Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:35 PM GMT

PDB ID	:	3U52
Title	:	X-ray Crystal Structure of Xenon-Pressurized Phenol Hydroxylase from Pseudomonas sp. OX1
Authors	:	McCormick, M.S.; Lippard, S.J.
Deposited on	:	2011-10-10
Resolution	:	1.95 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

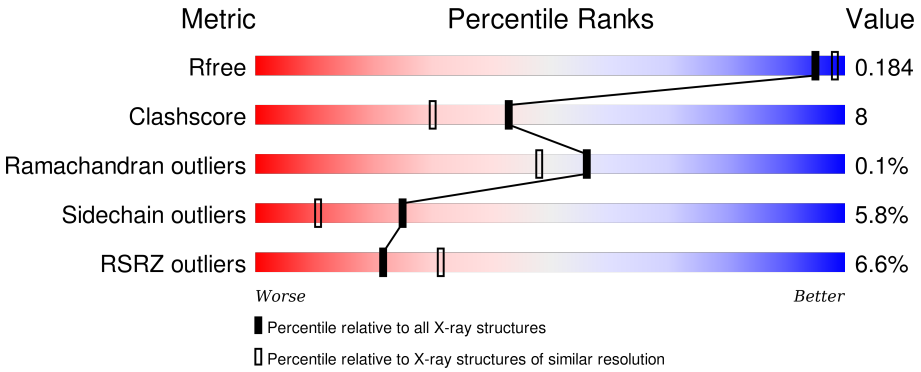
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 >=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 <=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	511	6% 82% 14%
1	B	511	9% 79% 15%
2	C	333	% 77% 14% 5%
2	D	333	8% 81% 14%
3	E	119	8% 75% 20%

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Mol	Chain	Length	Quality of chain
3	F	119	8% 77% 18%

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
10	EPE	B	517	-	-	X	X
7	GOL	A	516	-	-	-	X
7	GOL	A	519	-	-	-	X
7	GOL	B	518	-	-	-	X
7	GOL	D	334	-	-	X	X
8	XE	A	520	-	-	-	X
8	XE	A	521	-	-	X	-
8	XE	A	522	-	-	X	-
8	XE	B	520	-	-	-	X
8	XE	B	521	-	-	-	X
9	MPO	B	516	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16039 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 Phenol hydroxylase component phN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			4123	2652	693	754	24			
1	B	493	Total	C	N	O	S	0	0	0
			4110	2643	690	753	24			

- Molecule 2 is a protein called Phenol hydroxylase component phL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	318	Total	C	N	O	S	0	0	0
			2589	1630	449	492	18			
2	D	328	Total	C	N	O	S	0	0	0
			2659	1673	461	507	18			

- Molecule 3 is a protein called Phenol hydroxylase component phO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	118	Total	C	N	O	S	0	0	0
			925	602	145	173	5			
3	F	118	Total	C	N	O	S	0	0	0
			925	602	145	173	5			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Fe	0	0
			2	2		
4	A	2	Total	Fe	0	0
			2	2		

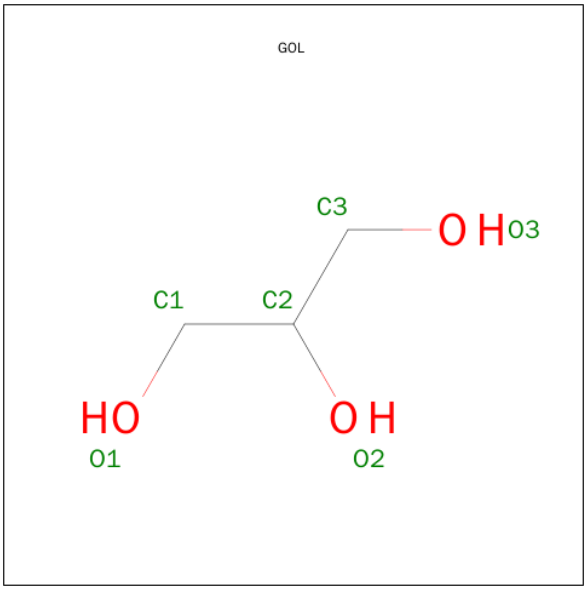
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cu 1 1	0	0
6	A	1	Total Cu 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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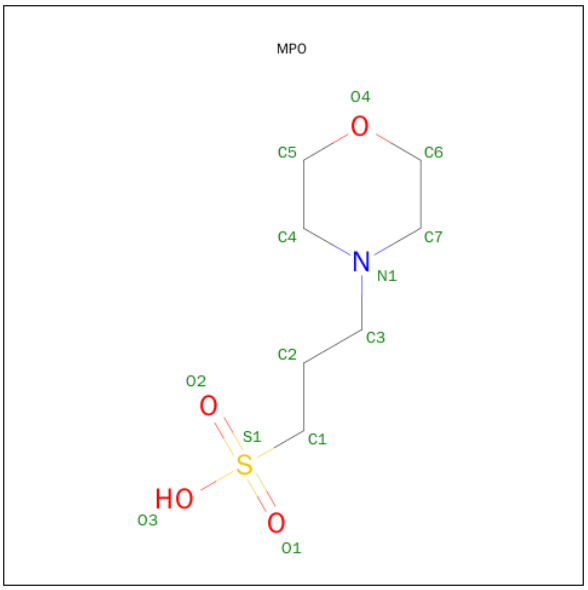
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	F	1	Total C O 6 3 3	0	0

- Molecule 8 is XENON (three-letter code: XE) (formula: Xe).

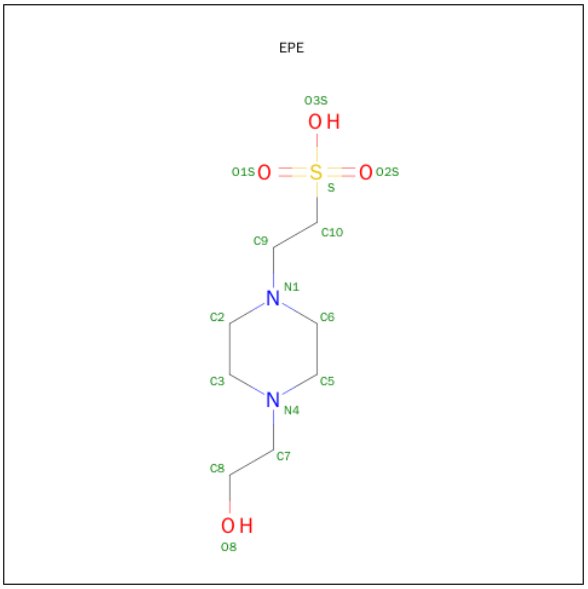
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	11	Total Xe 11 11	0	0
8	A	11	Total Xe 11 11	0	0
8	D	1	Total Xe 1 1	0	0
8	C	1	Total Xe 1 1	0	0

- Molecule 9 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O S 13 7 1 4 1	0	0

- Molecule 10 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 11 is water.

