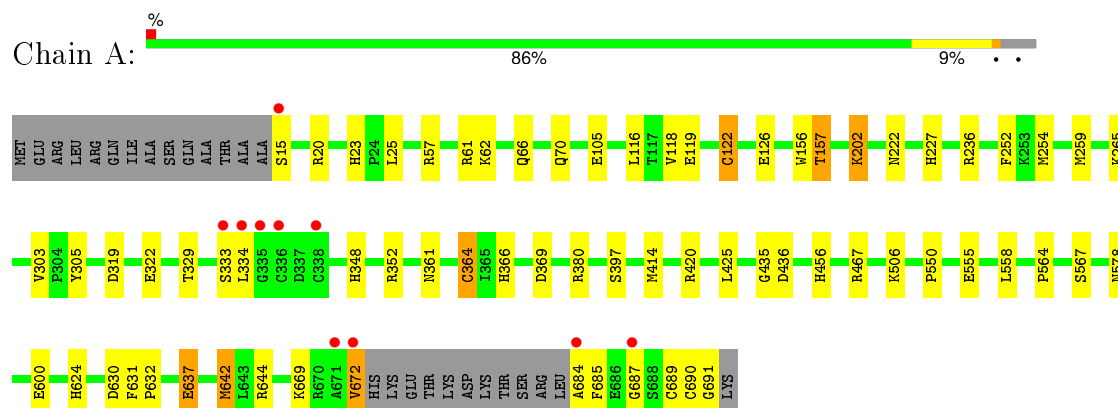


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1035	Total 1035	O 1035	0	0
5	B	1038	Total 1038	O 1038	0	0
5	C	1037	Total 1037	O 1037	0	0
5	D	1044	Total 1044	O 1044	0	0
5	E	1033	Total 1033	O 1033	0	0
5	F	1038	Total 1038	O 1038	0	0

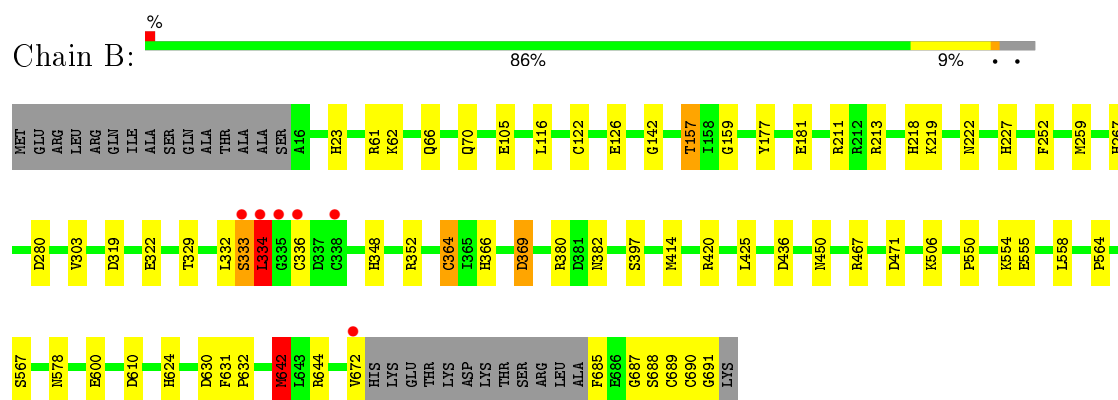
### 3 Residue-property plots

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.

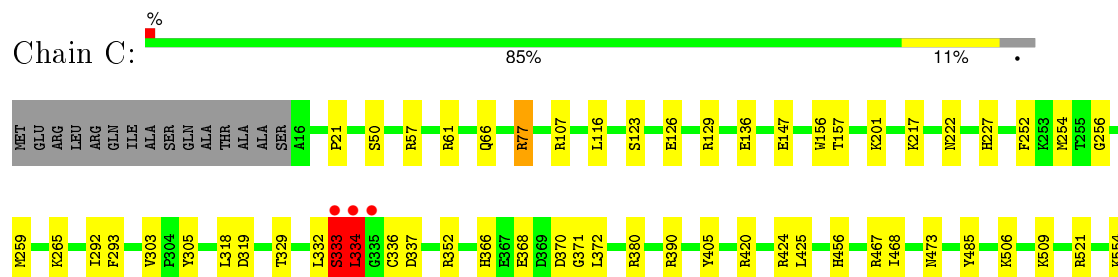
- Molecule 1: Peroxisomal primary amine oxidase



- Molecule 1: Peroxisomal primary amine oxidase

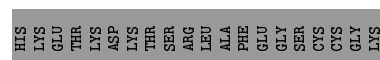
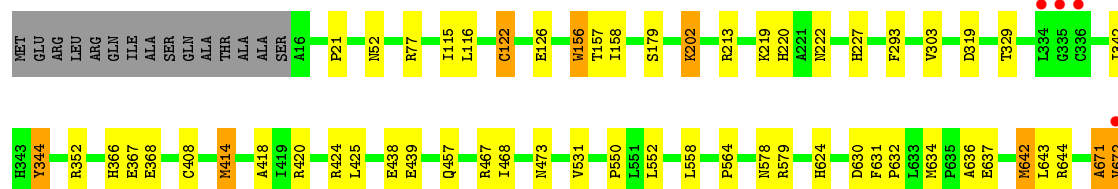
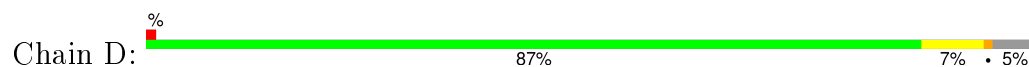


- Molecule 1: Peroxisomal primary amine oxidase

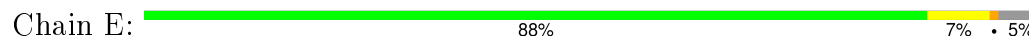




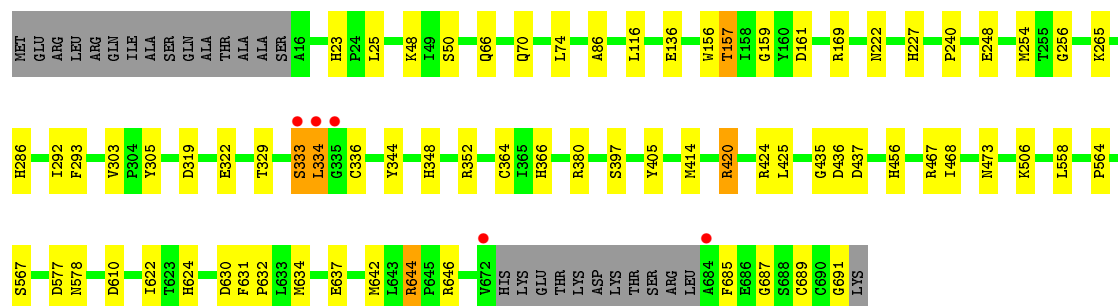
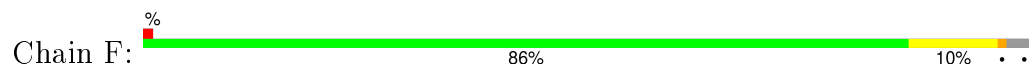
• Molecule 1: Peroxisomal primary amine oxidase



• Molecule 1: Peroxisomal primary amine oxidase



• Molecule 1: Peroxisomal primary amine oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.89Å 223.36Å 103.97Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	31.70 – 1.27 31.70 – 1.27	Depositor EDS
% Data completeness (in resolution range)	94.9 (31.70-1.27) 94.6 (31.70-1.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.108 , 0.138 0.107 , 0.138	Depositor DCC
$R_{free}$ test set	58671 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	7.8	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.2	EDS
Estimated twinning fraction	0.477 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 1169243 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	38975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, PO4, CO

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	0.91	9/5672 (0.2%)	0.94	11/7715 (0.1%)
1	B	0.90	10/5675 (0.2%)	0.94	17/7715 (0.2%)
1	C	0.87	3/5664 (0.1%)	0.94	15/7701 (0.2%)
1	D	0.87	2/5595 (0.0%)	0.92	11/7609 (0.1%)
1	E	0.90	4/5592 (0.1%)	0.90	9/7604 (0.1%)
1	F	0.86	5/5675 (0.1%)	0.93	18/7717 (0.2%)
All	All	0.88	33/33873 (0.1%)	0.93	81/46061 (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	B	0	2
1	C	0	4
1	D	0	3
1	F	0	1
All	All	0	12

