



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 PM UTC

PDB ID : 3U52 / pdb_00003u52
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

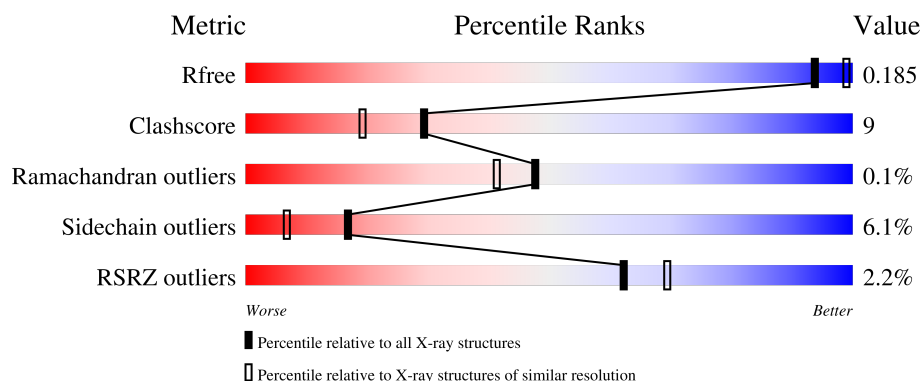
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	511	0% 81% 14% . .
1	B	511	2% 79% 15% . .
2	C	333	0% 77% 14% . 5%
2	D	333	5% 82% 13% . .
3	E	119	3% 75% 20% . .

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Mol	Chain	Length	Quality of chain
3	F	119	

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	-
7	GOL	D	334	-	-	X	-
8	XE	A	521	-	-	X	-
8	XE	A	522	-	-	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 (CCD ID: FE) (formula: Fe).

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

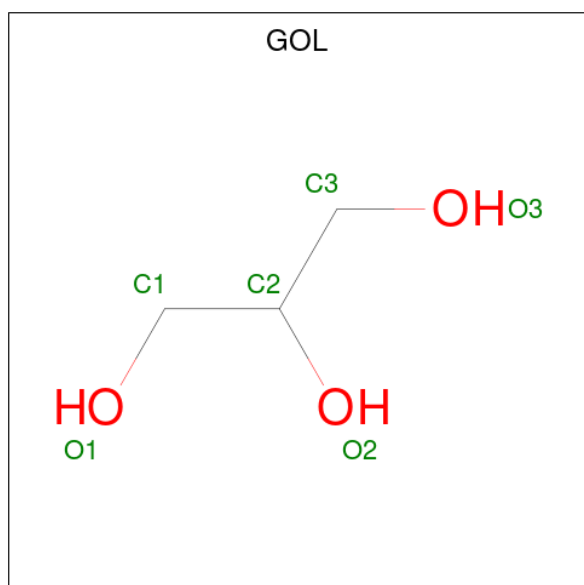
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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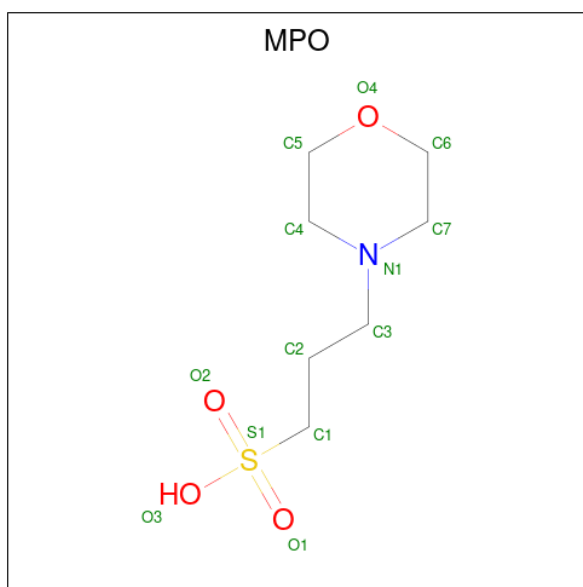
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is XENON (CCD ID: XE) (formula: Xe).

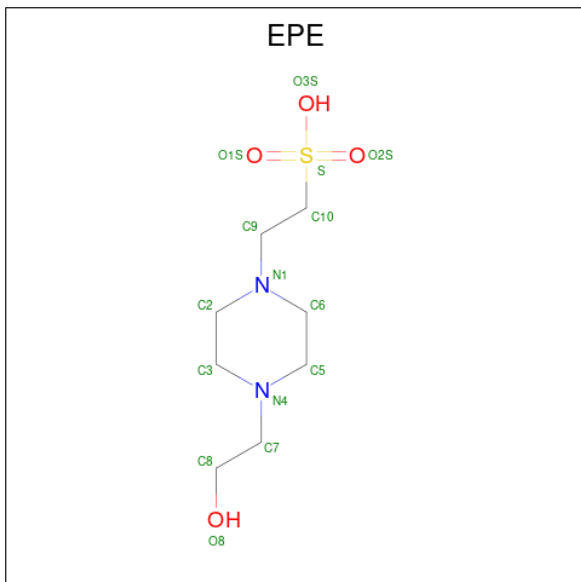
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total	Xe	0	0
			11	11		
8	B	11	Total	Xe	0	0
			11	11		
8	C	1	Total	Xe	0	0
			1	1		
8	D	1	Total	Xe	0	0
			1	1		

- Molecule 9 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: C₇H₁₅NO₄S).