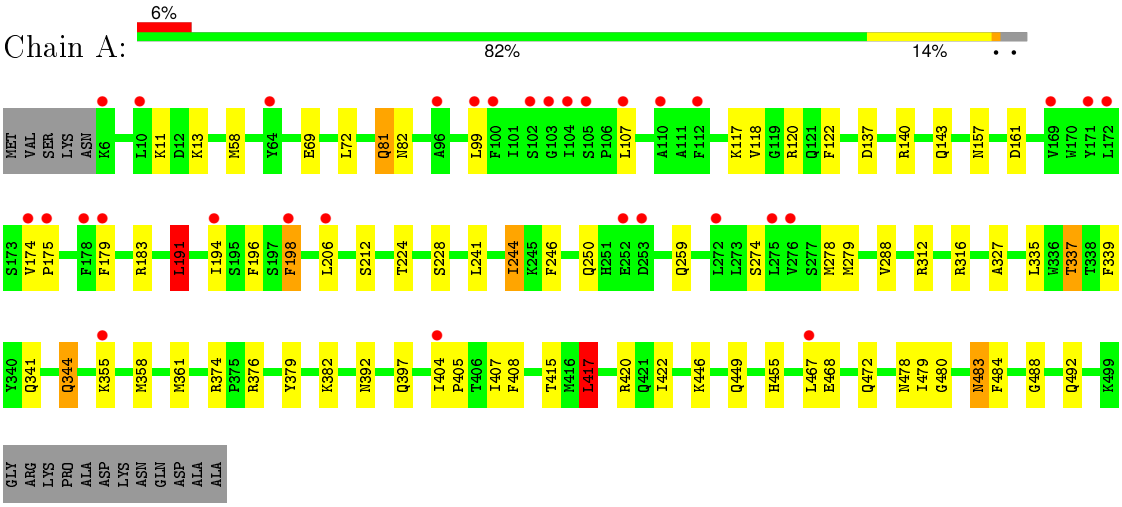
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	160	Total	O	0	0
			160	160		
11	B	139	Total	O	0	0
			139	139		
11	C	118	Total	O	0	0
			118	118		
11	D	99	Total	O	0	0
			99	99		
11	E	40	Total	O	0	0
			40	40		
11	F	32	Total	O	0	0
			32	32		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

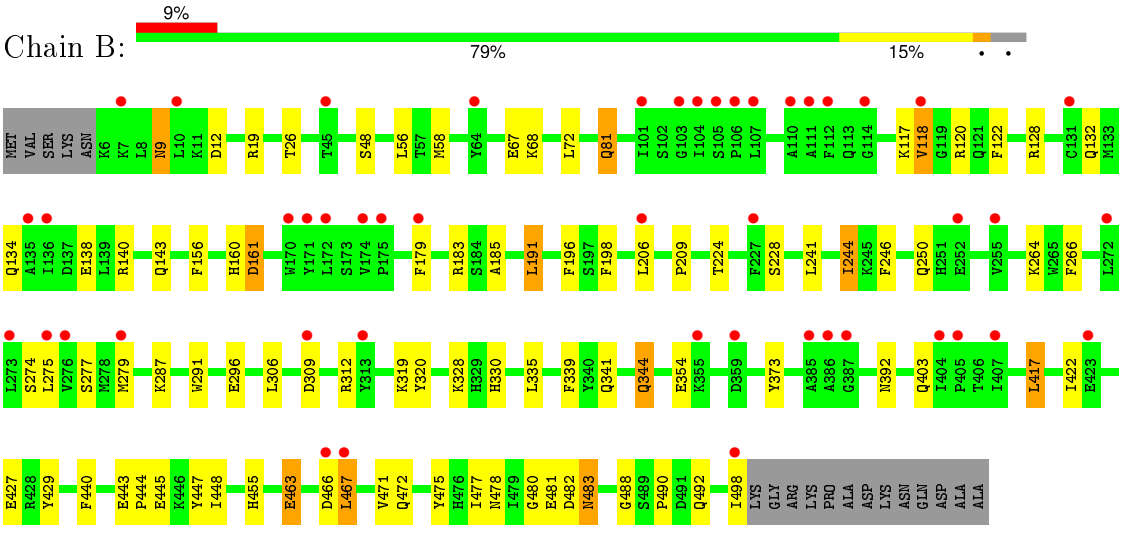
• Molecule 1: Phenol hydroxylase component phN

Chain A:



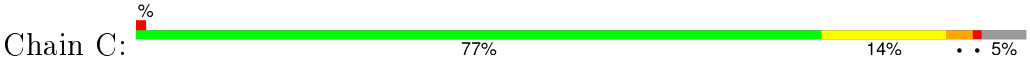
• Molecule 1: Phenol hydroxylase component phN

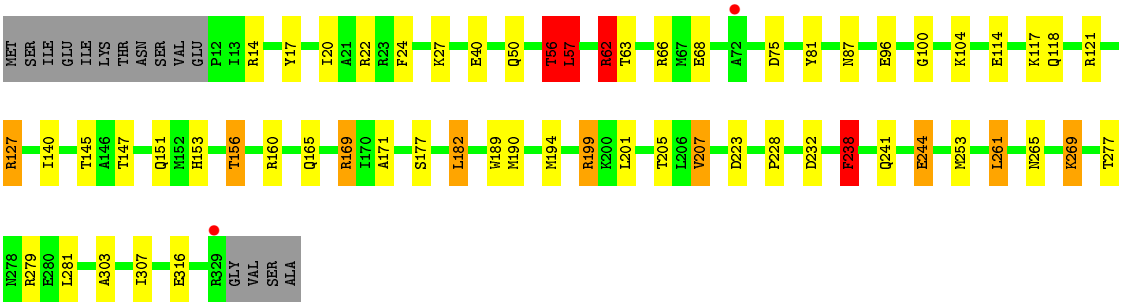
Chain B:



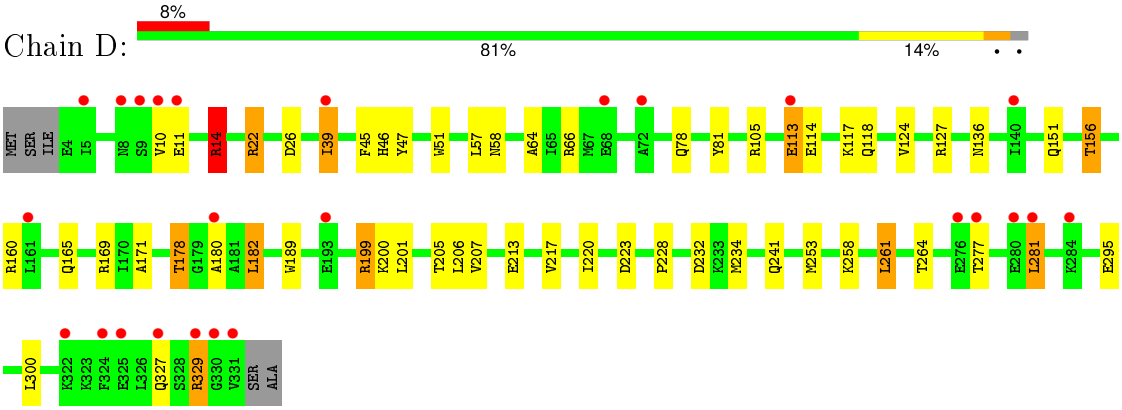
• Molecule 2: Phenol hydroxylase component phL

Chain C:

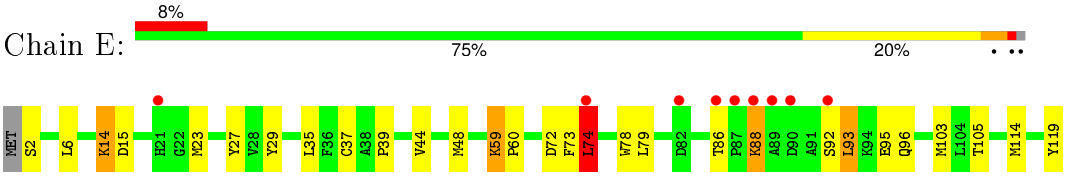




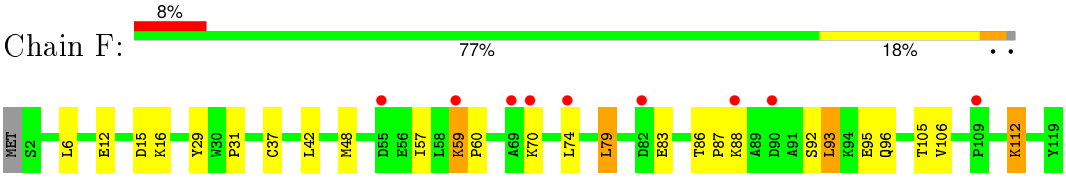
• Molecule 2: Phenol hydroxylase component phL



• Molecule 3: Phenol hydroxylase component phO



• Molecule 3: Phenol hydroxylase component phO



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.94Å 141.76Å 181.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 1.95 39.87 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (38.00-1.95) 92.5 (39.87-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.228 0.188 , 0.184	Depositor DCC
R_{free} test set	7399 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 145806 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16039	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ZN, MPO, XE, FE, EPE, CU