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364[A]	CYS	CB-SG	-9.00	1.67	1.82
1	B	364[B]	CYS	CB-SG	-9.00	1.67	1.82
1	E	122[A]	CYS	CB-SG	8.52	1.96	1.82
1	E	122[B]	CYS	CB-SG	8.52	1.96	1.82
1	A	364[A]	CYS	CB-SG	-8.46	1.67	1.82
1	A	364[B]	CYS	CB-SG	-8.46	1.67	1.82
1	A	122[A]	CYS	CB-SG	7.76	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122[B]	CYS	CB-SG	7.76	1.95	1.82
1	A	467	ARG	CB-CG	-7.41	1.32	1.52
1	B	642	MET	CB-CG	6.79	1.73	1.51
1	F	157[A]	THR	CA-CB	6.59	1.70	1.53
1	F	157[B]	THR	CA-CB	6.59	1.70	1.53
1	B	157[A]	THR	CB-CG2	-6.41	1.31	1.52
1	B	157[B]	THR	CB-CG2	-6.41	1.31	1.52
1	E	368	GLU	CB-CG	-6.09	1.40	1.52
1	B	642	MET	CG-SD	-6.00	1.65	1.81
1	F	157[A]	THR	CB-CG2	-5.98	1.32	1.52
1	F	157[B]	THR	CB-CG2	-5.98	1.32	1.52
1	B	157[A]	THR	CA-CB	5.97	1.68	1.53
1	B	157[B]	THR	CA-CB	5.97	1.68	1.53
1	D	439	GLU	CD-OE2	5.91	1.32	1.25
1	D	367	GLU	CD-OE2	-5.90	1.19	1.25
1	C	126	GLU	CG-CD	5.82	1.60	1.51
1	C	660	SER	CB-OG	5.61	1.49	1.42
1	B	600	GLU	CD-OE2	-5.56	1.19	1.25
1	F	333	SER	CA-C	-5.52	1.38	1.52
1	B	105	GLU	CB-CG	-5.38	1.42	1.52
1	E	382	ASN	CB-CG	5.16	1.62	1.51
1	C	554	LYS	CE-NZ	-5.14	1.36	1.49
1	A	119	GLU	CD-OE1	-5.10	1.20	1.25
1	A	637[A]	GLU	CD-OE1	-5.07	1.20	1.25
1	A	637[B]	GLU	CD-OE1	-5.07	1.20	1.25
1	A	105	GLU	CB-CG	-5.02	1.42	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	414[A]	MET	CG-SD-CE	-11.74	81.41	100.20
1	D	414[B]	MET	CG-SD-CE	-11.74	81.41	100.20
1	F	157[A]	THR	N-CA-CB	11.39	131.94	110.30
1	F	157[B]	THR	N-CA-CB	11.39	131.94	110.30
1	B	157[A]	THR	N-CA-CB	10.61	130.46	110.30
1	B	157[B]	THR	N-CA-CB	10.61	130.46	110.30
1	A	420	ARG	NE-CZ-NH1	-10.26	115.17	120.30
1	C	424[A]	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	C	424[B]	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	642[A]	MET	CG-SD-CE	-9.83	84.48	100.20
1	A	642[B]	MET	CG-SD-CE	-9.83	84.48	100.20
1	B	352	ARG	NE-CZ-NH1	8.22	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369[A]	ASP	CB-CG-OD2	8.08	125.58	118.30
1	B	369[B]	ASP	CB-CG-OD2	8.08	125.58	118.30
1	F	467	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	D	352	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	352	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	F	420[A]	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	F	420[B]	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	F	420[A]	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	420[B]	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	644[A]	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	644[B]	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	D	642[A]	MET	CG-SD-CE	-7.23	88.62	100.20
1	D	642[B]	MET	CG-SD-CE	-7.23	88.62	100.20
1	D	467	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	F	644[A]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	F	644[B]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	467	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	467	ARG	CG-CD-NE	-6.56	98.02	111.80
1	E	467	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	B	369[A]	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	B	369[B]	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	F	610	ASP	CB-CG-OD1	6.34	124.01	118.30
1	C	61	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	F	646	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	A	157[A]	THR	N-CA-CB	6.20	122.07	110.30
1	A	157[B]	THR	N-CA-CB	6.20	122.07	110.30
1	F	644[A]	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	F	644[B]	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	364[A]	CYS	CA-CB-SG	6.17	125.10	114.00
1	B	364[B]	CYS	CA-CB-SG	6.17	125.10	114.00
1	B	352	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	352	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	424[A]	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	424[B]	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	562	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	E	380	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	344	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	B	610	ASP	CB-CG-OD1	5.88	123.59	118.30
1	E	562	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	F	577	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	D	293	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	E	293	PHE	CB-CG-CD2	-5.58	116.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	157[A]	THR	OG1-CB-CG2	-5.50	97.36	110.00
1	F	157[B]	THR	OG1-CB-CG2	-5.50	97.36	110.00
1	A	364[A]	CYS	CA-CB-SG	5.47	123.85	114.00
1	A	364[B]	CYS	CA-CB-SG	5.47	123.85	114.00
1	B	642	MET	CB-CG-SD	-5.47	96.00	112.40
1	B	644	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	352	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	554[A]	LYS	CD-CE-NZ	5.40	124.12	111.70
1	B	554[B]	LYS	CD-CE-NZ	5.40	124.12	111.70
1	E	644	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	558[A]	LEU	N-CA-CB	-5.33	99.73	110.40
1	D	558[B]	LEU	N-CA-CB	-5.33	99.73	110.40
1	C	610	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	129	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	521	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	F	74	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	B	157[A]	THR	OG1-CB-CG2	-5.16	98.13	110.00
1	B	157[B]	THR	OG1-CB-CG2	-5.16	98.13	110.00
1	E	558[A]	LEU	N-CA-CB	-5.16	100.09	110.40
1	E	558[B]	LEU	N-CA-CB	-5.16	100.09	110.40
1	C	554	LYS	CA-CB-CG	-5.13	102.11	113.40
1	C	77	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	F	169	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	C	485	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	E	122[A]	CYS	CA-CB-SG	5.07	123.13	114.00
1	E	122[B]	CYS	CA-CB-SG	5.07	123.13	114.00
1	A	236	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	TRP	Peptide
1	A	684	ALA	Peptide
1	B	333	SER	Peptide
1	B	334	LEU	Peptide
1	C	156	TRP	Peptide
1	C	332	LEU	Peptide
1	C	333	SER	Peptide
1	C	334	LEU	Peptide
1	D	156	TRP	Peptide
1	D	579	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	671	ALA	Peptide
1	F	156	TRP	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	5423	0	5319	104	0
1	B	5441	0	5319	99	0
1	C	5427	0	5331	99	0
1	D	5368	0	5278	91	0
1	E	5355	0	5280	76	0
1	F	5426	0	5334	95	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	72	0	94	30	0
3	B	60	0	79	29	0
3	C	48	0	63	9	0
3	D	36	0	48	14	0
3	E	30	0	40	9	0
3	F	48	0	63	16	0
4	C	5	0	0	0	0