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

- Molecule 10 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: 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		

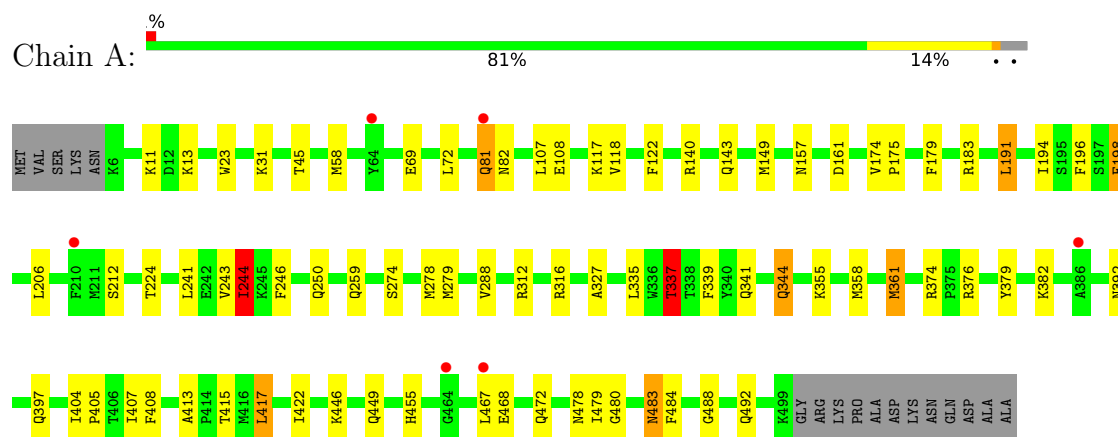
- Molecule 11 is water.

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		

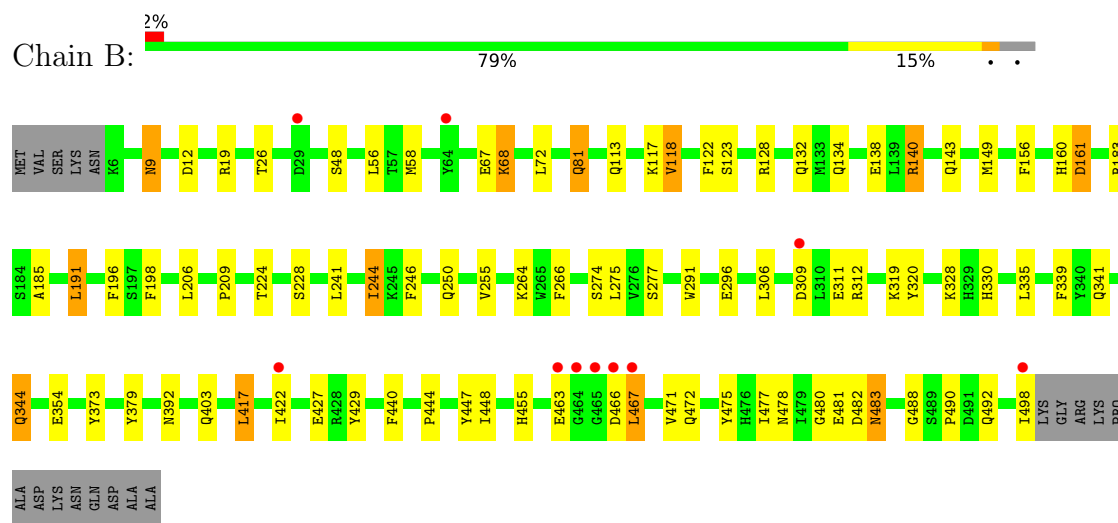
3 Residue-property plots

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

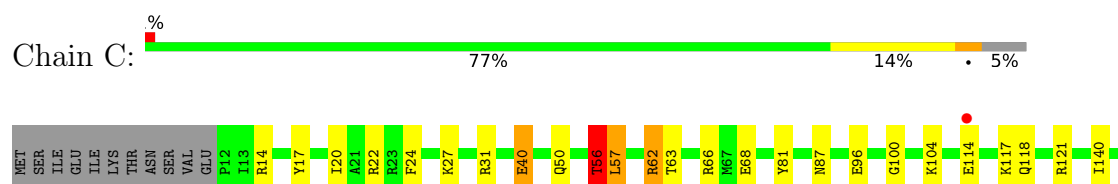
• Molecule 1: Phenol hydroxylase component pHN