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	0.89	0/4257	0.85	8/5766 (0.1%)
1	B	0.85	3/4244 (0.1%)	0.79	2/5751 (0.0%)
2	C	0.93	6/2648 (0.2%)	1.12	20/3580 (0.6%)
2	D	0.84	0/2718	0.95	13/3676 (0.4%)
3	E	0.83	0/953	0.87	2/1297 (0.2%)
3	F	0.79	0/953	0.76	0/1297
All	All	0.87	9/15773 (0.1%)	0.90	45/21367 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	316	GLU	CB-CG	5.94	1.63	1.52
2	C	238	PHE	CG-CD2	5.80	1.47	1.38
2	C	199	ARG	CD-NE	-5.48	1.37	1.46
1	B	445	GLU	CG-CD	5.48	1.60	1.51
2	C	238	PHE	CE1-CZ	5.41	1.47	1.37
1	B	463	GLU	CG-CD	5.20	1.59	1.51
2	C	62	ARG	CG-CD	5.08	1.64	1.51
2	C	316	GLU	CG-CD	5.04	1.59	1.51
1	B	443	GLU	CG-CD	5.02	1.59	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	199	ARG	NE-CZ-NH2	-22.56	109.02	120.30
2	C	22	ARG	NE-CZ-NH2	-15.90	112.35	120.30
2	D	199	ARG	NE-CZ-NH2	-15.68	112.46	120.30
2	C	199	ARG	NE-CZ-NH1	14.56	127.58	120.30
2	D	22	ARG	NE-CZ-NH2	-11.65	114.48	120.30
2	C	22	ARG	NE-CZ-NH1	11.64	126.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	22	ARG	NE-CZ-NH1	9.65	125.12	120.30
2	D	14	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	C	169	ARG	NE-CZ-NH1	-9.30	115.65	120.30
2	D	169	ARG	NE-CZ-NH2	-8.47	116.06	120.30
2	C	169	ARG	NE-CZ-NH2	8.07	124.33	120.30
2	D	199	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	279	MET	CG-SD-CE	7.59	112.35	100.20
2	C	199	ARG	CG-CD-NE	-7.51	96.03	111.80
2	C	62	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	D	199	ARG	CG-CD-NE	-6.92	97.27	111.80
3	E	74	LEU	CA-CB-CG	6.67	130.64	115.30
2	C	22	ARG	CG-CD-NE	-6.58	97.98	111.80
1	A	137	ASP	CB-CG-OD1	6.47	124.13	118.30
2	C	199	ARG	CD-NE-CZ	6.41	132.58	123.60
1	B	279	MET	CG-SD-CE	6.06	109.90	100.20
2	C	57	LEU	CB-CG-CD1	5.98	121.16	111.00
2	C	127	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	C	279	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	D	14	ARG	NE-CZ-NH1	5.85	123.23	120.30
2	C	56	THR	N-CA-CB	-5.81	99.26	110.30
2	C	75	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	120	ARG	NE-CZ-NH2	-5.67	117.46	120.30
2	D	105	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	D	14	ARG	CG-CD-NE	-5.63	99.97	111.80
1	A	467	LEU	CB-CA-C	5.62	120.87	110.20
1	A	120	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	417	LEU	CB-CG-CD1	5.52	120.38	111.00
2	C	22	ARG	CD-NE-CZ	5.47	131.26	123.60
2	C	261	LEU	CB-CG-CD1	5.45	120.26	111.00
2	C	62	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	420	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	C	127	ARG	NE-CZ-NH1	5.35	122.97	120.30
3	E	72	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	191	LEU	CB-CG-CD1	5.28	119.97	111.00
1	A	99	LEU	CA-CB-CG	5.24	127.35	115.30
2	D	261	LEU	CA-CB-CG	5.15	127.14	115.30
2	D	169	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	D	26	ASP	CB-CG-OD1	5.05	122.85	118.30
2	C	207	VAL	CG1-CB-CG2	5.04	118.96	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4123	0	3866	65	0
1	B	4110	0	3842	82	0
2	C	2589	0	2501	54	0
2	D	2659	0	2571	44	0
3	E	925	0	898	22	0
3	F	925	0	898	13	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	24	0	32	5	0
7	B	12	0	16	1	0
7	C	12	0	16	0	0
7	D	6	0	8	4	0
7	F	6	0	8	0	0
8	A	11	0	0	6	0
8	B	11	0	0	3	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	13	0	11	9	0
10	B	15	0	17	7	0
11	A	160	0	0	2	0
11	B	139	0	0	6	0
11	C	118	0	0	3	0
11	D	99	0	0	3	0
11	E	40	0	0	1	0
11	F	32	0	0	0	0
All	All	16039	0	14684	248	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (248) 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)
3:E:73:PHE:O	3:E:74:LEU:HB2	1.43	1.17
1:A:198:PHE:CE1	8:A:521:XE:XE	2.83	1.09
1:B:118:VAL:HG23	9:B:516:MPO:H61	1.19	1.08
1:A:337:THR:HG21	1:A:376:ARG:HH11	1.14	1.08
2:C:189:TRP:CD1	2:C:190:MET:CE	2.36	1.08
1:A:198:PHE:CD1	8:A:521:XE:XE	2.86	1.07
3:E:73:PHE:O	3:E:74:LEU:CB	2.02	1.04
1:B:183:ARG:HD2	9:B:516:MPO:O1	1.60	0.99
1:B:117:LYS:HD3	9:B:516:MPO:H12	1.43	0.98
1:A:344:GLN:HE21	1:A:344:GLN:H	1.11	0.97
2:C:62:ARG:HG2	2:C:62:ARG:HH11	1.30	0.96
1:A:198:PHE:HE1	8:A:521:XE:XE	2.26	0.94
1:A:337:THR:HG21	1:A:376:ARG:NH1	1.83	0.93
2:C:189:TRP:CD1	2:C:190:MET:HE2	2.04	0.90
1:B:274:SER:HB2	1:B:335:LEU:HD11	1.53	0.90
2:C:194:MET:HE2	2:C:303:ALA:HB2	1.52	0.89
1:B:344:GLN:HE21	1:B:344:GLN:H	1.20	0.88
1:B:196:PHE:CD1	1:B:244:ILE:HG12	2.08	0.88
1:A:408:PHE:HB3	7:A:519:GOL:H11	1.55	0.87
2:C:189:TRP:CD1	2:C:190:MET:HE3	2.10	0.87
1:A:198:PHE:HD1	8:A:521:XE:XE	2.31	0.86
2:C:87:ASN:HB2	11:C:556:HOH:O	1.76	0.85
2:C:189:TRP:HD1	2:C:190:MET:CE	1.86	0.85
1:A:196:PHE:CD1	1:A:244:ILE:HG12	2.10	0.85
1:B:275:LEU:HD12	8:B:521:XE:XE	2.56	0.83
2:C:17:TYR:HB2	2:C:20:ILE:HD12	1.61	0.82
3:F:92:SER:OG	3:F:95:GLU:HG2	1.79	0.82
2:C:189:TRP:HD1	2:C:190:MET:HE3	1.39	0.81
2:D:45:PHE:HB2	7:D:334:GOL:H12	1.63	0.81
1:B:68:LYS:HB2	1:B:68:LYS:HZ2	1.45	0.80
1:A:480:GLY:H	1:A:483:ASN:HD21	1.28	0.80
1:A:58:MET:H	2:C:165:GLN:HE22	1.26	0.80
3:F:59:LYS:HB3	3:F:60:PRO:HD3	1.64	0.79
2:C:62:ARG:CG	2:C:62:ARG:HH11	1.96	0.79
3:E:88:LYS:H	3:E:96:GLN:HE22	1.30	0.78
2:C:194:MET:HE2	2:C:303:ALA:CB	2.14	0.76
1:B:140:ARG:HG3	2:D:81:TYR:CE2	2.20	0.76
11:B:570:HOH:O	2:D:10:VAL:HG11	1.86	0.75
1:A:472:GLN:HE22	1:A:478:ASN:HD22	1.32	0.74
1:B:118:VAL:HG23	9:B:516:MPO:C6	2.10	0.74
1:A:483:ASN:H	1:A:483:ASN:HD22	1.32	0.74
2:C:171:ALA:HB3	2:C:182:LEU:HD13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:OD1	2:C:14:ARG:NH2	2.21	0.74
1:B:480:GLY:H	1:B:483:ASN:HD21	1.34	0.74
1:B:58:MET:H	2:D:165:GLN:HE22	1.36	0.73
2:C:194:MET:CE	2:C:303:ALA:CB	2.68	0.72
2:D:200:LYS:NZ	11:D:496:HOH:O	2.23	0.71
1:A:397:GLN:NE2	3:E:103:MET:HE3	2.05	0.70
1:A:344:GLN:N	1:A:344:GLN:HE21	1.86	0.70
1:B:341:GLN:HE21	1:B:392:ASN:HD22	1.37	0.70
2:C:121:ARG:NH2	2:C:194:MET:HE3	2.08	0.68
2:C:265:ASN:O	2:C:269:LYS:HG3	1.92	0.68
1:A:259:GLN:HE22	1:A:316:ARG:H	1.40	0.67
2:D:329:ARG:HB2	2:D:329:ARG:HH11	1.59	0.67
2:C:62:ARG:HD3	11:C:357:HOH:O	1.94	0.67
1:B:341:GLN:NE2	1:B:392:ASN:HD22	1.92	0.67
1:B:68:LYS:NZ	1:B:68:LYS:CB	2.58	0.67
1:B:81:GLN:NE2	11:B:606:HOH:O	2.26	0.66
2:D:45:PHE:CB	7:D:334:GOL:H12	2.26	0.66
1:A:341:GLN:HE21	1:A:392:ASN:HD22	1.42	0.66
1:B:68:LYS:CB	1:B:68:LYS:HZ2	2.06	0.66
1:A:397:GLN:HE22	3:E:103:MET:HE3	1.60	0.65
3:F:48:MET:HG2	3:F:93:LEU:HD22	1.78	0.65
1:B:160:HIS:HD2	11:B:535:HOH:O	1.79	0.65
1:B:185:ALA:O	9:B:516:MPO:H51	1.97	0.65
1:A:488:GLY:H	1:A:492:GLN:NE2	1.96	0.64
2:C:56:THR:HG22	2:C:57:LEU:O	1.98	0.64
2:D:10:VAL:HG12	2:D:11:GLU:N	2.13	0.64
1:A:72:LEU:HD12	1:A:224:THR:HG22	1.81	0.63
2:D:160:ARG:NH1	2:D:223:ASP:OD2	2.32	0.63
1:A:143:GLN:HE22	2:C:151:GLN:HE22	1.47	0.63
2:C:56:THR:CG2	2:C:57:LEU:O	2.47	0.62
2:C:100:GLY:O	2:C:104:LYS:HD3	1.99	0.62
1:B:483:ASN:HD22	1:B:483:ASN:H	1.47	0.62
1:B:472:GLN:HE22	1:B:478:ASN:HD22	1.46	0.62
2:D:47:TYR:O	7:D:334:GOL:H11	1.99	0.62
1:B:140:ARG:HG2	2:D:81:TYR:CD2	2.35	0.62
1:B:156:PHE:O	2:D:14:ARG:NH2	2.33	0.62
1:A:196:PHE:CE1	1:A:244:ILE:HG12	2.35	0.62
3:F:12:GLU:OE2	3:F:16:LYS:NZ	2.25	0.61
1:B:68:LYS:HZ1	1:B:140:ARG:NH2	1.99	0.61
2:C:171:ALA:CB	2:C:182:LEU:HD13	2.31	0.61
1:B:330:HIS:HD2	1:B:373:TYR:OH	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:CD	9:B:516:MPO:H12	2.27	0.61
1:A:117:LYS:CE	7:A:517:GOL:H11	2.31	0.60
1:A:327:ALA:HB2	7:A:519:GOL:H31	1.83	0.60
1:A:274:SER:HB2	1:A:335:LEU:HD11	1.83	0.60
2:C:62:ARG:CG	2:C:62:ARG:NH1	2.63	0.60
2:C:62:ARG:HG2	2:C:62:ARG:NH1	2.09	0.59
1:B:19:ARG:HD2	10:B:517:EPE:H32	1.84	0.59
1:A:455:HIS:HD2	3:E:15:ASP:OD1	1.84	0.59
1:A:143:GLN:HE22	2:C:151:GLN:NE2	2.01	0.58