4	F	5	0	0	0	0
5	A	1035	0	0	51	0
5	B	1038	0	0	47	1
5	C	1037	0	0	38	0
5	D	1044	0	0	22	1
5	E	1033	0	0	42	0
5	F	1038	0	0	40	0
All	All	38975	0	32248	556	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (556) 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:292:ILE:HG22	1:C:293[B]:PHE:CD2	1.59	1.37
1:F:292:ILE:HG22	1:F:293[B]:PHE:CD2	1.59	1.37
1:B:425[B]:LEU:HD21	5:B:1629:HOH:O	1.24	1.35
1:A:685:PHE:CZ	5:B:1745:HOH:O	1.79	1.33
1:B:157[B]:THR:CG2	5:B:1655:HOH:O	1.76	1.32
1:E:157[A]:THR:CG2	5:E:1657:HOH:O	1.67	1.32
1:B:414[B]:MET:CE	5:B:1628:HOH:O	1.77	1.32
1:A:685:PHE:CE2	5:B:1745:HOH:O	1.84	1.31
5:A:1606:HOH:O	1:B:550[B]:PRO:HG3	1.30	1.30
1:F:414[A]:MET:HE2	5:F:1656:HOH:O	1.29	1.29
5:E:1740:HOH:O	1:F:685:PHE:CE1	1.70	1.29
1:F:157[B]:THR:CG2	5:F:1653:HOH:O	1.67	1.29
1:F:425[B]:LEU:HD21	5:F:1599:HOH:O	1.33	1.28
1:D:425[A]:LEU:HD21	5:D:1642:HOH:O	1.32	1.27
1:E:414[A]:MET:CE	5:E:1568:HOH:O	1.73	1.26
1:F:414[A]:MET:CE	5:F:1656:HOH:O	1.80	1.26
5:A:1743:HOH:O	1:B:685:PHE:CZ	1.77	1.26
1:B:578[B]:ASN:ND2	5:B:1724:HOH:O	1.65	1.26
1:A:157[B]:THR:CG2	5:A:1626:HOH:O	1.63	1.25
1:A:425[B]:LEU:HD21	5:A:1628:HOH:O	1.16	1.25
1:F:578[B]:ASN:ND2	5:F:1584:HOH:O	1.68	1.25
1:F:292:ILE:HG22	1:F:293[B]:PHE:CE2	1.72	1.25
1:E:352[A]:ARG:HD3	5:E:1688:HOH:O	1.09	1.24
1:A:550[B]:PRO:HG3	5:B:1908:HOH:O	1.29	1.24
1:F:292:ILE:CG2	1:F:293[B]:PHE:CE2	2.22	1.23
1:A:414[B]:MET:CE	5:A:1678:HOH:O	1.77	1.22
3:A:807:GOL:H32	5:A:1490:HOH:O	1.09	1.20
1:E:425[B]:LEU:HD21	5:E:1637:HOH:O	1.41	1.20
3:E:806:GOL:H31	5:F:1037:HOH:O	1.38	1.19
1:B:688:SER:OG	5:B:1756:HOH:O	1.56	1.19
1:E:414[A]:MET:HE2	5:E:1568:HOH:O	1.28	1.18
1:C:425[B]:LEU:HD21	5:C:1633:HOH:O	1.44	1.18
5:A:1743:HOH:O	1:B:685:PHE:CE1	1.86	1.17
1:C:292:ILE:HG22	1:C:293[B]:PHE:CE2	1.80	1.17
1:E:425[B]:LEU:HD23	1:E:637[B]:GLU:OE1	1.40	1.16
1:E:550[B]:PRO:HG3	5:F:1586:HOH:O	1.43	1.16
1:F:425[B]:LEU:HD23	1:F:637[B]:GLU:OE2	1.43	1.16
1:C:292:ILE:CG2	1:C:293[B]:PHE:CE2	2.30	1.15
1:B:550[A]:PRO:HG2	5:B:1669:HOH:O	1.46	1.15
1:B:690:CYS:HB2	5:B:1750:HOH:O	1.49	1.13
5:E:1740:HOH:O	1:F:685:PHE:CZ	1.77	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ASN:HB2	5:E:1146:HOH:O	1.46	1.12
1:F:558[B]:LEU:HD23	3:F:808:GOL:H2	1.30	1.12
1:D:578[B]:ASN:ND2	5:D:1714:HOH:O	1.80	1.11
1:A:550[A]:PRO:HG2	5:A:1665:HOH:O	1.50	1.11
1:C:564:PRO:HG3	5:C:1670:HOH:O	1.50	1.11
1:E:126[B]:GLU:OE1	1:F:685:PHE:O	1.69	1.11
5:C:1101:HOH:O	3:D:806:GOL:H31	1.50	1.11
1:C:558[A]:LEU:HD23	3:C:809:GOL:H2	1.33	1.10
1:E:578[B]:ASN:ND2	5:E:1685:HOH:O	1.81	1.10
1:F:157[B]:THR:HG22	5:F:1653:HOH:O	1.32	1.10
1:A:690:CYS:HB2	5:A:1747:HOH:O	1.52	1.09
1:B:157[B]:THR:HG22	5:B:1655:HOH:O	1.39	1.08
1:D:219:LYS:H	3:D:806:GOL:H11	1.19	1.08
1:C:425[B]:LEU:HD23	1:C:637[B]:GLU:OE1	1.54	1.07
1:F:437:ASP:HB2	5:F:1367:HOH:O	1.54	1.07
1:B:506[A]:LYS:HE2	5:B:1455:HOH:O	1.53	1.07
1:C:685:PHE:O	1:D:126[B]:GLU:OE1	1.70	1.06
1:B:369[A]:ASP:OD1	5:B:1627:HOH:O	1.75	1.04
1:D:424[C]:ARG:HD2	1:D:636:ALA:HB1	1.38	1.04
1:C:578[B]:ASN:ND2	5:C:1717:HOH:O	1.88	1.04
1:B:414[A]:MET:SD	1:B:420[A]:ARG:NH1	2.31	1.03
1:F:564:PRO:HG3	5:F:1629:HOH:O	1.58	1.03
1:A:369[B]:ASP:OD1	5:A:1625:HOH:O	1.75	1.03
1:E:265[B]:LYS:NZ	5:E:1756:HOH:O	1.90	1.02
1:F:414[B]:MET:SD	1:F:420[B]:ARG:NH1	2.33	1.01
1:D:550:PRO:HG2	5:D:1676:HOH:O	1.57	1.00
1:E:219:LYS:H	3:E:806:GOL:H11	1.22	1.00
1:F:558[B]:LEU:HD21	3:F:808:GOL:H31	1.44	1.00
1:C:624[B]:HIS:CD2	1:C:637[B]:GLU:OE2	2.14	1.00
1:C:644[A]:ARG:HD2	5:C:1721:HOH:O	1.60	1.00
1:E:213[A]:ARG:NH1	5:E:1645:HOH:O	1.95	0.99
1:D:424[B]:ARG:NH1	3:D:803[B]:GOL:H12	1.76	0.98
1:C:292:ILE:CG2	1:C:293[B]:PHE:CD2	2.45	0.98
1:F:624[B]:HIS:CD2	1:F:637[B]:GLU:OE1	2.16	0.98
1:A:644[B]:ARG:HG3	5:A:1926:HOH:O	1.62	0.97
1:B:414[B]:MET:HE2	5:B:1628:HOH:O	1.50	0.97
1:F:292:ILE:CG2	1:F:293[B]:PHE:CD2	2.44	0.97
1:D:157[B]:THR:CA	1:D:158:ILE:N	2.27	0.97
1:E:550[A]:PRO:HG2	5:E:1665:HOH:O	1.64	0.96
1:F:157[A]:THR:HG23	1:F:159:GLY:H	1.30	0.96
1:C:642[A]:MET:HE1	5:C:1923:HOH:O	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558[B]:LEU:HD23	3:A:810:GOL:H2	1.47	0.96
1:B:425[B]:LEU:CD2	5:B:1629:HOH:O	1.91	0.95
1:F:425[B]:LEU:CD2	5:F:1599:HOH:O	1.94	0.94
1:E:157[A]:THR:HG22	5:E:1657:HOH:O	1.43	0.94
1:A:564:PRO:HG3	5:A:1461:HOH:O	1.66	0.94
1:D:414[B]:MET:SD	1:D:420[B]:ARG:NH1	2.41	0.94
1:A:425[B]:LEU:HD23	1:A:637[B]:GLU:OE2	1.67	0.94
1:D:424[B]:ARG:CZ	5:D:1522:HOH:O	2.17	0.93
1:B:550[A]:PRO:CG	5:B:1669:HOH:O	2.08	0.93
1:B:23:HIS:HE2	3:B:805[B]:GOL:H31	1.33	0.92
1:A:414[B]:MET:HE3	5:A:1678:HOH:O	1.52	0.92
1:E:23:HIS:HD2	1:E:25:LEU:H	1.15	0.92
1:C:558[A]:LEU:CD2	3:C:809:GOL:H2	1.99	0.92
1:A:425[B]:LEU:CD2	5:A:1628:HOH:O	1.78	0.92
1:E:425[B]:LEU:CD2	5:E:1637:HOH:O	2.04	0.92
1:F:558[B]:LEU:CD2	3:F:808:GOL:H2	1.99	0.92
1:C:425[B]:LEU:CD2	5:C:1633:HOH:O	2.07	0.91
1:F:23:HIS:HD2	1:F:25:LEU:H	1.16	0.91
1:A:23:HIS:HD2	1:A:25:LEU:H	1.13	0.89
1:A:550[A]:PRO:CG	5:A:1665:HOH:O	2.12	0.89
1:B:506[B]:LYS:HE3	5:B:1659:HOH:O	1.71	0.88
1:F:70:GLN:HG2	5:F:1858:HOH:O	1.74	0.88
1:C:333:SER:HB2	1:C:334:LEU:CA	2.03	0.88
1:B:558[A]:LEU:HD23	3:B:807:GOL:H2	1.55	0.88
1:B:157[A]:THR:HG23	1:B:159:GLY:H	1.40	0.87
1:A:157[B]:THR:HG22	5:A:1626:HOH:O	1.39	0.87
1:E:424[B]:ARG:CZ	5:E:1613:HOH:O	2.21	0.86
1:B:564:PRO:HG3	5:B:1514:HOH:O	1.74	0.86
1:B:157[B]:THR:HG21	5:B:1655:HOH:O	1.54	0.86
1:D:220:HIS:ND1	3:D:805:GOL:H2	1.90	0.85
1:A:558[B]:LEU:HD21	3:A:810:GOL:H12	1.58	0.85
1:B:414[B]:MET:HE1	5:B:1628:HOH:O	1.58	0.85
5:C:1101:HOH:O	3:D:806:GOL:C3	2.15	0.84
1:D:550:PRO:CG	5:D:1676:HOH:O	2.21	0.84
1:C:333:SER:CB	1:C:334:LEU:CA	2.54	0.84
1:E:420[A]:ARG:NH2	5:E:1656:HOH:O	2.10	0.84
1:C:558[A]:LEU:HD21	3:C:809:GOL:H12	1.58	0.84
1:A:436:ASP:H	3:A:802[B]:GOL:H32	1.38	0.84
1:D:420[B]:ARG:NH2	5:D:1671:HOH:O	2.09	0.84
3:B:806:GOL:H32	5:B:1901:HOH:O	1.77	0.83
1:C:116:LEU:CD1	1:C:157[A]:THR:HB	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:506:LYS:HE2	5:F:1905:HOH:O	1.80	0.82
1:E:213[A]:ARG:CZ	5:E:1645:HOH:O	2.27	0.82
1:D:634[B]:MET:CE	1:D:637[B]:GLU:CD	2.49	0.82
1:E:624[B]:HIS:CD2	1:E:637[B]:GLU:OE2	2.33	0.81
1:A:61:ARG:HH11	3:A:804:GOL:H32	1.46	0.81
1:B:558[A]:LEU:HD21	3:B:807:GOL:H31	1.60	0.81
3:F:809:GOL:H31	5:F:1857:HOH:O	1.79	0.81
1:A:122[A]:CYS:SG	5:B:1750:HOH:O	2.38	0.81
1:F:292:ILE:HG21	1:F:293[B]:PHE:CE2	2.13	0.81
1:B:420[A]:ARG:NH2	5:B:1805:HOH:O	2.14	0.81
1:E:122[A]:CYS:SG	5:E:1502:HOH:O	2.39	0.81