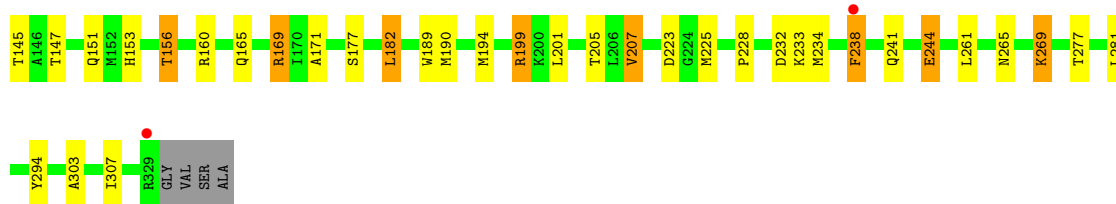


• Molecule 1: Phenol hydroxylase component pHN

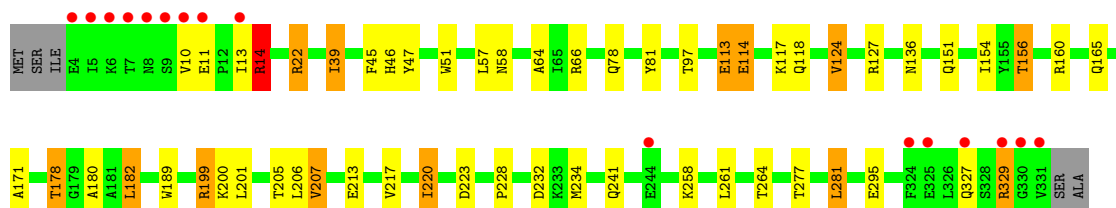
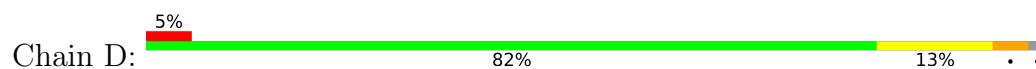


• Molecule 2: Phenol hydroxylase component pHL

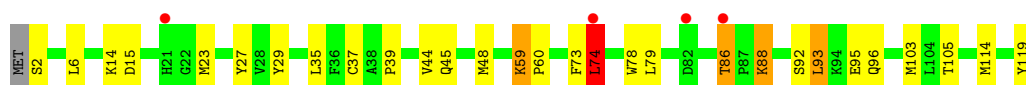
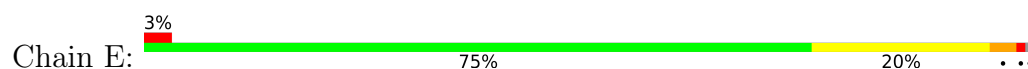




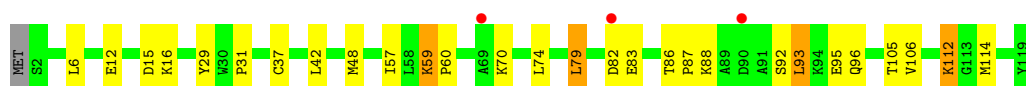
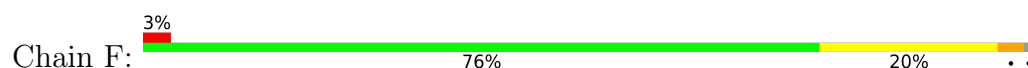
• Molecule 2: Phenol hydroxylase component phL



• Molecule 3: Phenol hydroxylase component phO



• Molecule 3: Phenol hydroxylase component phO



4 Data and refinement statistics

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 38.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (38.00-1.95) 92.5 (38.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.228 (Not available) , 0.185	Depositor DCC
R_{free} test set	7399 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, FE, EPE, ZN, MPO, XE, GOL