3:E:92:SER:OG	3:E:95:GLU:HG2	2.03	0.58
1:A:341:GLN:NE2	1:A:392:ASN:HD22	2.02	0.58
1:B:19:ARG:CD	10:B:517:EPE:H32	2.34	0.57
2:C:118:GLN:HE22	2:C:241:GLN:HE21	1.50	0.57
1:B:196:PHE:CE1	1:B:244:ILE:HG12	2.39	0.57
2:C:62:ARG:CD	11:C:357:HOH:O	2.51	0.56
1:A:397:GLN:NE2	3:E:103:MET:CE	2.67	0.56
1:A:339:PHE:CZ	8:A:522:XE:XE	3.37	0.56
2:D:171:ALA:HB3	2:D:182:LEU:HD13	1.88	0.56
1:A:122:PHE:CZ	1:A:191:LEU:HD22	2.41	0.56
1:A:397:GLN:HE22	3:E:103:MET:CE	2.18	0.55
1:B:117:LYS:HG2	9:B:516:MPO:H62	1.87	0.55
1:B:9:ASN:C	1:B:9:ASN:HD22	2.08	0.55
1:A:358:MET:CE	1:A:374:ARG:HG3	2.37	0.55
1:B:160:HIS:HE1	1:B:482:ASP:OD1	1.89	0.54
1:B:206:LEU:O	1:B:209:PRO:HD2	2.08	0.54
2:D:136:ASN:HD21	2:D:206:LEU:HD23	1.71	0.54
1:A:337:THR:HG23	11:E:122:HOH:O	2.06	0.54
1:A:259:GLN:NE2	1:A:316:ARG:H	2.04	0.54
1:B:296:GLU:OE1	1:B:328:LYS:HE3	2.07	0.54
1:B:341:GLN:HE22	3:F:37:CYS:H	1.55	0.54
2:C:194:MET:CE	2:C:303:ALA:HB2	2.28	0.53
1:A:69:GLU:OE1	1:A:140:ARG:NH1	2.41	0.53
11:B:573:HOH:O	2:D:39:ILE:HD11	2.08	0.53
1:B:480:GLY:H	1:B:483:ASN:ND2	2.04	0.53
1:A:58:MET:H	2:C:165:GLN:NE2	2.02	0.53
1:A:468:GLU:HG3	1:A:479:ILE:HD13	1.91	0.53
2:D:234:MET:HE1	2:D:300:LEU:HG	1.91	0.53
1:B:330:HIS:CD2	1:B:373:TYR:OH	2.61	0.53
9:B:516:MPO:H11	2:D:51:TRP:CZ2	2.44	0.52
2:C:121:ARG:HH22	2:C:194:MET:HE3	1.75	0.52
1:B:160:HIS:CD2	11:B:535:HOH:O	2.59	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:TYR:C	7:D:334:GOL:H11	2.30	0.52
1:B:472:GLN:HE22	1:B:478:ASN:ND2	2.07	0.52
1:B:274:SER:O	1:B:335:LEU:HD13	2.10	0.52
1:B:344:GLN:HE21	1:B:344:GLN:N	1.98	0.52
2:D:118:GLN:HE22	2:D:241:GLN:NE2	2.08	0.52
3:E:73:PHE:O	3:E:74:LEU:HB3	2.02	0.51
1:B:455:HIS:HD2	3:F:15:ASP:OD2	1.92	0.51
2:C:194:MET:HE1	2:C:303:ALA:CB	2.40	0.51
1:B:140:ARG:CG	2:D:81:TYR:CD2	2.94	0.51
3:E:88:LYS:H	3:E:96:GLN:NE2	2.05	0.51
1:B:488:GLY:H	1:B:492:GLN:NE2	2.08	0.51
2:D:45:PHE:CZ	2:D:58:ASN:HB2	2.46	0.51
1:B:198:PHE:HE2	7:B:519:GOL:H32	1.76	0.51
1:A:13:LYS:NZ	2:C:177:SER:OG	2.44	0.51
1:B:140:ARG:CG	2:D:81:TYR:CE2	2.93	0.50
1:B:48:SER:HA	10:B:517:EPE:H31	1.92	0.50
2:C:40:GLU:HG2	2:C:145:THR:O	2.12	0.50
2:C:156:THR:O	2:C:160:ARG:HG2	2.12	0.50
1:B:9:ASN:ND2	1:B:12:ASP:H	2.09	0.50
1:B:417:LEU:HD22	3:F:29:TYR:CE2	2.47	0.49
1:B:68:LYS:NZ	1:B:140:ARG:NH2	2.61	0.49
1:A:212:SER:OG	1:A:288:VAL:HG11	2.13	0.49
1:B:122:PHE:CZ	1:B:191:LEU:HD22	2.47	0.49
1:B:26:THR:CB	2:D:199:ARG:HH22	2.25	0.49
2:D:10:VAL:CG1	2:D:11:GLU:N	2.76	0.49
1:B:481:GLU:HA	1:B:490:PRO:HG2	1.95	0.48
2:D:118:GLN:HE22	2:D:241:GLN:HE21	1.59	0.48
1:B:140:ARG:NH1	11:B:576:HOH:O	2.47	0.48
2:D:156:THR:O	2:D:160:ARG:HG2	2.12	0.48
2:D:189:TRP:CZ2	2:D:199:ARG:HG3	2.48	0.48
2:C:118:GLN:HE22	2:C:241:GLN:NE2	2.09	0.48
2:C:244:GLU:H	2:C:244:GLU:HG3	1.36	0.48
2:D:171:ALA:CB	2:D:182:LEU:HD13	2.44	0.48
1:A:122:PHE:CE2	1:A:191:LEU:HD22	2.48	0.48
1:B:134:GLN:O	1:B:138:GLU:HG2	2.13	0.48
1:B:422:ILE:HD11	1:B:440:PHE:CE2	2.48	0.48
1:A:449:GLN:O	3:E:14:LYS:HG3	2.14	0.48
1:B:477:ILE:HG23	1:B:482:ASP:HB2	1.96	0.47
3:E:48:MET:HG2	3:E:93:LEU:HD22	1.95	0.47
1:A:405:PRO:HB2	1:A:407:ILE:HG23	1.96	0.47
2:C:160:ARG:NH1	2:C:223:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LYS:HE3	1:B:447:TYR:OH	2.14	0.47
1:A:341:GLN:HE22	3:E:37:CYS:H	1.63	0.47
1:B:140:ARG:HG3	2:D:81:TYR:CZ	2.50	0.47
1:B:143:GLN:HE22	2:D:151:GLN:HE22	1.62	0.47
2:C:171:ALA:HB3	2:C:182:LEU:CD1	2.40	0.47
2:D:178:THR:CG2	2:D:180:ALA:H	2.29	0.46
2:D:66:ARG:NH2	11:D:353:HOH:O	2.48	0.46
2:D:136:ASN:ND2	2:D:206:LEU:HD23	2.31	0.46
3:E:79:LEU:HB2	3:E:105:THR:HB	1.97	0.46
1:B:274:SER:HB2	1:B:335:LEU:CD1	2.36	0.46
2:C:194:MET:HE1	2:C:303:ALA:HB1	1.98	0.46
2:D:124:VAL:O	2:D:127:ARG:HG2	2.16	0.46
2:C:201:LEU:O	2:C:205:THR:HG23	2.16	0.46
2:C:63:THR:O	2:C:66:ARG:NH2	2.49	0.46
2:C:118:GLN:HB3	2:C:238:PHE:HZ	1.81	0.45
1:A:244:ILE:H	1:A:244:ILE:HG13	1.70	0.45
3:E:59:LYS:HB3	3:E:60:PRO:HD3	1.98	0.45
1:B:244:ILE:HG13	1:B:244:ILE:H	1.69	0.45
2:C:228:PRO:O	2:C:232:ASP:HB3	2.17	0.45
1:B:309:ASP:OD1	1:B:312:ARG:NH1	2.50	0.45
1:B:48:SER:HB2	10:B:517:EPE:H31	1.99	0.45
1:B:403:GLN:HE22	2:D:46:HIS:CD2	2.34	0.45
2:C:140:ILE:HG21	2:C:153:HIS:CD2	2.52	0.45
1:A:417:LEU:HD22	3:E:29:TYR:CE2	2.51	0.45
3:F:79:LEU:HB2	3:F:105:THR:HB	1.99	0.45
1:A:183:ARG:HD2	11:A:621:HOH:O	2.17	0.45
1:A:81:GLN:HE21	1:A:82:ASN:HD21	1.64	0.45
1:A:379:TYR:CD1	3:E:114:MET:CE	2.99	0.45
1:A:140:ARG:CD	2:C:81:TYR:CE2	2.99	0.44
1:B:319:LYS:HG2	1:B:320:TYR:CD1	2.52	0.44
1:B:339:PHE:CZ	8:B:522:XE:XE	3.48	0.44
1:A:483:ASN:N	1:A:483:ASN:HD22	2.00	0.44
3:F:31:PRO:HD2	3:F:106:VAL:O	2.18	0.44
9:B:516:MPO:H11	2:D:51:TRP:HZ2	1.83	0.44
2:D:78:GLN:NE2	11:D:404:HOH:O	2.36	0.44
2:D:228:PRO:O	2:D:232:ASP:HB2	2.18	0.44
1:A:278:MET:SD	1:A:339:PHE:CD1	3.11	0.44
3:E:74:LEU:H	3:E:78:TRP:HE1	1.66	0.44
1:B:444:PRO:O	1:B:448:ILE:HG23	2.18	0.44
3:F:92:SER:O	3:F:96:GLN:HG2	2.18	0.43
2:C:96:GLU:CD	2:C:169:ARG:HH12	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:THR:HG23	2:C:57:LEU:O	2.17	0.43
2:C:96:GLU:OE1	2:C:169:ARG:NH1	2.48	0.43
1:A:174:VAL:HB	1:A:175:PRO:CD	2.49	0.43
2:D:201:LEU:O	2:D:205:THR:HG23	2.17	0.43
1:A:194:ILE:O	1:A:198:PHE:HB3	2.19	0.42
3:F:42:LEU:HD13	3:F:57:ILE:HG21	2.01	0.42
1:A:404:ILE:HG23	8:A:522:XE:XE	2.97	0.42
1:B:306:LEU:O	1:B:309:ASP:HB3	2.18	0.42
1:A:246:PHE:O	1:A:250:GLN:HG2	2.17	0.42
1:A:117:LYS:HE3	7:A:517:GOL:H11	1.99	0.42
2:C:189:TRP:CE2	2:C:199:ARG:HG3	2.55	0.42
2:D:113:GLU:O	2:D:117:LYS:HD3	2.19	0.42
1:B:483:ASN:N	1:B:483:ASN:HD22	2.12	0.42
1:A:122:PHE:CE2	1:A:191:LEU:CD2	3.03	0.42
1:B:48:SER:CB	10:B:517:EPE:H31	2.50	0.42
1:A:472:GLN:HE22	1:A:478:ASN:ND2	2.10	0.42
2:D:213:GLU:O	2:D:217:VAL:HG23	2.20	0.42
1:B:19:ARG:HD3	10:B:517:EPE:H32	2.02	0.41
2:C:189:TRP:O	2:C:199:ARG:HD2	2.20	0.41
1:B:19:ARG:HH21	10:B:517:EPE:H32	1.85	0.41
2:C:24:PHE:O	2:C:27:LYS:HE3	2.21	0.41
1:A:446:LYS:NZ	2:C:50:GLN:NE2	2.68	0.41
2:D:220:ILE:CD1	2:D:264:THR:HB	2.50	0.41
3:E:39:PRO:HB3	3:E:103:MET:HE2	2.02	0.41
1:B:427:GLU:HB2	1:B:429:TYR:CE2	2.56	0.41
1:B:246:PHE:O	1:B:250:GLN:HG2	2.20	0.41
1:A:483:ASN:O	1:A:484:PHE:HB2	2.20	0.41
1:B:72:LEU:HD12	1:B:224:THR:HG22	2.02	0.41
3:F:86:THR:HA	3:F:87:PRO:HD2	1.97	0.41
1:A:455:HIS:CE1	3:E:27:TYR:OH	2.74	0.41
2:D:64:ALA:HB3	2:D:281:LEU:HD11	2.03	0.41
1:A:408:PHE:CB	7:A:519:GOL:H11	2.40	0.40
1:B:266:PHE:HB2	8:B:528:XE:XE	3.00	0.40
1:A:337:THR:HG22	11:A:613:HOH:O	2.21	0.40
1:B:471:VAL:O	1:B:475:TYR:HB2	2.21	0.40
1:B:128:ARG:O	1:B:132:GLN:HG3	2.21	0.40
1:B:277:SER:HB2	1:B:291:TRP:CG	2.56	0.40
2:C:40:GLU:HG3	2:C:147:THR:OG1	2.21	0.40
1:B:466:ASP:O	1:B:467:LEU:HB2	2.21	0.40
1:B:161:ASP:OD1	2:D:22:ARG:NH2	2.48	0.40
3:E:35:LEU:HA	3:E:119:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:112:LYS:HE2	3:F:112:LYS:HB3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	492/511 (96%)	477 (97%)	15 (3%)	0	100 100
1	B	491/511 (96%)	473 (96%)	17 (4%)	1 (0%)	52 43
2	C	316/333 (95%)	313 (99%)	3 (1%)	0	100 100
2	D	326/333 (98%)	319 (98%)	7 (2%)	0	100 100
3	E	116/119 (98%)	113 (97%)	2 (2%)	1 (1%)	21 9
3	F	116/119 (98%)	111 (96%)	5 (4%)	0	100 100
All	All	1857/1926 (96%)	1806 (97%)	49 (3%)	2 (0%)	56 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	74	LEU
1	B	467	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	434/447 (97%)	412 (95%)	22 (5%)	29 13
1	B	432/447 (97%)	414 (96%)	18 (4%)	36 21
2	C	272/285 (95%)	254 (93%)	18 (7%)	21 7
2	D	280/285 (98%)	263 (94%)	17 (6%)	23 9
3	E	98/99 (99%)	88 (90%)	10 (10%)	9 2
3	F	98/99 (99%)	89 (91%)	9 (9%)	11 3
All	All	1614/1662 (97%)	1520 (94%)	94 (6%)	25 10