1:D:425[A]:LEU:CD2	5:D:1642:HOH:O	2.03	0.80
5:A:1747:HOH:O	1:B:122[B]:CYS:SG	2.39	0.80
1:D:564:PRO:HG3	5:D:1718:HOH:O	1.81	0.80
1:E:352[A]:ARG:CD	5:E:1688:HOH:O	1.87	0.79
1:D:468:ILE:H	1:D:473:ASN:HD21	1.30	0.79
1:A:319[B]:ASP:OD1	5:A:1685:HOH:O	2.01	0.79
1:D:156:TRP:C	1:D:157[B]:THR:CA	2.51	0.79
1:F:558[B]:LEU:HD21	3:F:808:GOL:C3	2.13	0.79
1:B:506[B]:LYS:HE2	5:B:1509:HOH:O	1.82	0.79
1:E:564:PRO:HG3	5:E:1697:HOH:O	1.81	0.79
1:E:157[A]:THR:HG21	5:E:1657:HOH:O	1.45	0.78
1:D:219:LYS:N	3:D:806:GOL:H11	1.98	0.78
1:C:371:GLY:HA3	1:D:424[C]:ARG:NH2	1.99	0.77
1:E:550[A]:PRO:CG	5:E:1665:HOH:O	2.23	0.77
1:E:315:LYS:HZ2	1:E:430:ASN:HD21	1.33	0.77
1:F:50:SER:HB2	1:F:352:ARG:HG3	1.65	0.77
1:D:634[B]:MET:HE1	1:D:637[B]:GLU:CD	2.06	0.76
1:B:550[A]:PRO:CD	5:B:1669:HOH:O	2.33	0.76
1:C:372:LEU:N	1:D:424[C]:ARG:HH21	1.83	0.76
1:C:468:ILE:H	1:C:473:ASN:HD21	1.33	0.76
1:B:122[B]:CYS:SG	5:B:1396:HOH:O	2.44	0.75
1:F:558[B]:LEU:CD2	3:F:808:GOL:C2	2.65	0.75
1:C:292:ILE:HG21	1:C:293[B]:PHE:CE2	2.21	0.75
1:F:157[B]:THR:HG21	5:F:1653:HOH:O	1.46	0.75
1:A:624[B]:HIS:HE1	1:A:630:ASP:OD2	1.69	0.75
1:A:558[B]:LEU:CD2	3:A:810:GOL:H2	2.15	0.75
1:A:157[B]:THR:HG21	5:A:1626:HOH:O	1.45	0.75
1:A:506:LYS:HE2	5:A:1835:HOH:O	1.85	0.75
1:A:122[A]:CYS:SG	5:A:1346:HOH:O	2.43	0.74
1:C:624[B]:HIS:NE2	1:C:637[B]:GLU:OE2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:HG3	3:B:806:GOL:H12	1.69	0.74
1:B:567[B]:SER:OG	5:B:1646:HOH:O	2.04	0.74
1:D:122[B]:CYS:SG	5:D:1454:HOH:O	2.45	0.74
1:A:414[B]:MET:HE2	5:A:1678:HOH:O	1.59	0.74
3:C:808:GOL:H12	5:C:1837:HOH:O	1.87	0.73
1:F:624[B]:HIS:HE1	1:F:630:ASP:OD2	1.70	0.73
1:D:642[A]:MET:HG2	1:D:644:ARG:HG3	1.71	0.73
1:A:567[B]:SER:OG	5:A:1624:HOH:O	2.07	0.73
1:B:280:ASP:OD2	3:B:805[B]:GOL:H32	1.88	0.73
1:F:468:ILE:H	1:F:473:ASN:HD21	1.35	0.72
1:B:550[A]:PRO:HD2	5:B:1669:HOH:O	1.88	0.72
1:C:116:LEU:HD12	1:C:157[A]:THR:HB	1.69	0.72
1:A:57:ARG:HH22	3:A:809:GOL:C3	2.02	0.72
1:F:157[A]:THR:HG23	1:F:159:GLY:N	2.03	0.72
1:F:435:GLY:HA2	3:F:803:GOL:H32	1.72	0.72
1:D:624[B]:HIS:CD2	1:D:637[B]:GLU:OE1	2.44	0.71
1:A:118[A]:VAL:HG22	5:A:1143:HOH:O	1.88	0.71
1:D:220:HIS:H	3:D:805:GOL:C2	2.03	0.71
1:C:366:HIS:HD2	5:C:1810:HOH:O	1.73	0.71
1:F:366:HIS:HD2	5:F:1657:HOH:O	1.72	0.71
1:D:157[A]:THR:OG1	5:D:1633:HOH:O	2.07	0.71
1:E:23:HIS:CD2	1:E:25:LEU:H	2.06	0.71
1:F:558[B]:LEU:HD23	3:F:808:GOL:C2	2.17	0.71
1:B:23:HIS:HE2	3:B:805[B]:GOL:C3	2.03	0.70
1:B:425[B]:LEU:HD23	5:B:1919:HOH:O	1.91	0.70
1:C:333:SER:HB3	1:C:337:ASP:H	1.55	0.70
1:D:624[B]:HIS:HE1	1:D:630:ASP:OD2	1.73	0.70
1:C:624[B]:HIS:HE1	1:C:630:ASP:OD2	1.73	0.70
1:B:332:LEU:O	1:B:334:LEU:CB	2.40	0.70
1:E:219:LYS:N	3:E:806:GOL:H11	2.03	0.69
1:D:116:LEU:CD1	1:D:157[B]:THR:HB	2.22	0.69
1:A:642[B]:MET:HE1	5:A:1449:HOH:O	1.90	0.69
1:A:23:HIS:CD2	1:A:25:LEU:H	2.04	0.69
1:C:644[B]:ARG:NH1	5:C:1721:HOH:O	2.25	0.69
1:A:672:VAL:CG2	1:A:672:VAL:O	2.40	0.69
1:A:691:GLY:HA2	1:B:122[A]:CYS:SG	2.33	0.69
1:D:624[A]:HIS:CE1	5:D:1745:HOH:O	2.25	0.69
1:D:634[B]:MET:HE2	1:D:637[B]:GLU:HG3	1.74	0.69
1:A:366:HIS:HD2	5:A:1653:HOH:O	1.75	0.69
1:A:600[B]:GLU:OE2	5:A:1759:HOH:O	2.11	0.69
1:C:405:TYR:HE2	1:C:634[B]:MET:CE	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:CD1	1:A:157[A]:THR:HB	2.22	0.68
1:A:62:LYS:NZ	1:A:66[A]:GLN:OE1	2.17	0.68
1:D:319[B]:ASP:OD1	5:D:1290:HOH:O	2.11	0.68
1:C:319[B]:ASP:OD1	5:C:1626:HOH:O	2.10	0.68
1:B:624[B]:HIS:HE1	1:B:630:ASP:OD2	1.77	0.68
1:C:147[B]:GLU:OE2	5:C:1506:HOH:O	2.11	0.68
1:B:578[B]:ASN:OD1	5:B:1764:HOH:O	2.11	0.68
1:B:319[B]:ASP:OD1	5:B:1380:HOH:O	2.12	0.68
1:C:558[A]:LEU:CD2	3:C:809:GOL:C2	2.72	0.67
1:E:286:HIS:HD2	5:E:1757:HOH:O	1.75	0.67
1:B:558[A]:LEU:CD2	3:B:807:GOL:H2	2.23	0.67
1:C:567[B]:SER:OG	5:C:1671:HOH:O	2.12	0.67
1:F:624[A]:HIS:CE1	5:F:1705:HOH:O	2.27	0.67
1:F:624[B]:HIS:NE2	1:F:637[B]:GLU:OE1	2.28	0.67
1:E:550[A]:PRO:HD2	5:E:1665:HOH:O	1.93	0.67
1:D:303:VAL:HG23	5:D:1290:HOH:O	1.94	0.67
1:A:20:ARG:HD2	5:A:1689:HOH:O	1.94	0.67
1:C:644[B]:ARG:CZ	5:C:1721:HOH:O	2.43	0.67
1:A:23:HIS:HE1	3:A:807:GOL:C1	2.07	0.67
1:F:506:LYS:HD2	5:F:1344:HOH:O	1.94	0.67
1:D:634[B]:MET:HE2	1:D:637[B]:GLU:CD	2.15	0.66
1:F:567[A]:SER:OG	5:F:1635:HOH:O	2.12	0.66
1:B:23:HIS:NE2	3:B:805[B]:GOL:H31	2.08	0.66
1:F:405:TYR:HE2	1:F:634[A]:MET:HE1	1.60	0.66
1:E:116:LEU:CD1	1:E:157[B]:THR:HB	2.26	0.66
1:A:558[B]:LEU:CD2	3:A:810:GOL:C2	2.74	0.66
1:B:303:VAL:HG23	5:B:1380:HOH:O	1.95	0.66
1:F:624[B]:HIS:NE2	5:F:1348:HOH:O	2.29	0.66
1:E:624[B]:HIS:HE1	1:E:630:ASP:OD2	1.79	0.66
1:D:424[B]:ARG:HH12	3:D:803[B]:GOL:H12	1.59	0.66
1:E:315:LYS:NZ	1:E:430:ASN:HD21	1.93	0.65
1:D:213[B]:ARG:CZ	1:D:438:GLU:OE1	2.44	0.65
1:A:265:LYS:HE2	3:A:807:GOL:H31	1.79	0.65
1:D:219:LYS:H	3:D:806:GOL:C1	2.03	0.65
1:D:634[B]:MET:CE	1:D:637[B]:GLU:HG3	2.26	0.65
1:C:644[B]:ARG:NH2	5:C:1721:HOH:O	2.30	0.65
1:B:558[A]:LEU:HD23	3:B:807:GOL:C2	2.27	0.65
1:D:179[B]:SER:OG	3:D:805:GOL:H32	1.97	0.65
1:C:50:SER:HB2	1:C:352:ARG:HG3	1.78	0.65
1:B:157[A]:THR:HG23	1:B:159:GLY:N	2.11	0.65
1:F:23:HIS:CD2	1:F:25:LEU:H	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:HE2	3:B:806:GOL:H12	1.79	0.64
1:D:642[B]:MET:CE	5:D:1458:HOH:O	2.45	0.64
1:A:436:ASP:N	3:A:802[B]:GOL:H32	2.11	0.64
1:E:348:HIS:HD2	5:E:1086:HOH:O	1.79	0.64
1:F:334:LEU:HD22	5:F:1521:HOH:O	1.96	0.64
1:B:558[A]:LEU:CD2	3:B:807:GOL:C2	2.76	0.63
1:A:118[A]:VAL:CG2	5:A:1143:HOH:O	2.44	0.63
1:E:265[A]:LYS:HE2	3:E:802:GOL:H2	1.81	0.63
1:D:634[B]:MET:HE2	1:D:637[B]:GLU:CG	2.28	0.63
1:C:624[B]:HIS:NE2	5:C:1646:HOH:O	2.31	0.63
1:C:265:LYS:HE2	3:C:806:GOL:H2	1.80	0.63
1:E:642[A]:MET:HE1	5:E:1435:HOH:O	1.99	0.62
1:E:219:LYS:H	3:E:806:GOL:C1	2.05	0.62
1:A:303:VAL:HG23	5:A:1685:HOH:O	1.98	0.62
1:A:61:ARG:NH1	3:A:804:GOL:H32	2.14	0.62
1:D:642[A]:MET:HG2	1:D:644:ARG:CG	2.29	0.62
1:E:218:HIS:HD2	3:E:806:GOL:O3	1.81	0.62
1:F:265:LYS:HE2	3:F:802:GOL:H2	1.82	0.62
1:A:348:HIS:HD2	5:A:1135:HOH:O	1.81	0.61
1:B:23:HIS:HE2	3:B:805[A]:GOL:C3	2.08	0.61
1:E:218:HIS:HE1	5:E:1278:HOH:O	1.82	0.61
1:A:122[B]:CYS:SG	1:B:691:GLY:HA2	2.41	0.61
1:E:303:VAL:HG23	5:E:1347:HOH:O	1.99	0.61
1:F:116:LEU:CD1	1:F:157[A]:THR:HB	2.30	0.61
1:C:558[A]:LEU:HD21	3:C:809:GOL:C1	2.28	0.61
1:D:179[A]:SER:OG	3:D:805:GOL:H12	2.01	0.61
1:A:506:LYS:HD2	5:A:1383:HOH:O	1.99	0.61
1:C:371:GLY:CA	1:D:424[C]:ARG:NH2	2.64	0.60
1:F:292:ILE:HG21	1:F:293[B]:PHE:HE2	1.60	0.60