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	1.06	2/4257 (0.0%)	1.07	9/5766 (0.2%)
1	B	0.99	1/4244 (0.0%)	1.03	3/5751 (0.1%)
2	C	1.08	1/2648 (0.0%)	1.16	12/3580 (0.3%)
2	D	1.04	2/2718 (0.1%)	1.07	6/3676 (0.2%)
3	E	1.00	1/953 (0.1%)	1.05	1/1297 (0.1%)
3	F	0.93	0/953	0.94	0/1297
All	All	1.03	7/15773 (0.0%)	1.07	31/21367 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	VAL	CA-CB	8.49	1.58	1.54
1	A	243	VAL	CA-CB	6.54	1.61	1.54
2	C	199	ARG	CD-NE	-6.51	1.37	1.46
2	D	220	ILE	CA-CB	6.34	1.60	1.55
2	D	124	VAL	CA-CB	6.14	1.58	1.53
1	A	337	THR	CA-C	5.71	1.60	1.52
3	E	74	LEU	N-CA	5.68	1.53	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	199	ARG	NE-CZ-NH2	-11.31	109.02	119.20
2	C	56	THR	N-CA-CB	-7.82	99.26	110.44
1	A	108	GLU	N-CA-C	-7.65	102.94	111.28
2	C	22	ARG	NE-CZ-NH2	-7.61	112.35	119.20
2	D	199	ARG	NE-CZ-NH2	-7.49	112.46	119.20
3	E	86	THR	CB-CA-C	7.29	118.27	110.17
2	C	199	ARG	CG-CD-NE	-7.26	96.03	112.00
1	A	413	ALA	CA-C-N	7.09	127.24	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ALA	C-N-CA	7.09	127.24	119.87
2	C	207	VAL	N-CA-CB	-7.05	103.16	112.26
1	A	337	THR	CB-CA-C	6.92	122.28	110.79
2	C	207	VAL	CB-CA-C	6.91	119.76	111.20
2	D	207	VAL	N-CA-CB	-6.82	103.46	112.26
2	D	199	ARG	CG-CD-NE	-6.70	97.27	112.00
2	C	22	ARG	CG-CD-NE	-6.37	97.98	112.00
2	C	199	ARG	NE-CZ-NH1	6.08	127.58	121.50
2	C	169	ARG	NE-CZ-NH1	-5.85	115.65	121.50
2	C	199	ARG	CD-NE-CZ	5.84	132.58	124.40
2	D	207	VAL	CB-CA-C	5.71	118.28	111.20
2	C	169	ARG	NE-CZ-NH2	5.71	124.33	119.20
1	B	113	GLN	N-CA-C	5.66	117.12	111.07
1	A	244	ILE	N-CA-CB	5.58	118.94	110.58
2	D	14	ARG	CG-CD-NE	-5.47	99.97	112.00
1	A	361	MET	N-CA-C	5.36	117.12	111.28
2	D	22	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	A	467	LEU	CB-CA-C	5.21	120.87	109.99
1	A	279	MET	CG-SD-CE	5.20	112.35	100.90
1	B	123	SER	CA-C-N	-5.11	117.75	122.29
1	B	123	SER	C-N-CA	-5.11	117.75	122.29
2	C	233	LYS	N-CA-C	5.08	116.62	111.14
1	A	244	ILE	CB-CA-C	-5.02	105.29	112.22

There are no chirality outliers.

There are no planarity outliers.

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	4123	0	3866	70	0
1	B	4110	0	3842	84	0
2	C	2589	0	2501	58	0
2	D	2659	0	2571	45	0
3	E	925	0	898	23	0
3	F	925	0	898	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	0
8	B	11	0	0	4	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	3	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	258	0