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	81	GLN
1	A	107	LEU
1	A	118	VAL
1	A	161	ASP
1	A	179	PHE
1	A	191	LEU
1	A	198	PHE
1	A	206	LEU
1	A	228	SER
1	A	241	LEU
1	A	244	ILE
1	A	312	ARG
1	A	337	THR
1	A	344	GLN
1	A	355	LYS
1	A	361	MET
1	A	382	LYS
1	A	415	THR
1	A	417	LEU
1	A	422	ILE
1	A	483	ASN
1	B	9	ASN
1	B	56	LEU
1	B	67	GLU
1	B	81	GLN
1	B	118	VAL
1	B	161	ASP
1	B	179	PHE
1	B	191	LEU

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Mol	Chain	Res	Type
1	B	228	SER
1	B	241	LEU
1	B	244	ILE
1	B	287	LYS
1	B	344	GLN
1	B	354	GLU
1	B	417	LEU
1	B	463	GLU
1	B	483	ASN
1	B	498	ILE
2	C	56	THR
2	C	57	LEU
2	C	62	ARG
2	C	68	GLU
2	C	114	GLU
2	C	117	LYS
2	C	127	ARG
2	C	156	THR
2	C	182	LEU
2	C	207	VAL
2	C	238	PHE
2	C	244	GLU
2	C	253	MET
2	C	261	LEU
2	C	269	LYS
2	C	277	THR
2	C	281	LEU
2	C	307	ILE
2	D	14	ARG
2	D	39	ILE
2	D	57	LEU
2	D	113	GLU
2	D	114	GLU
2	D	156	THR
2	D	178	THR
2	D	182	LEU
2	D	207	VAL
2	D	253	MET
2	D	258	LYS
2	D	261	LEU
2	D	277	THR
2	D	281	LEU