1:D:634[B]:MET:CE	1:D:637[B]:GLU:CG	2.78	0.60
1:B:348:HIS:HD2	5:B:1217:HOH:O	1.84	0.60
1:D:116:LEU:HD11	1:D:157[B]:THR:HB	1.83	0.60
1:B:366:HIS:HD2	5:B:1644:HOH:O	1.83	0.60
1:B:267:HIS:HB2	3:B:805[A]:GOL:H31	1.84	0.60
1:B:116:LEU:CD1	1:B:157[A]:THR:HB	2.31	0.59
1:B:366:HIS:CE1	5:B:1643:HOH:O	2.55	0.59
1:A:672:VAL:HG22	1:A:672:VAL:O	2.01	0.59
1:C:506[B]:LYS:HE2	5:C:1350:HOH:O	2.01	0.59
1:F:366:HIS:CD2	5:F:1657:HOH:O	2.52	0.59
1:A:550[A]:PRO:HD2	5:A:1665:HOH:O	2.02	0.59
1:C:624[A]:HIS:CE1	5:C:1731:HOH:O	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624[B]:HIS:CE1	1:A:630:ASP:OD2	2.54	0.59
1:A:558[B]:LEU:HD21	3:A:810:GOL:C1	2.29	0.59
1:A:687:GLY:HA3	1:B:126[A]:GLU:HB2	1.83	0.59
1:A:23:HIS:HE1	3:A:807:GOL:H11	1.67	0.59
1:A:57:ARG:HH22	3:A:809:GOL:H32	1.68	0.58
1:C:107:ARG:CZ	5:C:1705:HOH:O	2.49	0.58
1:A:578:ASN:HB3	5:A:1719:HOH:O	2.02	0.58
1:A:624[A]:HIS:CE1	5:A:1736:HOH:O	2.19	0.58
1:B:366:HIS:HE1	5:B:1515:HOH:O	1.86	0.58
1:A:550[A]:PRO:CD	5:A:1665:HOH:O	2.45	0.58
1:E:550[A]:PRO:CD	5:E:1665:HOH:O	2.43	0.58
1:E:126[B]:GLU:OE1	1:F:685:PHE:C	2.41	0.58
1:B:558[A]:LEU:CD2	3:B:807:GOL:H12	2.33	0.58
1:C:405:TYR:HE2	1:C:634[B]:MET:HE1	1.67	0.58
1:D:179[B]:SER:OG	3:D:805:GOL:C3	2.52	0.58
1:A:116:LEU:HD11	1:A:157[A]:THR:HB	1.86	0.57
1:C:642[A]:MET:CE	5:C:1923:HOH:O	2.36	0.57
1:C:691:GLY:HA2	1:D:122[A]:CYS:SG	2.45	0.57
1:E:116:LEU:HD11	1:E:157[B]:THR:HB	1.85	0.57
1:F:558[B]:LEU:HD21	3:F:808:GOL:C2	2.34	0.57
1:F:348:HIS:HD2	5:F:1198:HOH:O	1.88	0.57
1:E:211:ARG:HB3	5:E:1645:HOH:O	2.05	0.57
1:B:558[A]:LEU:HD21	3:B:807:GOL:C3	2.31	0.57
1:F:303:VAL:HG23	5:F:1292:HOH:O	2.05	0.57
1:A:23:HIS:CE1	3:A:807:GOL:H11	2.39	0.57
1:C:509:LYS:CE	5:C:1457:HOH:O	2.52	0.57
1:D:424[B]:ARG:HH11	3:D:803[B]:GOL:H12	1.64	0.57
1:A:118[A]:VAL:CG2	5:A:1623:HOH:O	2.52	0.57
1:F:136[B]:GLU:HG3	5:F:915:HOH:O	2.04	0.57
1:D:671:ALA:O	1:D:672:VAL:HB	2.03	0.56
1:A:118[A]:VAL:HG22	5:A:921:HOH:O	2.05	0.56
1:C:405:TYR:CE2	1:C:634[B]:MET:HE1	2.41	0.56
1:B:177:TYR:OH	3:B:808:GOL:H32	2.05	0.56
1:E:342:ILE:C	1:E:342:ILE:HD12	2.26	0.56
1:D:634[B]:MET:HE1	1:D:637[B]:GLU:OE1	2.05	0.56
1:C:333:SER:HB2	1:C:336[B]:CYS:SG	2.46	0.56
1:B:280:ASP:HB3	3:B:805[A]:GOL:H32	1.87	0.56
1:C:107:ARG:NH2	5:C:1705:HOH:O	2.39	0.56
1:E:424[B]:ARG:NH2	5:E:1683:HOH:O	2.28	0.55
1:B:218:HIS:ND1	3:B:806:GOL:H31	2.21	0.55
1:B:436:ASP:OD1	3:B:802[B]:GOL:H2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:GLY:C	1:D:424[C]:ARG:HH21	2.10	0.55
1:F:624[B]:HIS:CE1	1:F:630:ASP:OD2	2.56	0.55
1:A:57:ARG:HH22	3:A:809:GOL:H31	1.71	0.55
1:A:116:LEU:HD12	1:A:157[A]:THR:HB	1.88	0.55
1:C:506[B]:LYS:HD2	5:C:1414:HOH:O	2.05	0.55
1:C:303:VAL:HG23	5:C:1626:HOH:O	2.07	0.54
1:C:371:GLY:HA3	1:D:424[C]:ARG:HH22	1.70	0.54
1:E:122[B]:CYS:SG	1:F:691:GLY:HA2	2.47	0.54
1:E:315:LYS:HZ2	1:E:430:ASN:ND2	2.02	0.54
1:D:642[A]:MET:HG3	1:D:643:LEU:N	2.22	0.54
1:B:624[B]:HIS:CE1	1:B:630:ASP:OD2	2.61	0.54
1:E:567[A]:SER:OG	5:E:1664:HOH:O	2.07	0.54
1:E:388[B]:VAL:HG13	1:F:336[B]:CYS:HB3	1.87	0.54
1:C:564:PRO:CG	5:C:1670:HOH:O	2.30	0.54
1:C:685:PHE:C	1:D:126[B]:GLU:OE1	2.45	0.54
1:E:213[B]:ARG:NE	5:E:1645:HOH:O	1.90	0.54
1:C:405:TYR:CE2	1:C:634[B]:MET:CE	2.89	0.54
1:F:642[A]:MET:HG3	1:F:644[A]:ARG:HG3	1.90	0.54
3:A:807:GOL:C1	5:A:1490:HOH:O	2.51	0.54
1:E:624[A]:HIS:CE1	5:E:1731:HOH:O	2.39	0.54
3:B:802[B]:GOL:O2	5:B:1663:HOH:O	2.02	0.54
1:D:366:HIS:CD2	1:D:368:GLU:HG3	2.43	0.54
1:C:136:GLU:HG3	5:C:1064:HOH:O	2.06	0.54
1:A:61:ARG:HH11	3:A:804:GOL:C3	2.20	0.54
1:D:624[B]:HIS:CE1	1:D:630:ASP:OD2	2.59	0.53
1:D:550:PRO:CD	5:D:1676:HOH:O	2.52	0.53
1:D:550:PRO:HD2	5:D:1676:HOH:O	2.08	0.53
1:B:555[A]:GLU:HG3	5:B:1647:HOH:O	2.09	0.53
1:B:62:LYS:NZ	1:B:66[A]:GLN:OE1	2.19	0.53
1:F:116:LEU:HD12	1:F:157[A]:THR:HB	1.91	0.53
1:A:366:HIS:CE1	5:A:1415:HOH:O	2.62	0.53
1:D:424[C]:ARG:HD2	1:D:636:ALA:CB	2.25	0.53
3:B:809:GOL:H31	5:B:1792:HOH:O	2.08	0.53
1:F:286:HIS:HE1	5:F:975:HOH:O	1.92	0.53
1:D:156:TRP:O	1:D:157[B]:THR:CA	2.56	0.53
1:A:624[B]:HIS:CD2	1:A:637[B]:GLU:OE1	2.62	0.53
1:E:624[B]:HIS:CE1	1:E:630:ASP:OD2	2.61	0.53
1:B:382[B]:ASN:OD1	5:B:1716:HOH:O	2.19	0.53
1:B:506[A]:LYS:CE	5:B:1455:HOH:O	2.32	0.52
1:A:366:HIS:HE1	5:A:1416:HOH:O	1.91	0.52
1:C:333:SER:CB	1:C:336[B]:CYS:SG	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HD12	1:B:157[A]:THR:HB	1.91	0.52
1:F:436:ASP:H	3:F:803:GOL:H32	1.74	0.52
1:D:116:LEU:HD12	1:D:157[B]:THR:HB	1.89	0.52
1:A:558[B]:LEU:HD23	3:A:810:GOL:C2	2.27	0.52
1:E:414[A]:MET:HE3	5:E:1568:HOH:O	1.69	0.52
1:D:642[B]:MET:HE1	5:D:1458:HOH:O	2.09	0.52
1:B:334:LEU:CB	5:B:1732:HOH:O	2.58	0.52
1:F:23:HIS:HE1	3:F:802:GOL:O1	1.94	0.51
1:F:48:LYS:HE2	1:F:86:ALA:HB2	1.92	0.51
1:E:642[A]:MET:CE	5:E:1435:HOH:O	2.58	0.51
1:C:107:ARG:NH1	5:C:1705:HOH:O	2.43	0.51
1:F:380:ARG:O	1:F:689:CYS:HB3	2.09	0.51
1:A:265:LYS:CD	3:A:807:GOL:H31	2.40	0.51
1:A:126[A]:GLU:HB2	1:B:687:GLY:HA3	1.91	0.51
1:C:380:ARG:O	1:C:689:CYS:HB3	2.11	0.51
1:B:219:LYS:HG3	3:B:806:GOL:C1	2.39	0.51
1:C:624[B]:HIS:CE1	1:C:630:ASP:OD2	2.59	0.51
1:D:220:HIS:H	3:D:805:GOL:H2	1.75	0.50
1:F:157[A]:THR:HG21	1:F:322:GLU:OE2	2.10	0.50
1:F:634[B]:MET:HE1	5:F:1599:HOH:O	2.11	0.50
1:B:211:ARG:HD3	1:B:213[A]:ARG:HE	1.76	0.50
1:B:157[A]:THR:HG21	1:B:322:GLU:OE2	2.12	0.50
1:E:425[B]:LEU:HB3	1:E:637[B]:GLU:HB2	1.94	0.50
1:F:468:ILE:H	1:F:473:ASN:ND2	2.07	0.50
1:F:624[B]:HIS:CD2	5:F:1751:HOH:O	2.65	0.50
1:C:644[A]:ARG:CD	5:C:1721:HOH:O	2.35	0.50
1:C:333:SER:OG	1:C:334:LEU:CA	2.59	0.50
1:A:689:CYS:SG	5:A:1123:HOH:O	2.38	0.49
1:E:213[A]:ARG:HD2	5:E:1645:HOH:O	2.12	0.49
1:C:689:CYS:SG	5:C:1764:HOH:O	2.32	0.49
1:C:116:LEU:HD11	1:C:157[A]:THR:HB	1.91	0.49
1:C:292:ILE:HG21	1:C:293[B]:PHE:HE2	1.73	0.49
1:E:116:LEU:HD12	1:E:157[B]:THR:HB	1.95	0.49
1:F:436:ASP:H	3:F:803:GOL:C3	2.25	0.49
1:E:294:HIS:HD2	5:E:1579:HOH:O	1.94	0.49
1:A:23:HIS:HE1	3:A:807:GOL:O1	1.96	0.49
1:C:558[A]:LEU:HD21	3:C:809:GOL:C2	2.42	0.49
1:A:558[B]:LEU:HD21	3:A:810:GOL:C2	2.43	0.49
1:C:631:PHE:CG	1:C:632:PRO:HA	2.48	0.49
1:D:21:PRO:HG3	1:D:77:ARG:CZ	2.42	0.49
1:E:624[B]:HIS:NE2	1:E:637[B]:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230[B]:GLU:OE2	5:E:1389:HOH:O	2.19	0.49
1:A:265:LYS:CE	3:A:807:GOL:H31	2.43	0.49
1:C:644[A]:ARG:NH2	5:C:1785:HOH:O	2.46	0.49
1:C:468:ILE:H	1:C:473:ASN:ND2	2.07	0.49
1:E:388[B]:VAL:CG1	1:F:336[B]:CYS:HB3	2.43	0.48
1:B:471[A]:ASP:OD2	5:B:1742:HOH:O	2.19	0.48