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

All (258) 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
2:C:189:TRP:HD1	2:C:190:MET:HE3	1.19	1.06
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
2:C:194:MET:HE2	2:C:303:ALA:HB2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HD3	9:B:516:MPO:H12	1.43	0.98
2:C:189:TRP:CD1	2:C:190:MET:HE3	1.97	0.98
1:A:344:GLN:H	1:A:344:GLN:HE21	1.11	0.97
2:C:62:ARG:HH11	2:C:62:ARG:HG2	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:194:MET:HE2	2:C:303:ALA:CB	2.00	0.91
1:B:274:SER:HB2	1:B:335:LEU:HD11	1.53	0.90
1:B:344:GLN:H	1:B:344:GLN:HE21	1.20	0.88
1:A:379:TYR:CD1	3:E:114:MET:HE1	2.09	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
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
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: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:HH11	2:C:62:ARG:CG	1.96	0.79
3:E:88:LYS:H	3:E:96:GLN:HE22	1.30	0.78
1:B:140:ARG:HG3	2:D:81:TYR:CE2	2.20	0.76
2:C:189:TRP:CD1	2:C:190:MET:HE2	2.18	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:A:483:ASN:H	1:A:483:ASN:HD22	1.32	0.74
1:B:118:VAL:HG23	9:B:516:MPO:C6	2.10	0.74
2:C:171:ALA:HB3	2:C:182:LEU:HD13	1.69	0.74
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	0.71
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:HE21	1:A:344:GLN:N	1.86	0.70
1:B:341:GLN:HE21	1:B:392:ASN:HD22	1.37	0.70
2:C:265:ASN:O	2:C:269:LYS:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:HE22	1:A:316:ARG:H	1.40	0.67
2:C:225:MET:HE1	2:C:294:TYR:HA	1.77	0.67
2:D:329:ARG:HH11	2:D:329:ARG:HB2	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:CB	1:B:68:LYS:NZ	2.58	0.67
1:B:81:GLN:NE2	11:B:606:HOH:O	2.26	0.66
1:A:341:GLN:HE21	1:A:392:ASN:HD22	1.42	0.66
2:D:45:PHE:CB	7:D:334:GOL:H12	2.26	0.66
1:B:68:LYS:HZ2	1:B:68:LYS:CB	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
1:A:31:LYS:NZ	11:A:573:HOH:O	2.30	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
1:A:143:GLN:HE22	2:C:151:GLN:HE22	1.47	0.63
1:A:149:MET:HE3	8:A:527:XE:XE	2.76	0.63
2:D:160:ARG:NH1	2:D:223:ASP:OD2	2.32	0.63
1:B:379:TYR:CD1	3:F:114:MET:HE1	2.33	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
1:B:140:ARG:HG2	2:D:81:TYR:CD2	2.35	0.62
2:D:47:TYR:O	7:D:334:GOL:H11	1.99	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
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
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:274:SER:HB2	1:A:335:LEU:HD11	1.83	0.60
1:A:327:ALA:HB2	7:A:519:GOL:H31	1.83	0.60
2:C:62:ARG:CG	2:C:62:ARG:NH1	2.63	0.60
1:B:9:ASN:C	1:B:9:ASN:HD22	2.08	0.59
2:C:62:ARG:HG2	2:C:62:ARG:NH1	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:HIS:HD2	3:E:15:ASP:OD1	1.84	0.59
1:B:19:ARG:HD2	10:B:517:EPE:H32	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
2:C:121:ARG:NH2	2:C:194:MET:HE3	2.20	0.57
2:D:47:TYR:C	7:D:334:GOL:H11	2.30	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:B:149:MET:HE3	8:B:527:XE:XE	2.83	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: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
3:F:12:GLU:OE2	3:F:16:LYS:NZ	2.25	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
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
1:B:160:HIS:CD2	11:B:535:HOH:O	2.59	0.52
1:B:472:GLN:HE22	1:B:478:ASN:ND2	2.07	0.52
2:C:121:ARG:NH1	2:C:194:MET:HE1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:198:PHE:HE2	7:B:519:GOL:H32	1.76	0.51
2:D:45:PHE:CZ	2:D:58:ASN:HB2	2.46	0.51
1:A:13:LYS:NZ	2:C:177:SER:OG	2.44	0.51
1:B:48:SER:HA	10:B:517:EPE:H31	1.92	0.50
1:B:140:ARG:CG	2:D:81:TYR:CE2	2.93	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
2:C:189:TRP:HD1	2:C:190:MET:CE	1.86	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:A:23:TRP:CD1	2:C:190:MET:HE1	2.48	0.49
1:B:26:THR:CB	2:D:199:ARG:HH22	2.25	0.49
1:B:122:PHE:CZ	1:B:191:LEU:HD22	2.47	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
1:A:379:TYR:HD1	3:E:114:MET:HE1	1.73	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:C:96:GLU:CD	2:C:169:ARG:HH12	2.21	0.48
1:A:122:PHE:CE2	1:A:191:LEU:HD22	2.48	0.48
2:D:171:ALA:CB	2:D:182:LEU:HD13	2.44	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
1:A:405:PRO:HB2	1:A:407:ILE:HG23	1.96	0.47
3:E:48:MET:HG2	3:E:93:LEU:HD22	1.95	0.47
1:B:264:LYS:HE3	1:B:447:TYR:OH	2.14	0.47
2:C:160:ARG:NH1	2:C:223:ASP:OD2	2.46	0.47
1:A:341:GLN:HE22	3:E:37:CYS:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:66:ARG:NH2	11:D:353:HOH:O	2.48	0.46
2:D:178:THR:CG2	2:D:180:ALA:H	2.29	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: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:H	1:B:244:ILE:HG13	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
2:C:234:MET:HE3	2:C:234:MET:HB2	1.76	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: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
2:D:234:MET:HE3	2:D:234:MET:HB2	1.90	0.44
1:A:483:ASN:HD22	1:A:483:ASN:N	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
1:B:444:PRO:O	1:B:448:ILE:HG23	2.18	0.44
3:E:74:LEU:H	3:E:78:TRP:HE1	1.66	0.44
2:D:114:GLU:CD	2:D:114:GLU:H	2.25	0.43
3:F:92:SER:O	3:F:96:GLN:HG2	2.18	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:121:ARG:HH22	2:C:194:MET:HE3	1.83	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:246:PHE:O	1:A:250:GLN:HG2	2.17	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: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:A:122:PHE:CE2	1:A:191:LEU:CD2	3.03	0.42
1:B:483:ASN:HD22	1:B:483:ASN:N	2.12	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
1:B:19:ARG:HH21	10:B:517:EPE:H32	1.85	0.41
2:C:189:TRP:O	2:C:199:ARG:HD2	2.20	0.41
1:A:446:LYS:NZ	2:C:50:GLN:NE2	2.68	0.41
1:A:446:LYS:HZ2	2:C:50:GLN:HE22	1.68	0.41
2:C:24:PHE:O	2:C:27:LYS:HE3	2.21	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:246:PHE:O	1:B:250:GLN:HG2	2.20	0.41
1:B:427:GLU:HB2	1:B:429:TYR:CE2	2.56	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:C:40:GLU:CD	2:C:40:GLU:H	2.29	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:128:ARG:O	1:B:132:GLN:HG3	2.21	0.40
1:B:471:VAL:O	1:B:475:TYR:HB2	2.21	0.40
1:B:277:SER:HB2	1:B:291:TRP:CG	2.56	0.40
1:B:161:ASP:OD1	2:D:22:ARG:NH2	2.48	0.40
1:B:466:ASP:O	1:B:467:LEU:HB2	2.21	0.40
2:C:40:GLU:HG3	2:C:147:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:35:LEU:HA	3:E:119:TYR:CE2	2.56	0.40
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%)	43	36
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%)	14	6
3	F	116/119 (98%)	111 (96%)	5 (4%)	0	100	100
All	All	1857/1926 (96%)	1806 (97%)	49 (3%)	2 (0%)	48	41