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Mol	Chain	Res	Type
2	D	295	GLU
2	D	327	GLN
2	D	329	ARG
3	E	2	SER
3	E	6	LEU
3	E	14	LYS
3	E	23	MET
3	E	44	VAL
3	E	59	LYS
3	E	74	LEU
3	E	86	THR
3	E	88	LYS
3	E	93	LEU
3	F	6	LEU
3	F	59	LYS
3	F	70	LYS
3	F	74	LEU
3	F	79	LEU
3	F	83	GLU
3	F	88	LYS
3	F	93	LEU
3	F	112	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	49	GLN
1	A	65	GLN
1	A	81	GLN
1	A	87	ASN
1	A	153	ASN
1	A	259	GLN
1	A	334	GLN
1	A	341	GLN
1	A	344	GLN
1	A	393	ASN
1	A	397	GLN
1	A	400	GLN
1	A	455	HIS
1	A	478	ASN
1	A	483	ASN

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Mol	Chain	Res	Type
1	A	492	GLN
1	B	9	ASN
1	B	15	GLN
1	B	28	GLN
1	B	81	GLN
1	B	153	ASN
1	B	160	HIS
1	B	164	HIS
1	B	330	HIS
1	B	341	GLN
1	B	344	GLN
1	B	393	ASN
1	B	400	GLN
1	B	455	HIS
1	B	478	ASN
1	B	483	ASN
1	B	492	GLN
2	C	50	GLN
2	C	137	ASN
2	C	151	GLN
2	C	165	GLN
2	C	219	ASN
2	C	241	GLN
2	D	46	HIS
2	D	50	GLN
2	D	136	ASN
2	D	137	ASN
2	D	151	GLN
2	D	165	GLN
2	D	219	ASN
2	D	241	GLN
3	E	96	GLN

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 44 ligands modelled in this entry, 32 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
7	GOL	A	516	4	5,5,5	0.36	0	5,5,5	1.20	0
7	GOL	A	517	-	5,5,5	0.40	0	5,5,5	1.39	1 (20%)
7	GOL	A	518	-	5,5,5	0.30	0	5,5,5	0.39	0
7	GOL	A	519	-	5,5,5	0.58	0	5,5,5	1.08	0
9	MPO	B	516	-	12,13,13	4.39	3 (25%)	15,17,17	6.88	8 (53%)
10	EPE	B	517	-	14,15,15	0.47	0	18,20,20	2.21	6 (33%)
7	GOL	B	518	-	5,5,5	0.35	0	5,5,5	0.37	0
7	GOL	B	519	4	5,5,5	0.27	0	5,5,5	0.82	0
7	GOL	C	334	-	5,5,5	0.39	0	5,5,5	0.56	0
7	GOL	C	335	-	5,5,5	0.48	0	5,5,5	0.77	0
7	GOL	D	334	-	5,5,5	0.58	0	5,5,5	1.21	0
7	GOL	F	120	-	5,5,5	0.27	0	5,5,5	0.59	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
7	GOL	A	516	4	-	0/4/4/4	0/0/0/0
7	GOL	A	517	-	-	0/4/4/4	0/0/0/0
7	GOL	A	518	-	-	0/4/4/4	0/0/0/0
7	GOL	A	519	-	-	0/4/4/4	0/0/0/0
9	MPO	B	516	-	-	0/7/15/15	0/1/1/1
10	EPE	B	517	-	-	0/9/19/19	0/1/1/1
7	GOL	B	518	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	519	4	-	0/4/4/4	0/0/0/0
7	GOL	C	334	-	-	0/4/4/4	0/0/0/0
7	GOL	C	335	-	-	0/4/4/4	0/0/0/0
7	GOL	D	334	-	-	0/4/4/4	0/0/0/0
7	GOL	F	120	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	516	MPO	C3-N1	-11.34	1.20	1.47
9	B	516	MPO	C7-N1	-7.64	1.26	1.46
9	B	516	MPO	C2-C3	-6.06	1.25	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	517	GOL	C3-C2-C1	-2.72	100.44	111.12
9	B	516	MPO	C5-C4-N1	-2.17	106.84	110.12
10	B	517	EPE	O8-C8-C7	-2.10	101.63	111.28
10	B	517	EPE	C3-C2-N1	-2.07	106.93	110.63
10	B	517	EPE	C7-N4-C5	2.33	117.24	111.27
10	B	517	EPE	C7-N4-C3	2.47	117.61	111.27
9	B	516	MPO	O2-S1-C1	2.65	109.17	106.91
9	B	516	MPO	C3-N1-C4	3.46	120.14	111.27
9	B	516	MPO	C3-N1-C7	3.48	120.18	111.27
9	B	516	MPO	C6-C7-N1	3.87	115.99	110.12
9	B	516	MPO	C3-C2-C1	4.29	119.44	112.37
10	B	517	EPE	C5-N4-C3	4.47	118.57	108.90
9	B	516	MPO	C7-N1-C4	4.97	119.67	108.90
10	B	517	EPE	O1S-S-C10	6.16	112.16	106.91
9	B	516	MPO	C2-C3-N1	24.67	175.95	113.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	517	GOL	2	0
7	A	519	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	516	MPO	9	0
10	B	517	EPE	7	0
7	B	519	GOL	1	0
7	D	334	GOL	4	0