1:E:631:PHE:CG	1:E:632:PRO:HA	2.49	0.48
1:B:558[A]:LEU:HD21	3:B:807:GOL:C2	2.43	0.48
3:F:803:GOL:H2	5:F:1095:HOH:O	2.12	0.48
1:A:550[B]:PRO:CG	5:B:1908:HOH:O	2.13	0.48
1:D:631:PHE:CG	1:D:632:PRO:HA	2.49	0.48
1:A:631:PHE:CG	1:A:632:PRO:HA	2.49	0.48
1:F:631:PHE:CG	1:F:632:PRO:HA	2.49	0.48
1:E:126[A]:GLU:HB2	1:F:687:GLY:HA3	1.95	0.48
1:E:201:LYS:HG2	5:E:1238:HOH:O	2.13	0.48
1:A:435:GLY:HA2	3:A:802[B]:GOL:H32	1.96	0.47
1:B:631:PHE:CG	1:B:632:PRO:HA	2.48	0.47
1:D:414[B]:MET:HE3	1:D:418:ALA:HB3	1.96	0.47
1:A:118[A]:VAL:HG23	5:A:1623:HOH:O	2.13	0.47
1:F:564:PRO:CG	5:F:1629:HOH:O	2.37	0.47
1:B:558[A]:LEU:CD2	3:B:807:GOL:C1	2.92	0.47
1:D:366:HIS:NE2	1:D:368:GLU:HG3	2.28	0.47
1:B:61:ARG:HH22	1:B:467[A]:ARG:HG2	1.79	0.47
1:E:218:HIS:CD2	3:E:806:GOL:O3	2.65	0.47
1:C:687:GLY:HA3	1:D:126[A]:GLU:HB2	1.96	0.47
1:E:642[B]:MET:HG3	1:E:644:ARG:HG3	1.97	0.47
1:F:424:ARG:NE	5:F:1669:HOH:O	2.39	0.47
1:A:669:LYS:HE3	1:B:181:GLU:OE1	2.15	0.47
1:B:380:ARG:O	1:B:689:CYS:HB3	2.15	0.47
1:A:642[B]:MET:CE	5:A:1449:HOH:O	2.58	0.47
3:E:806:GOL:C3	5:F:1037:HOH:O	2.22	0.47
1:D:157[B]:THR:OG1	5:D:1633:HOH:O	0.47	0.47
1:E:23:HIS:HE1	3:E:802:GOL:O1	1.98	0.46
1:B:364[B]:CYS:SG	1:B:397[B]:SER:OG	2.74	0.46
1:D:457:GLN:HE22	1:D:552:LEU:H	1.61	0.46
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.50	0.46
1:C:333:SER:CB	1:C:337:ASP:H	2.24	0.46
1:F:319[B]:ASP:OD1	5:F:1292:HOH:O	2.20	0.46
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.51	0.46
1:F:425[B]:LEU:HD23	5:F:1599:HOH:O	1.85	0.46
1:E:222:ASN:HB3	1:E:227:HIS:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ILE:H	1:D:473:ASN:ND2	2.05	0.46
5:A:1606:HOH:O	1:B:550[B]:PRO:CG	2.15	0.45
1:B:348:HIS:HE1	5:B:1277:HOH:O	1.99	0.45
1:C:371:GLY:C	1:D:424[C]:ARG:NH2	2.68	0.45
1:A:348:HIS:HE1	5:A:1278:HOH:O	1.99	0.45
1:A:265:LYS:HG2	3:A:807:GOL:H31	1.99	0.45
1:C:371:GLY:HA2	1:C:390[A]:ARG:NH2	2.32	0.45
1:B:558[B]:LEU:HD13	3:B:807:GOL:H12	1.98	0.45
1:B:689:CYS:SG	5:B:1757:HOH:O	2.21	0.45
1:A:578:ASN:CB	5:A:1719:HOH:O	2.61	0.45
1:D:425[B]:LEU:HB2	1:D:637[B]:GLU:HB2	1.98	0.45
3:B:809:GOL:H11	5:B:1792:HOH:O	2.17	0.45
1:C:66:GLN:NE2	5:C:1508:HOH:O	2.48	0.45
1:B:642:MET:HE3	1:B:642:MET:HB3	1.53	0.45
1:E:230[A]:GLU:HG2	5:E:1263:HOH:O	2.16	0.45
1:A:66[B]:GLN:HG3	1:A:70:GLN:NE2	2.32	0.45
1:F:642[B]:MET:SD	1:F:644[B]:ARG:NH2	2.90	0.45
1:E:631:PHE:CD1	1:E:632:PRO:HA	2.52	0.45
1:A:157[A]:THR:HG21	1:A:322:GLU:OE2	2.17	0.44
1:C:644[B]:ARG:HD2	5:C:1166:HOH:O	2.18	0.44
1:B:218:HIS:HD2	1:B:450:ASN:HD22	1.65	0.44
1:C:217:LYS:HE3	5:C:1781:HOH:O	2.16	0.44
1:D:222:ASN:HB3	1:D:227:HIS:CG	2.53	0.44
1:A:425[B]:LEU:HD23	5:A:1628:HOH:O	1.78	0.44
1:C:420[B]:ARG:NH1	5:C:1634:HOH:O	2.44	0.44
1:D:425[A]:LEU:HG	1:D:634[A]:MET:HE3	1.99	0.44
1:A:436:ASP:H	3:A:802[A]:GOL:H32	1.81	0.44
1:D:408:CYS:HB2	1:D:424[C]:ARG:HB2	1.99	0.44
1:F:424:ARG:HG2	5:F:1669:HOH:O	2.16	0.44
1:F:222:ASN:HB3	1:F:227:HIS:CG	2.53	0.44
1:D:202:LYS:HE3	1:D:202:LYS:HB2	1.74	0.44
1:A:333:SER:HA	1:A:334:LEU:HA	1.60	0.44
1:B:142:GLY:O	3:B:808:GOL:O2	2.36	0.44
1:B:116:LEU:HD11	1:B:157[A]:THR:HB	2.00	0.43
1:E:642[B]:MET:CG	1:E:644:ARG:HG3	2.48	0.43
1:F:334:LEU:HD23	1:F:344:TYR:OH	2.18	0.43
1:D:531[A]:VAL:HG23	5:D:1499:HOH:O	2.19	0.43
1:D:52:ASN:HD21	1:D:115:ILE:HG22	1.83	0.43
1:F:425[A]:LEU:HD12	1:F:622:ILE:HD11	2.01	0.43
1:D:642[B]:MET:HE3	5:D:1458:HOH:O	2.13	0.43
1:F:66:GLN:NE2	5:F:1442:HOH:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644[B]:ARG:NH1	5:C:1923:HOH:O	1.93	0.43
1:A:380:ARG:O	1:A:689:CYS:HB3	2.19	0.43
1:F:624[B]:HIS:HD2	1:F:637[B]:GLU:OE1	1.94	0.43
1:C:624[B]:HIS:CD2	5:D:1651:HOH:O	2.72	0.43
1:D:631:PHE:CD1	1:D:632:PRO:HA	2.54	0.43
1:C:425[A]:LEU:HD12	1:C:622:ILE:HD11	2.01	0.42
1:A:558[B]:LEU:CD2	3:A:810:GOL:H31	2.49	0.42
1:A:305:TYR:CD2	1:A:456:HIS:HB3	2.54	0.42
3:F:804[A]:GOL:H2	5:F:1703:HOH:O	2.19	0.42
1:B:222:ASN:HB3	1:B:227:HIS:CG	2.54	0.42
3:A:802[A]:GOL:H2	5:A:1031:HOH:O	2.18	0.42
1:F:305:TYR:CD2	1:F:456:HIS:HB3	2.54	0.42
1:D:425[A]:LEU:HG	1:D:634[A]:MET:CE	2.50	0.42
1:B:280:ASP:OD2	3:B:805[A]:GOL:H32	2.19	0.42
1:D:468:ILE:N	1:D:473:ASN:HD21	2.08	0.42
1:A:364[B]:CYS:SG	1:A:397[B]:SER:OG	2.77	0.42
3:C:802:GOL:H12	5:C:1170:HOH:O	2.19	0.42
1:A:202:LYS:HB2	1:A:202:LYS:HE3	1.38	0.42
1:C:333:SER:HB3	1:C:336[B]:CYS:SG	2.60	0.42
1:D:564:PRO:CG	5:D:1718:HOH:O	2.54	0.42
1:C:123[A]:SER:HB3	1:C:201:LYS:HE2	2.01	0.42
1:F:116:LEU:HD11	1:F:157[A]:THR:HB	2.01	0.42
1:F:634[A]:MET:HE3	1:F:634[A]:MET:HB3	1.63	0.42
1:F:435:GLY:CA	3:F:803:GOL:H32	2.45	0.42
1:C:366:HIS:NE2	1:C:368[A]:GLU:CD	2.73	0.42
1:C:333:SER:OG	1:C:334:LEU:C	2.58	0.42
1:C:372:LEU:N	1:D:424[C]:ARG:NH2	2.61	0.42
1:B:334:LEU:CB	1:B:336:CYS:H	2.32	0.42
1:D:366:HIS:HE2	1:D:368:GLU:CG	2.33	0.42
1:B:66[B]:GLN:HG3	1:B:70:GLN:NE2	2.34	0.41
1:B:467[B]:ARG:HE	1:B:471[B]:ASP:CG	2.23	0.41
1:A:631:PHE:CD1	1:A:632:PRO:HA	2.55	0.41
1:C:57:ARG:NH1	5:C:1684:HOH:O	2.30	0.41
1:C:370:ASP:O	1:D:424[C]:ARG:NH2	2.42	0.41
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.55	0.41
1:C:222:ASN:HB3	1:C:227:HIS:ND1	2.36	0.41
1:F:254[B]:MET:HE3	1:F:256:GLY:O	2.20	0.41
1:F:348:HIS:HE1	5:F:1232:HOH:O	2.03	0.41
1:F:161[A]:ASP:OD2	5:F:1282:HOH:O	2.21	0.41
1:D:642[A]:MET:HB2	1:D:642[A]:MET:HE2	1.86	0.41
1:E:21:PRO:HG3	1:E:77:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:HB2	1:A:259:MET:SD	2.61	0.41
1:D:624[B]:HIS:NE2	1:D:637[B]:GLU:OE1	2.53	0.41
1:E:352[A]:ARG:CG	5:E:1688:HOH:O	2.50	0.41
1:F:50:SER:HB2	1:F:352:ARG:CG	2.45	0.41
1:C:123[A]:SER:CB	1:C:201:LYS:HE2	2.51	0.41
1:C:252:PHE:HB2	1:C:259:MET:SD	2.61	0.41
1:F:405:TYR:CE2	1:F:634[A]:MET:HE1	2.47	0.41
1:A:265:LYS:CG	3:A:807:GOL:H31	2.50	0.41
1:B:218:HIS:CD2	1:B:450:ASN:HD22	2.39	0.41
1:C:366:HIS:CD2	1:C:368[A]:GLU:CG	3.04	0.41
1:F:248:GLU:OE1	5:F:1693:HOH:O	2.22	0.41
1:F:222:ASN:HB3	1:F:227:HIS:ND1	2.36	0.41
1:C:254[A]:MET:HE3	1:C:256:GLY:O	2.21	0.41
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.51	0.41
1:A:126[B]:GLU:HB2	1:B:687:GLY:HA3	1.84	0.40
1:B:252:PHE:HB2	1:B:259:MET:SD	2.61	0.40
1:E:558[A]:LEU:HA	1:E:558[A]:LEU:HD12	1.91	0.40
1:A:555[A]:GLU:HG3	5:A:1605:HOH:O	2.20	0.40
1:A:361:ASN:ND2	5:A:1519:HOH:O	2.53	0.40
1:C:305:TYR:CD2	1:C:456:HIS:HB3	2.56	0.40
1:F:364[A]:CYS:SG	1:F:397[A]:SER:OG	2.79	0.40
1:D:342:ILE:HD11	1:D:344:TYR:CE2	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1586:HOH:O	5:D:1105:HOH:O[1_556]	2.14	0.06