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%)	21	10
1	B	432/447 (97%)	413 (96%)	19 (4%)	25	15
2	C	272/285 (95%)	254 (93%)	18 (7%)	15	5
2	D	280/285 (98%)	261 (93%)	19 (7%)	14	5
3	E	98/99 (99%)	88 (90%)	10 (10%)	7	1
3	F	98/99 (99%)	88 (90%)	10 (10%)	7	1
All	All	1614/1662 (97%)	1516 (94%)	98 (6%)	17	7

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	45	THR
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	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	68	LYS
1	B	81	GLN
1	B	118	VAL
1	B	140	ARG
1	B	161	ASP

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Mol	Chain	Res	Type
1	B	191	LEU
1	B	228	SER
1	B	241	LEU
1	B	244	ILE
1	B	311	GLU
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	31	ARG
2	C	40	GLU
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	156	THR
2	C	182	LEU
2	C	207	VAL
2	C	238	PHE
2	C	244	GLU
2	C	261	LEU
2	C	269	LYS
2	C	277	THR
2	C	281	LEU
2	C	307	ILE
2	D	13	ILE
2	D	14	ARG
2	D	39	ILE
2	D	57	LEU
2	D	97	THR
2	D	113	GLU
2	D	114	GLU
2	D	154	ILE
2	D	156	THR
2	D	178	THR
2	D	182	LEU
2	D	207	VAL
2	D	258	LYS