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^{th} 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^2)	Q<0.9
1	A	494/511 (96%)	0.24	31 (6%) 23 33	15, 24, 37, 51	0
1	B	493/511 (96%)	0.44	47 (9%) 10 17	18, 28, 41, 54	0
2	C	318/333 (95%)	0.09	2 (0%) 90 94	16, 24, 35, 58	0
2	D	328/333 (98%)	0.41	25 (7%) 17 26	18, 28, 46, 71	0
3	E	118/119 (99%)	0.33	9 (7%) 17 26	19, 32, 42, 46	0
3	F	118/119 (99%)	0.49	9 (7%) 17 26	22, 35, 47, 53	0
All	All	1869/1926 (97%)	0.32	123 (6%) 22 31	15, 27, 42, 71	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	331	VAL	7.3
2	D	10	VAL	7.2
1	B	386	ALA	6.1
2	D	9	SER	5.7
2	D	8	ASN	5.0
2	D	11	GLU	4.6
2	D	324	PHE	4.5
3	E	21	HIS	4.2
1	A	64	TYR	4.1
1	B	385	ALA	3.9
1	B	107	LEU	3.8
1	B	498	ILE	3.7
1	A	6	LYS	3.6
1	B	313	TYR	3.6
1	B	467	LEU	3.6
1	B	103	GLY	3.5
2	D	280	GLU	3.5
1	B	276	VAL	3.4
1	A	275	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	275	LEU	3.4
3	F	74	LEU	3.4
2	D	327	GLN	3.4
1	A	99	LEU	3.4
1	A	355	LYS	3.3
1	A	174	VAL	3.3
1	A	175	PRO	3.3
1	B	104	ILE	3.2
1	A	104	ILE	3.1
2	D	325	GLU	3.1
1	B	273	LEU	3.1
1	B	64	TYR	3.1
1	B	355	LYS	3.1
1	B	466	ASP	3.1
3	E	88	LYS	3.0
1	B	131	CYS	3.0
1	B	404	ILE	3.0
1	B	175	PRO	2.9
1	B	309	ASP	2.9
1	A	169	VAL	2.9
1	B	252	GLU	2.9
1	B	135	ALA	2.9
1	B	172	LEU	2.8
1	B	112	PHE	2.8
1	A	103	GLY	2.8
1	B	387	GLY	2.8
1	A	272	LEU	2.8
3	F	90	ASP	2.8
1	A	172	LEU	2.8
1	B	110	ALA	2.8
2	D	276	GLU	2.8
1	A	179	PHE	2.8
3	F	88	LYS	2.8
3	E	89	ALA	2.7
1	A	206	LEU	2.7
1	B	407	ILE	2.7
1	A	178	PHE	2.7
1	A	107	LEU	2.7
3	F	59	LYS	2.7
2	C	72	ALA	2.7
1	A	100	PHE	2.7
1	B	10	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	F	69	ALA	2.6
1	B	101	ILE	2.6
2	D	281	LEU	2.6
1	A	404	ILE	2.6
3	E	90	ASP	2.6
1	B	118	VAL	2.6
2	D	329	ARG	2.6
2	D	5	ILE	2.6
1	A	253	ASP	2.6
1	B	171	TYR	2.5
1	B	106	PRO	2.5
1	B	179	PHE	2.5
1	A	102	SER	2.5
1	B	105	SER	2.5
1	B	111	ALA	2.5
2	D	113	GLU	2.5
3	F	70	LYS	2.5
1	A	105	SER	2.4
2	D	322	LYS	2.4
2	D	39	ILE	2.4
1	B	227	PHE	2.4
2	D	330	GLY	2.4
3	F	82	ASP	2.3
3	E	87	PRO	2.3
1	B	7	LYS	2.3
1	A	276	VAL	2.3
2	D	180	ALA	2.3
1	A	198	PHE	2.3
3	F	109	PRO	2.3
1	B	136	ILE	2.3
1	A	110	ALA	2.3
1	B	255	VAL	2.3
3	E	92	SER	2.3
2	D	277	THR	2.3
1	B	114	GLY	2.2
1	A	194	ILE	2.2
2	D	68	GLU	2.2
1	A	171	TYR	2.2
1	A	252	GLU	2.2
3	E	86	THR	2.2
1	B	405	PRO	2.2
1	A	10	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	72	ALA	2.2
1	A	112	PHE	2.2
1	B	206	LEU	2.2
1	A	96	ALA	2.1
1	A	467	LEU	2.1
1	B	423	GLU	2.1
2	D	193	GLU	2.1
3	E	82	ASP	2.1
3	E	74	LEU	2.1
2	D	284	LYS	2.1
2	D	140	ILE	2.1
2	D	161	LEU	2.1
2	C	329	ARG	2.1
1	B	170	TRP	2.1
1	B	272	LEU	2.1
1	B	45	THR	2.1
1	B	174	VAL	2.0
1	B	279	MET	2.0
1	B	359	ASP	2.0
3	F	55	ASP	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^{th} 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^2)	Q<0.9
7	GOL	D	334	6/6	0.93	0.30	7.28	22,35,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	EPE	B	517	15/15	0.62	0.28	4.52	47,68,82,82	0
7	GOL	A	519	6/6	0.93	0.21	3.60	30,36,37,38	0
7	GOL	A	516	6/6	0.89	0.31	3.36	37,40,43,44	0
8	XE	A	520	1/1	0.88	0.33	2.84	49,49,49,49	1
8	XE	B	520	1/1	0.94	0.30	2.80	56,56,56,56	1
7	GOL	B	518	6/6	0.63	0.26	2.45	59,65,68,70	0
8	XE	B	521	1/1	0.95	0.33	2.37	53,53,53,53	1
7	GOL	A	517	6/6	0.90	0.20	1.88	32,40,42,42	0
7	GOL	B	519	6/6	0.93	0.25	1.61	43,45,46,50	0
9	MPO	B	516	13/13	0.84	0.22	1.38	50,54,67,69	0
7	GOL	A	518	6/6	0.94	0.11	0.62	30,33,34,36	0
8	XE	A	530	1/1	0.88	0.12	0.59	53,53,53,53	1
8	XE	B	530	1/1	0.92	0.12	0.11	50,50,50,50	1
4	FE	A	513	1/1	0.96	0.14	-0.01	34,34,34,34	0
7	GOL	C	335	6/6	0.96	0.11	-0.02	25,32,36,39	0
4	FE	B	513	1/1	0.97	0.13	-0.31	36,36,36,36	0
4	FE	B	512	1/1	1.00	0.13	-0.36	31,31,31,31	0
4	FE	A	512	1/1	0.99	0.12	-0.82	33,33,33,33	0
7	GOL	F	120	6/6	0.96	0.07	-1.01	31,35,36,38	0
5	ZN	A	514	1/1	1.00	0.09	-1.10	19,19,19,19	0
5	ZN	B	514	1/1	0.99	0.09	-1.17	23,23,23,23	0
6	CU	B	515	1/1	0.98	0.04	-1.26	33,33,33,33	0
8	XE	B	524	1/1	0.96	0.05	-1.52	45,45,45,45	0
8	XE	D	335	1/1	0.99	0.03	-1.57	49,49,49,49	0
8	XE	B	527	1/1	0.97	0.06	-1.71	46,46,46,46	1
8	XE	B	525	1/1	0.99	0.03	-1.74	44,44,44,44	0
8	XE	B	526	1/1	0.99	0.02	-1.75	49,49,49,49	0
8	XE	A	526	1/1	0.98	0.03	-1.78	48,48,48,48	0
8	XE	A	525	1/1	1.00	0.03	-1.78	40,40,40,40	0
8	XE	B	529	1/1	0.98	0.05	-1.80	43,43,43,43	0
6	CU	A	515	1/1	0.99	0.04	-1.87	32,32,32,32	0
8	XE	A	527	1/1	0.99	0.03	-1.89	44,44,44,44	1
8	XE	B	522	1/1	0.96	0.15	-2.00	46,46,46,46	1
8	XE	A	524	1/1	0.95	0.05	-2.05	42,42,42,42	0
8	XE	A	522	1/1	0.95	0.10	-2.07	42,42,42,42	1
8	XE	A	521	1/1	0.98	0.10	-2.27	47,47,47,47	1
8	XE	A	528	1/1	0.99	0.04	-2.42	36,36,36,36	0
8	XE	A	529	1/1	0.99	0.03	-2.54	41,41,41,41	0
8	XE	B	528	1/1	1.00	0.03	-3.39	40,40,40,40	0
8	XE	C	336	1/1	0.99	0.02	-5.34	41,41,41,41	0
8	XE	B	523	1/1	0.99	0.04	-	37,37,37,37	0
8	XE	A	523	1/1	0.99	0.05	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	GOL	C	334	6/6	0.74	0.19	-	48,55,56,58	0

6.5 Other polymers (i)

There are no such residues in this entry.