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	696/692 (101%)	673 (97%)	23 (3%)	0	100	100
1	B	695/692 (100%)	675 (97%)	19 (3%)	1 (0%)	56	21
1	C	694/692 (100%)	670 (96%)	22 (3%)	2 (0%)	46	17
1	D	685/692 (99%)	665 (97%)	20 (3%)	0	100	100
1	E	684/692 (99%)	667 (98%)	17 (2%)	0	100	100
1	F	695/692 (100%)	672 (97%)	23 (3%)	0	100	100
All	All	4149/4152 (100%)	4022 (97%)	124 (3%)	3 (0%)	56	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	334	LEU
1	C	333	SER
1	C	334	LEU

### 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	605/594 (102%)	599 (99%)	6 (1%)	82	51
1	B	605/594 (102%)	601 (99%)	4 (1%)	88	64
1	C	603/594 (102%)	602 (100%)	1 (0%)	95	79
1	D	596/594 (100%)	591 (99%)	5 (1%)	86	60
1	E	595/594 (100%)	591 (99%)	4 (1%)	88	64
1	F	605/594 (102%)	601 (99%)	4 (1%)	88	64
All	All	3609/3564 (101%)	3585 (99%)	24 (1%)	90	64

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	202	LYS

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Mol	Chain	Res	Type
1	A	254[A]	MET
1	A	254[B]	MET
1	A	329	THR
1	A	672	VAL
1	B	329	THR
1	B	333	SER
1	B	642	MET
1	B	672	VAL
1	C	329	THR
1	D	122[A]	CYS
1	D	122[B]	CYS
1	D	202	LYS
1	D	329	THR
1	D	672	VAL
1	E	210	ASN
1	E	213[A]	ARG
1	E	213[B]	ARG
1	E	329	THR
1	F	240	PRO
1	F	329	THR
1	F	333	SER
1	F	334	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	70	GLN
1	A	348	HIS
1	A	361	ASN
1	A	366	HIS
1	A	382	ASN
1	B	70	GLN
1	B	288	ASN
1	B	348	HIS
1	B	361	ASN
1	B	366	HIS
1	B	450	ASN
1	C	66	GLN
1	C	361	ASN
1	C	382	ASN
1	C	473	ASN