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Mol	Chain	Res	Type
2	D	261	LEU
2	D	277	THR
2	D	281	LEU
2	D	295	GLU
2	D	327	GLN
2	D	329	ARG
3	E	2	SER
3	E	6	LEU
3	E	23	MET
3	E	44	VAL
3	E	45	GLN
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	82	ASP
3	F	83	GLU
3	F	88	LYS
3	F	93	LEU
3	F	112	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	65	GLN
1	A	81	GLN
1	A	87	ASN
1	A	259	GLN
1	A	334	GLN
1	A	341	GLN
1	A	344	GLN
1	A	424	HIS
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	160	HIS
1	B	164	HIS
1	B	166	HIS
1	B	330	HIS
1	B	341	GLN
1	B	344	GLN
1	B	393	ASN
1	B	400	GLN
1	B	403	GLN
1	B	424	HIS
1	B	455	HIS
1	B	472	GLN
1	B	483	ASN
1	B	492	GLN
2	C	15	HIS
2	C	50	GLN
2	C	87	ASN
2	C	92	GLN
2	C	137	ASN
2	C	151	GLN
2	C	165	GLN
2	C	219	ASN
2	C	241	GLN
2	D	50	GLN
2	D	92	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
2	D	288	HIS
3	E	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	518	-	5,5,5	0.35	0	5,5,5	0.46	0
7	GOL	A	519	-	5,5,5	0.59	0	5,5,5	1.13	0
7	GOL	A	516	4	5,5,5	0.43	0	5,5,5	1.28	0
7	GOL	C	334	-	5,5,5	0.43	0	5,5,5	0.58	0
7	GOL	D	334	-	5,5,5	0.65	0	5,5,5	1.29	0
7	GOL	B	518	-	5,5,5	0.40	0	5,5,5	0.39	0
10	EPE	B	517	-	15,15,15	1.04	1 (6%)	19,20,20	1.82	5 (26%)
9	MPO	B	516	-	13,13,13	4.88	5 (38%)	17,17,17	5.79	6 (35%)
7	GOL	A	517	-	5,5,5	0.39	0	5,5,5	1.56	1 (20%)
7	GOL	F	120	-	5,5,5	0.29	0	5,5,5	0.62	0
7	GOL	B	519	4	5,5,5	0.28	0	5,5,5	0.89	0
7	GOL	C	335	-	5,5,5	0.48	0	5,5,5	0.83	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	518	-	-	2/4/4/4	-
7	GOL	A	519	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	516	4	-	2/4/4/4	-
7	GOL	C	334	-	-	2/4/4/4	-
7	GOL	D	334	-	-	3/4/4/4	-
7	GOL	B	518	-	-	0/4/4/4	-
10	EPE	B	517	-	-	3/9/19/19	0/1/1/1
9	MPO	B	516	-	-	5/7/15/15	0/1/1/1
7	GOL	A	517	-	-	0/4/4/4	-
7	GOL	F	120	-	-	0/4/4/4	-
7	GOL	B	519	4	-	2/4/4/4	-
7	GOL	C	335	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	516	MPO	C3-N1	-11.72	1.20	1.47
9	B	516	MPO	C1-S1	-7.87	1.66	1.77
9	B	516	MPO	C7-N1	-7.72	1.26	1.46
9	B	516	MPO	C2-C3	-6.55	1.25	1.51
10	B	517	EPE	C10-S	3.53	1.82	1.77
9	B	516	MPO	O2-S1	2.14	1.51	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	516	MPO	C2-C3-N1	22.06	175.95	113.93
9	B	516	MPO	C7-N1-C4	5.03	119.67	108.84
10	B	517	EPE	C5-N4-C3	4.52	118.57	108.84
9	B	516	MPO	C6-C7-N1	3.86	115.99	110.12
10	B	517	EPE	O1S-S-C10	3.60	112.16	106.73
9	B	516	MPO	C3-N1-C7	3.36	120.18	111.24
9	B	516	MPO	C3-N1-C4	3.34	120.14	111.24
7	A	517	GOL	C3-C2-C1	-3.10	100.44	111.80
10	B	517	EPE	C7-N4-C3	2.39	117.61	111.24
10	B	517	EPE	O8-C8-C7	-2.33	101.63	111.22
10	B	517	EPE	C7-N4-C5	2.25	117.24	111.24
9	B	516	MPO	C5-C4-N1	-2.16	106.84	110.12

