



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:23 AM GMT

PDB ID : 4EV5
Title : Crystal structure of copper amine oxidase-1 from Hansenula polymorpha in complex with benzylamine
Authors : Klema, V.J.; Solheid, C.J.; Wilmot, C.M.
Deposited on : 2012-04-25
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

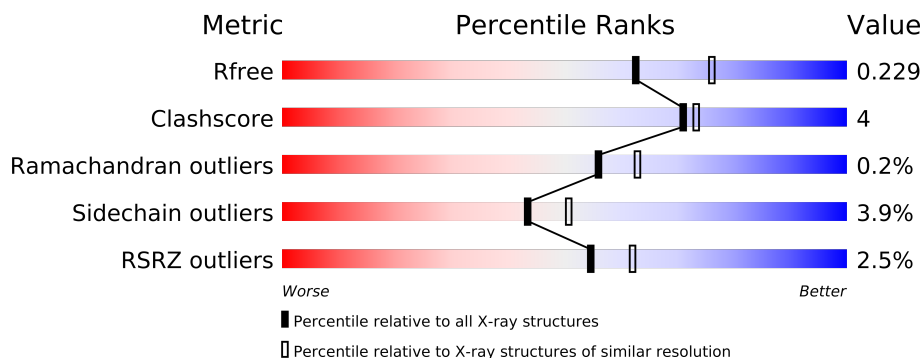
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	692	
1	B	692	
1	C	692	
1	D	692	
1	E	692	
1	F	692	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	703	-	X
2	GOL	A	705	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	706	-	X
2	GOL	B	701	-	X
2	GOL	B	704	-	X
2	GOL	B	705	-	X
2	GOL	C	703	-	X
2	GOL	C	704	-	X
2	GOL	C	706	-	X
2	GOL	C	707	-	X
2	GOL	D	702	-	X
2	GOL	D	703	-	X
2	GOL	D	704	-	X
2	GOL	D	705	-	X
2	GOL	E	702	-	X
2	GOL	E	703	-	X
2	GOL	E	704	-	X
2	GOL	F	702	-	X
2	GOL	F	703	-	X
2	GOL	F	704	-	X
2	GOL	F	706	-	X
4	PEO	B	708	-	X
4	PEO	F	707	-	X

2 Entry composition

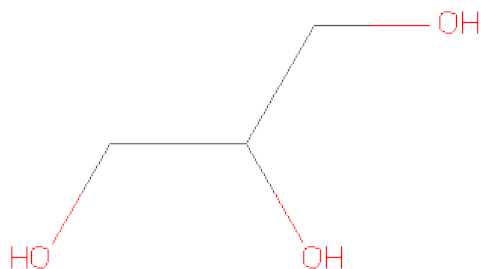
There are 6 unique types of molecules in this entry. The entry contains 34660 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	11	0
			5227	3333	891	979	24			
1	B	655	Total	C	N	O	S	0	8	0
			5227	3328	897	977	25			
1	C	655	Total	C	N	O	S	0	10	0
			5228	3330	891	981	26			
1	D	655	Total	C	N	O	S	0	8	0
			5223	3325	896	977	25			
1	E	654	Total	C	N	O	S	0	13	0
			5245	3343	899	978	25			
1	F	655	Total	C	N	O	S	0	8	0
			5227	3330	896	975	26			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

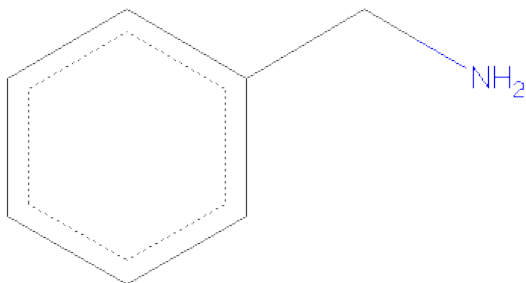
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Cu 1 1	0	0
3	E	1	Total Cu 1 1	0	0
3	B	1	Total Cu 1 1	0	0
3	C	1	Total Cu 1 1	0	0
3	A	1	Total Cu 1 1	0	0
3	F	1	Total Cu 1 1	0	0

- Molecule 4 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	B	1	Total O 2 2	0	0
4	E	1	Total O 2 2	0	0
4	F	1	Total O 2 2	0	0

- Molecule 5 is BENZYLAMINE (three-letter code: ABN) (formula: C₇H₉N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 8 7 1	0	0
5	B	1	Total C N 8 7 1	0	0
5	C	1	Total C N 8 7 1	0	0
5	D	1	Total C N 8 7 1	0	0
5	E	1	Total C N 8 7 1	0	0
5	F	1	Total C N 8 7 1	0	0

- Molecule 6 is water.