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Mol	Chain	Res	Type
1	C	547	GLN
1	D	52	ASN
1	D	70	GLN
1	D	286	HIS
1	D	288	ASN
1	D	457	GLN
1	D	473	ASN
1	E	23	HIS
1	E	70	GLN
1	E	210	ASN
1	E	218	HIS
1	E	286	HIS
1	E	294	HIS
1	E	348	HIS
1	E	361	ASN
1	E	430	ASN
1	F	23	HIS
1	F	66	GLN
1	F	70	GLN
1	F	286	HIS
1	F	348	HIS
1	F	361	ASN
1	F	382	ASN
1	F	473	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 6 are monoatomic - leaving 51 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	GOL	A	802[A]	-	5,5,5	0.79	0	5,5,5	1.04	0
3	GOL	A	802[B]	-	5,5,5	0.75	0	5,5,5	0.68	0
3	GOL	A	803[A]	-	5,5,5	0.48	0	5,5,5	0.67	0
3	GOL	A	803[B]	-	5,5,5	0.45	0	5,5,5	0.54	0
3	GOL	A	804	-	5,5,5	0.48	0	5,5,5	0.75	0
3	GOL	A	805	-	5,5,5	0.60	0	5,5,5	0.31	0
3	GOL	A	806	-	5,5,5	0.40	0	5,5,5	0.80	0
3	GOL	A	807	-	5,5,5	1.30	1 (20%)	5,5,5	3.00	3 (60%)
3	GOL	A	808	-	5,5,5	0.38	0	5,5,5	0.46	0
3	GOL	A	809	-	5,5,5	0.48	0	5,5,5	1.00	0
3	GOL	A	810	-	5,5,5	1.23	1 (20%)	5,5,5	0.52	0
3	GOL	A	811	-	5,5,5	0.82	0	5,5,5	1.91	3 (60%)
3	GOL	B	802[A]	-	5,5,5	0.40	0	5,5,5	1.11	0
3	GOL	B	802[B]	-	5,5,5	0.21	0	5,5,5	0.95	0
3	GOL	B	803	-	5,5,5	0.61	0	5,5,5	0.68	0
3	GOL	B	804	-	5,5,5	0.51	0	5,5,5	0.65	0
3	GOL	B	805[A]	-	5,5,5	0.69	0	5,5,5	1.28	1 (20%)
3	GOL	B	805[B]	-	5,5,5	0.37	0	5,5,5	1.40	1 (20%)
3	GOL	B	806	-	5,5,5	0.68	0	5,5,5	0.94	0
3	GOL	B	807	-	5,5,5	1.36	1 (20%)	5,5,5	0.73	0
3	GOL	B	808	-	5,5,5	0.61	0	5,5,5	1.44	2 (40%)
3	GOL	B	809	-	5,5,5	0.81	0	5,5,5	1.15	0
3	GOL	C	802	-	5,5,5	0.96	0	5,5,5	4.40	4 (80%)
3	GOL	C	803	-	5,5,5	0.31	0	5,5,5	0.93	0
4	PO4	C	804	-	4,4,4	0.78	0	6,6,6	0.46	0
3	GOL	C	805	-	5,5,5	0.43	0	5,5,5	0.74	0
3	GOL	C	806	-	5,5,5	0.34	0	5,5,5	0.96	0
3	GOL	C	807	-	5,5,5	0.56	0	5,5,5	0.56	0
3	GOL	C	808	-	5,5,5	0.57	0	5,5,5	0.94	0
3	GOL	C	809	-	5,5,5	1.86	2 (40%)	5,5,5	1.20	0
3	GOL	C	810	-	5,5,5	0.36	0	5,5,5	0.98	0
3	GOL	D	802	-	5,5,5	0.33	0	5,5,5	0.98	1 (20%)
3	GOL	D	803[A]	-	5,5,5	0.47	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	803[B]	-	5,5,5	0.35	0	5,5,5	0.54	0
3	GOL	D	804	-	5,5,5	0.39	0	5,5,5	0.44	0
3	GOL	D	805	-	5,5,5	0.99	0	5,5,5	3.60	4 (80%)
3	GOL	D	806	-	5,5,5	0.82	0	5,5,5	2.79	2 (40%)
3	GOL	E	802	-	5,5,5	0.41	0	5,5,5	0.87	0
3	GOL	E	803	-	5,5,5	0.63	0	5,5,5	1.32	1 (20%)
3	GOL	E	804	-	5,5,5	0.34	0	5,5,5	0.75	0
3	GOL	E	805	-	5,5,5	0.24	0	5,5,5	0.49	0
3	GOL	E	806	-	5,5,5	0.62	0	5,5,5	2.81	2 (40%)
3	GOL	F	802	-	5,5,5	0.35	0	5,5,5	0.75	0
3	GOL	F	803	-	5,5,5	0.93	0	5,5,5	1.23	0
3	GOL	F	804[A]	-	5,5,5	0.43	0	5,5,5	0.52	0
3	GOL	F	804[B]	-	5,5,5	0.50	0	5,5,5	0.78	0
3	GOL	F	805	-	5,5,5	0.44	0	5,5,5	0.81	0
4	PO4	F	806	-	4,4,4	1.04	0	6,6,6	0.44	0
3	GOL	F	807	-	5,5,5	0.38	0	5,5,5	0.38	0
3	GOL	F	808	-	5,5,5	1.65	1 (20%)	5,5,5	0.92	0
3	GOL	F	809	-	5,5,5	0.67	0	5,5,5	0.82	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
3	GOL	A	802[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	802[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
3	GOL	A	805	-	-	0/4/4/4	0/0/0/0
3	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	GOL	A	807	-	-	0/4/4/4	0/0/0/0
3	GOL	A	808	-	-	0/4/4/4	0/0/0/0
3	GOL	A	809	-	-	0/4/4/4	0/0/0/0
3	GOL	A	810	-	-	0/4/4/4	0/0/0/0
3	GOL	A	811	-	-	0/4/4/4	0/0/0/0
3	GOL	B	802[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	B	802[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	B	803	-	-	0/4/4/4	0/0/0/0
3	GOL	B	804	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	805[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	B	805[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	B	806	-	-	0/4/4/4	0/0/0/0
3	GOL	B	807	-	-	0/4/4/4	0/0/0/0
3	GOL	B	808	-	-	0/4/4/4	0/0/0/0
3	GOL	B	809	-	-	0/4/4/4	0/0/0/0
3	GOL	C	802	-	-	0/4/4/4	0/0/0/0
3	GOL	C	803	-	-	0/4/4/4	0/0/0/0
4	PO4	C	804	-	-	0/0/0/0	0/0/0/0
3	GOL	C	805	-	-	0/4/4/4	0/0/0/0
3	GOL	C	806	-	-	0/4/4/4	0/0/0/0
3	GOL	C	807	-	-	0/4/4/4	0/0/0/0
3	GOL	C	808	-	-	0/4/4/4	0/0/0/0
3	GOL	C	809	-	-	0/4/4/4	0/0/0/0
3	GOL	C	810	-	-	0/4/4/4	0/0/0/0
3	GOL	D	802	-	-	0/4/4/4	0/0/0/0
3	GOL	D	803[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	D	803[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	D	804	-	-	0/4/4/4	0/0/0/0
3	GOL	D	805	-	-	0/4/4/4	0/0/0/0
3	GOL	D	806	-	-	0/4/4/4	0/0/0/0
3	GOL	E	802	-	-	0/4/4/4	0/0/0/0
3	GOL	E	803	-	-	0/4/4/4	0/0/0/0
3	GOL	E	804	-	-	0/4/4/4	0/0/0/0
3	GOL	E	805	-	-	0/4/4/4	0/0/0/0
3	GOL	E	806	-	-	0/4/4/4	0/0/0/0
3	GOL	F	802	-	-	0/4/4/4	0/0/0/0
3	GOL	F	803	-	-	0/4/4/4	0/0/0/0
3	GOL	F	804[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	F	804[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	F	805	-	-	0/4/4/4	0/0/0/0
4	PO4	F	806	-	-	0/0/0/0	0/0/0/0
3	GOL	F	807	-	-	0/4/4/4	0/0/0/0
3	GOL	F	808	-	-	0/4/4/4	0/0/0/0
3	GOL	F	809	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	809	GOL	O3-C3	-3.11	1.29	1.42
3	F	808	GOL	O1-C1	-2.91	1.29	1.42
3	A	807	GOL	O1-C1	-2.73	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	807	GOL	O1-C1	-2.29	1.32	1.42
3	A	810	GOL	O3-C3	-2.18	1.33	1.42
3	C	809	GOL	O2-C2	-2.03	1.37	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	GOL	O2-C2-C1	-6.87	77.16	108.65
3	D	805	GOL	O2-C2-C3	-6.67	78.06	108.65
3	A	807	GOL	O1-C1-C2	-5.23	84.81	110.18
3	C	802	GOL	C3-C2-C1	-4.67	92.81	111.12
3	D	806	GOL	O2-C2-C3	-4.60	87.56	108.65
3	E	806	GOL	O2-C2-C3	-4.25	89.16	108.65
3	A	807	GOL	O3-C3-C2	-2.72	97.00	110.18
3	A	807	GOL	C3-C2-C1	-2.62	100.85	111.12
3	B	805[B]	GOL	O3-C3-C2	-2.29	99.06	110.18
3	B	808	GOL	O3-C3-C2	-2.27	99.18	110.18
3	B	805[A]	GOL	O3-C3-C2	-2.21	99.47	110.18
3	B	808	GOL	O2-C2-C3	-2.07	99.15	108.65
3	D	802	GOL	O3-C3-C2	-2.04	100.29	110.18
3	E	803	GOL	O2-C2-C1	2.04	118.03	108.65
3	A	811	GOL	C3-C2-C1	2.09	119.31	111.12
3	D	805	GOL	O2-C2-C1	2.10	118.28	108.65
3	D	805	GOL	O1-C1-C2	2.14	120.56	110.18
3	A	811	GOL	O2-C2-C3	2.35	119.41	108.65
3	A	811	GOL	O3-C3-C2	2.48	122.22	110.18
3	C	802	GOL	O2-C2-C3	3.11	122.90	108.65
3	D	805	GOL	O3-C3-C2	3.30	126.18	110.18
3	C	802	GOL	O3-C3-C2	3.81	128.65	110.18
3	D	806	GOL	O2-C2-C1	3.93	126.65	108.65
3	E	806	GOL	O2-C2-C1	3.96	126.81	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802[A]	GOL	2	0
3	A	802[B]	GOL	3	0
3	A	804	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	807	GOL	11	0
3	A	809	GOL	3	0
3	A	810	GOL	8	0
3	B	802[B]	GOL	2	0
3	B	805[A]	GOL	4	0
3	B	805[B]	GOL	4	0
3	B	806	GOL	5	0
3	B	807	GOL	10	0
3	B	808	GOL	2	0
3	B	809	GOL	2	0
3	C	802	GOL	1	0
3	C	806	GOL	1	0
3	C	808	GOL	1	0
3	C	809	GOL	6	0
3	D	803[B]	GOL	3	0
3	D	805	GOL	6	0
3	D	806	GOL	5	0
3	E	802	GOL	2	0
3	E	806	GOL	7	0
3	F	802	GOL	2	0
3	F	803	GOL	5	0
3	F	804[A]	GOL	1	0
3	F	808	GOL	7	0
3	F	809	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	666/692 (96%)	-0.77	10 (1%) 76 73	5, 8, 21, 44	8 (1%)
1	B	664/692 (95%)	-0.78	6 (0%) 85 84	5, 8, 20, 46	7 (1%)
1	C	666/692 (96%)	-0.78	4 (0%) 90 88	5, 8, 23, 49	11 (1%)
1	D	657/692 (94%)	-0.82	4 (0%) 90 88	5, 8, 20, 52	1 (0%)
1	E	656/692 (94%)	-0.84	2 (0%) 94 92	5, 8, 19, 38	2 (0%)
1	F	665/692 (96%)	-0.77	5 (0%) 87 86	5, 8, 23, 51	8 (1%)
All	All	3974/4152 (95%)	-0.79	31 (0%) 87 86	5, 8, 21, 52	37 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	LEU	8.9
1	B	334	LEU	7.5
1	B	335	GLY	5.3
1	F	333	SER	5.3
1	F	672	VAL	4.8
1	F	334	LEU	4.7
1	F	335	GLY	4.6
1	A	333	SER	4.3
1	D	335	GLY	3.9
1	C	334	LEU	3.8
1	B	333	SER	3.8
1	C	333	SER	3.6
1	F	684	ALA	3.3
1	C	335	GLY	3.3
1	E	335	GLY	3.1
1	A	672	VAL	3.0
1	A	15	SER	2.9
1	A	684	ALA	2.8
1	A	335[A]	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	672	VAL	2.7
1	B	672	VAL	2.7
1	C	672	VAL	2.5
1	D	334	LEU	2.5
1	B	336	CYS	2.5
1	D	336	CYS	2.4
1	A	336[A]	CYS	2.3
1	E	336	CYS	2.3
1	B	338	CYS	2.1
1	A	671	ALA	2.1
1	A	338	CYS	2.0
1	A	687	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	E	804	6/6	0.92	0.12	29.08	32,35,37,43	0
3	GOL	D	804	6/6	0.86	0.12	20.21	36,37,42,48	0
3	GOL	C	808	6/6	0.97	0.15	19.13	17,22,25,30	0
3	GOL	B	804	6/6	0.94	0.11	17.84	28,31,33,39	0
3	GOL	C	805	6/6	0.90	0.14	17.20	25,32,38,43	0
3	GOL	A	807	6/6	0.96	0.19	16.58	16,26,31,38	0
3	GOL	A	810	6/6	0.95	0.15	16.43	10,17,19,21	0
3	GOL	B	807	6/6	0.96	0.14	16.16	10,17,19,21	0
3	GOL	F	805	6/6	0.93	0.12	15.50	34,36,42,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	805[B]	6/6	0.85	0.25	14.98	7,16,24,28	6
3	GOL	B	805[A]	6/6	0.85	0.25	14.68	11,22,25,29	6
3	GOL	A	805	6/6	0.97	0.16	14.65	10,18,22,31	0
3	GOL	C	809	6/6	0.94	0.13	14.12	10,16,20,21	0
3	GOL	E	806	6/6	0.90	0.20	13.88	11,27,30,31	0
3	GOL	F	809	6/6	0.95	0.11	12.85	18,21,25,31	0
3	GOL	A	806	6/6	0.87	0.12	12.57	27,29,37,43	0
3	GOL	B	809	6/6	0.98	0.12	12.16	21,25,27,31	0
3	GOL	C	807	6/6	0.98	0.12	11.69	10,18,22,29	0
3	GOL	A	811	6/6	0.83	0.18	9.26	30,31,33,40	0
3	GOL	D	805	6/6	0.95	0.17	9.05	12,24,27,32	0
3	GOL	B	808	6/6	0.90	0.12	8.59	25,30,33,37	0
3	GOL	A	804	6/6	0.94	0.13	8.39	20,32,40,40	0
3	GOL	F	808	6/6	0.97	0.13	7.62	10,17,20,21	0
3	GOL	A	802[B]	6/6	0.85	0.15	7.37	17,20,24,26	6
3	GOL	F	803	6/6	0.82	0.14	7.07	21,23,34,35	0
3	GOL	F	804[B]	6/6	0.89	0.15	7.00	16,22,24,29	6
3	GOL	D	806	6/6	0.93	0.17	6.76	11,27,29,30	0
3	GOL	A	809	6/6	0.89	0.14	6.64	18,23,38,40	0
3	GOL	F	804[A]	6/6	0.89	0.15	6.62	12,18,20,24	6
3	GOL	E	802	6/6	0.93	0.14	6.55	14,18,20,29	0
3	GOL	A	803[A]	6/6	0.87	0.13	5.70	15,17,20,20	6
3	GOL	C	803	6/6	0.81	0.16	5.57	22,26,28,28	0
3	GOL	A	803[B]	6/6	0.87	0.13	5.14	13,19,22,25	6
3	GOL	D	802	6/6	0.94	0.11	4.82	14,19,21,28	0
3	GOL	C	806	6/6	0.98	0.09	4.66	15,20,22,31	0
3	GOL	A	802[A]	6/6	0.85	0.15	4.53	17,24,25,26	6
3	GOL	F	802	6/6	0.96	0.08	3.71	15,20,22,32	0
3	GOL	B	803	6/6	0.94	0.12	3.55	17,20,20,29	0
3	GOL	D	803[B]	6/6	0.94	0.12	3.54	13,25,26,35	6
3	GOL	E	803	6/6	0.88	0.13	2.90	21,24,26,28	0
3	GOL	C	802	6/6	0.91	0.10	2.82	19,24,29,35	0
3	GOL	D	803[A]	6/6	0.94	0.12	2.64	11,16,17,21	6
3	GOL	B	802[B]	6/6	0.87	0.15	2.23	17,20,23,23	6
3	GOL	B	802[A]	6/6	0.87	0.15	2.23	19,21,26,32	6
3	GOL	E	805	6/6	0.91	0.10	1.18	22,23,25,34	0
2	CO	F	801	1/1	1.00	0.04	-1.42	6,6,6,6	1
2	CO	C	801	1/1	1.00	0.03	-1.62	6,6,6,6	1
2	CO	D	801	1/1	1.00	0.03	-1.66	7,7,7,7	1
2	CO	B	801	1/1	1.00	0.03	-1.79	8,8,8,8	1
2	CO	A	801	1/1	1.00	0.03	-2.16	8,8,8,8	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO	E	801	1/1	1.00	0.02	-2.26	7,7,7,7	1
3	GOL	C	810	6/6	0.93	0.17	-	32,38,41,45	0
3	GOL	B	806	6/6	0.93	0.12	-	20,42,49,55	0
4	PO4	F	806	5/5	0.97	0.12	-	12,16,24,25	5
4	PO4	C	804	5/5	0.96	0.14	-	13,18,25,26	5
3	GOL	A	808	6/6	0.93	0.08	-	20,30,32,38	0
3	GOL	F	807	6/6	0.92	0.09	-	40,41,43,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.