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	516	GOL	C1-C2-C3-O3
7	A	519	GOL	C1-C2-C3-O3
7	A	519	GOL	O2-C2-C3-O3
7	B	519	GOL	C1-C2-C3-O3
7	C	334	GOL	O1-C1-C2-C3
7	C	335	GOL	O1-C1-C2-C3
7	D	334	GOL	C1-C2-C3-O3
7	D	334	GOL	O2-C2-C3-O3
10	B	517	EPE	S-C10-C9-N1
9	B	516	MPO	C2-C1-S1-O3
7	B	519	GOL	O2-C2-C3-O3
9	B	516	MPO	S1-C1-C2-C3
7	A	518	GOL	C1-C2-C3-O3
7	A	519	GOL	O1-C1-C2-C3
7	A	519	GOL	O1-C1-C2-O2
10	B	517	EPE	C8-C7-N4-C5
7	A	516	GOL	O2-C2-C3-O3
7	C	334	GOL	O1-C1-C2-O2
9	B	516	MPO	C2-C1-S1-O1
9	B	516	MPO	C2-C1-S1-O2
7	C	335	GOL	O1-C1-C2-O2
10	B	517	EPE	N4-C7-C8-O8
9	B	516	MPO	C2-C3-N1-C7
7	A	518	GOL	O2-C2-C3-O3
7	D	334	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	519	GOL	3	0
7	D	334	GOL	4	0
10	B	517	EPE	7	0
9	B	516	MPO	9	0
7	A	517	GOL	2	0
7	B	519	GOL	1	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, 95th 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%)	-0.14	6 (1%) 76 82	15, 24, 37, 51	0
1	B	493/511 (96%)	0.08	10 (2%) 65 72	18, 28, 41, 54	0
2	C	318/333 (95%)	-0.09	3 (0%) 81 85	16, 24, 35, 58	0
2	D	328/333 (98%)	0.20	16 (4%) 35 41	18, 28, 46, 71	0
3	E	118/119 (99%)	0.43	4 (3%) 48 54	19, 32, 42, 46	0
3	F	118/119 (99%)	0.56	3 (2%) 58 65	22, 35, 47, 53	0
All	All	1869/1926 (97%)	0.07	42 (2%) 62 69	15, 27, 42, 71	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	331	VAL	7.9
1	B	467	LEU	5.0
2	D	10	VAL	4.6
1	B	498	ILE	4.5
3	E	21	HIS	4.4
2	D	5	ILE	4.3
2	D	4	GLU	4.0
1	B	309	ASP	3.7
3	F	82	ASP	3.4
1	A	64	TYR	3.2
1	B	466	ASP	3.1
3	F	69	ALA	3.1
2	D	6	LYS	3.0
2	C	238	PHE	3.0
1	A	464	GLY	3.0
1	B	64	TYR	2.9
1	A	467	LEU	2.9
2	C	329	ARG	2.8
1	A	81	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	74	LEU	2.7
2	D	325	GLU	2.7
2	D	330	GLY	2.6
2	C	114	GLU	2.5
2	D	9	SER	2.5
2	D	7	THR	2.5
2	D	329	ARG	2.4
2	D	244	GLU	2.4
3	E	82	ASP	2.3
1	A	386	ALA	2.3
1	A	210	PHE	2.2
2	D	324	PHE	2.2
1	B	29	ASP	2.2
2	D	11	GLU	2.2
1	B	422	ILE	2.2
2	D	13	ILE	2.2
1	B	465	GLY	2.2
2	D	327	GLN	2.1
1	B	464	GLY	2.1
3	F	90	ASP	2.1
3	E	86	THR	2.0
1	B	463	GLU	2.0
2	D	8	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	EPE	B	517	15/15	0.75	0.21	47,68,82,82	0
7	GOL	C	334	6/6	0.77	0.19	48,55,56,58	0
9	MPO	B	516	13/13	0.85	0.16	50,54,67,69	0
7	GOL	B	518	6/6	0.85	0.18	59,65,68,70	0
7	GOL	B	519	6/6	0.86	0.13	43,45,46,50	0
7	GOL	A	516	6/6	0.86	0.10	37,40,43,44	0
7	GOL	A	517	6/6	0.89	0.12	32,40,42,42	0
8	XE	A	530	1/1	0.89	0.09	53,53,53,53	1
7	GOL	A	519	6/6	0.90	0.19	30,36,37,38	0
8	XE	A	520	1/1	0.91	0.16	49,49,49,49	1
8	XE	B	521	1/1	0.91	0.12	53,53,53,53	1
7	GOL	F	120	6/6	0.92	0.11	31,35,36,38	0
8	XE	B	522	1/1	0.92	0.08	46,46,46,46	1
8	XE	B	530	1/1	0.92	0.08	50,50,50,50	1
7	GOL	A	518	6/6	0.92	0.09	30,33,34,36	0
7	GOL	D	334	6/6	0.92	0.20	22,35,41,44	0
8	XE	B	520	1/1	0.93	0.14	56,56,56,56	1
4	FE	B	513	1/1	0.94	0.04	36,36,36,36	0
7	GOL	C	335	6/6	0.94	0.09	25,32,36,39	0
8	XE	A	522	1/1	0.95	0.09	42,42,42,42	1
8	XE	B	529	1/1	0.97	0.09	43,43,43,43	0
4	FE	A	513	1/1	0.97	0.04	34,34,34,34	0
8	XE	A	524	1/1	0.97	0.09	42,42,42,42	0
8	XE	B	524	1/1	0.97	0.10	45,45,45,45	0
8	XE	B	523	1/1	0.98	0.07	37,37,37,37	0
8	XE	A	527	1/1	0.98	0.12	44,44,44,44	1
8	XE	B	527	1/1	0.98	0.06	46,46,46,46	1
8	XE	A	521	1/1	0.98	0.10	47,47,47,47	1
6	CU	B	515	1/1	0.98	0.04	33,33,33,33	0
6	CU	A	515	1/1	0.98	0.07	32,32,32,32	0
8	XE	A	526	1/1	0.98	0.09	48,48,48,48	0
5	ZN	B	514	1/1	0.99	0.02	23,23,23,23	0
8	XE	A	528	1/1	0.99	0.06	36,36,36,36	0
8	XE	B	525	1/1	0.99	0.08	44,44,44,44	0
8	XE	B	526	1/1	0.99	0.09	49,49,49,49	0
8	XE	A	529	1/1	0.99	0.09	41,41,41,41	0
8	XE	B	528	1/1	0.99	0.09	40,40,40,40	0
8	XE	A	523	1/1	0.99	0.05	32,32,32,32	0
4	FE	B	512	1/1	0.99	0.03	31,31,31,31	0
8	XE	C	336	1/1	0.99	0.10	41,41,41,41	0
8	XE	D	335	1/1	0.99	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	XE	A	525	1/1	0.99	0.10	40,40,40,40	0
4	FE	A	512	1/1	0.99	0.03	33,33,33,33	0
5	ZN	A	514	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.