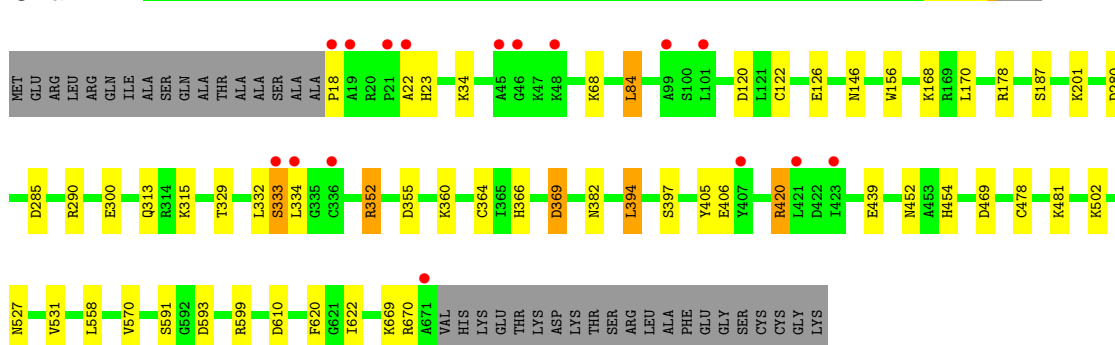
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	527	Total O 529 529	0	2
6	B	579	Total O 583 583	0	4
6	C	497	Total O 499 499	0	2
6	D	462	Total O 465 465	0	3
6	E	460	Total O 462 462	0	2
6	F	501	Total O 503 503	0	2

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.

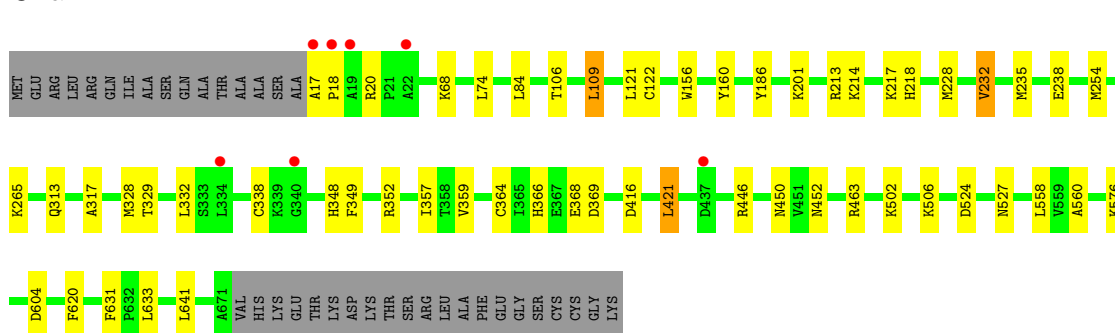
- Molecule 1: Peroxisomal primary amine oxidase

Chain A:



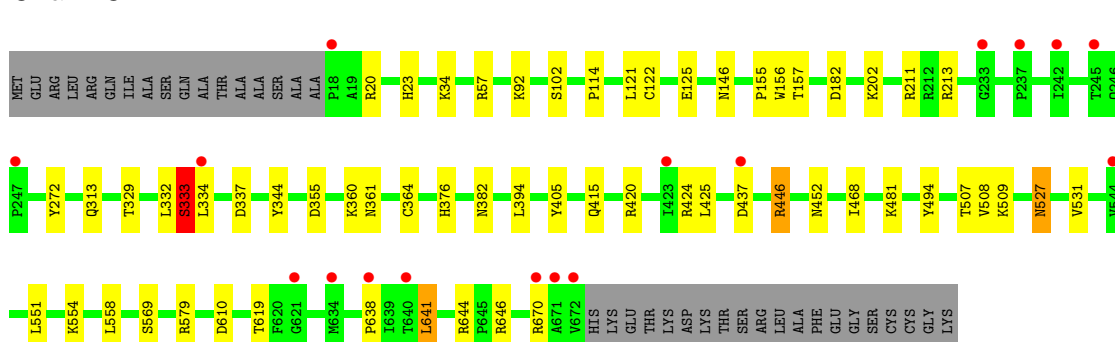
- Molecule 1: Peroxisomal primary amine oxidase

Chain B:



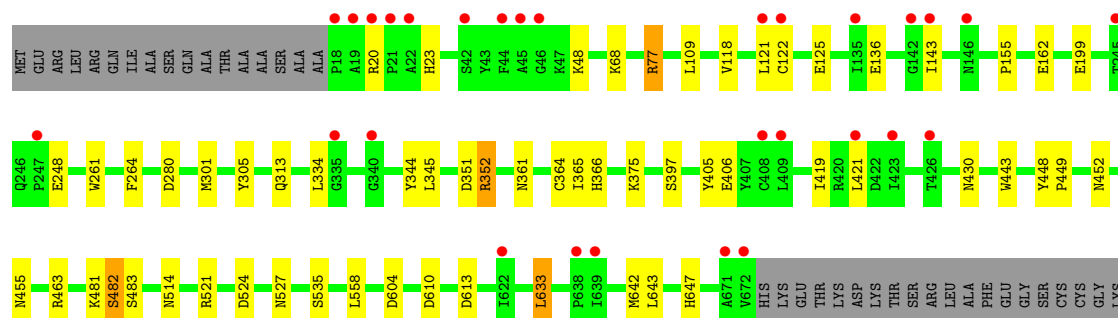
- Molecule 1: Peroxisomal primary amine oxidase

Chain C:



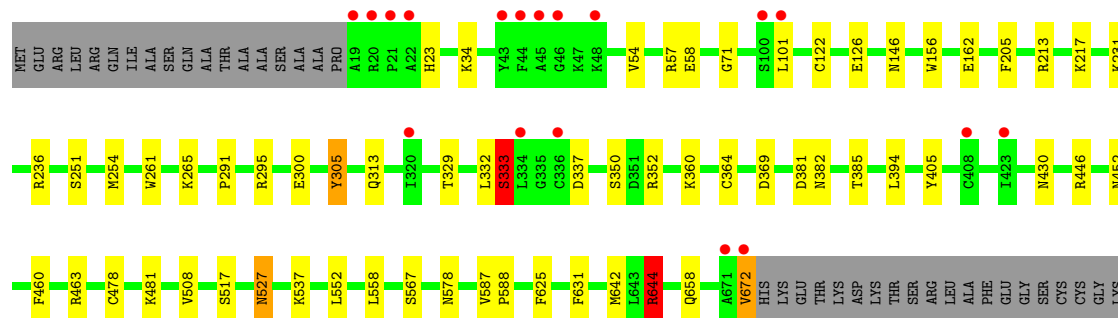
- Molecule 1: Peroxisomal primary amine oxidase

Chain D:



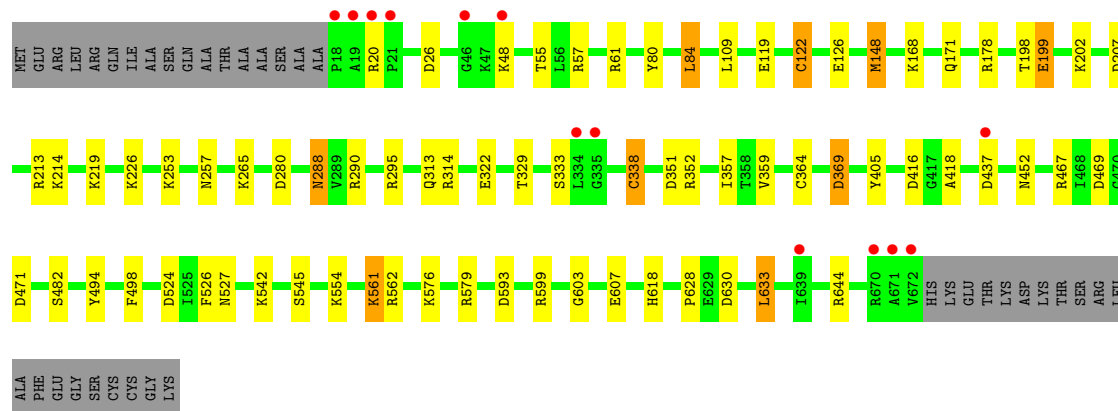
- Molecule 1: Peroxisomal primary amine oxidase

Chain E:



- Molecule 1: Peroxisomal primary amine oxidase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.24Å 233.71Å 105.05Å 90.00° 96.57° 90.00°	Depositor
Resolution (Å)	48.90 – 2.25 48.90 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.90-2.25) 98.8 (48.90-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.169 , 0.230 0.169 , 0.229	Depositor DCC
R_{free} test set	11654 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.5	EDS
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 232566 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34660	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEO, CU, TYQ, ABN

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	1.09	6/5395 (0.1%)	0.95	10/7340 (0.1%)
1	B	1.21	8/5387 (0.1%)	1.01	11/7328 (0.2%)
1	C	1.05	2/5396 (0.0%)	0.95	9/7343 (0.1%)
1	D	0.98	1/5382 (0.0%)	0.90	11/7323 (0.2%)
1	E	1.13	11/5418 (0.2%)	0.98	9/7372 (0.1%)
1	F	1.10	7/5386 (0.1%)	0.98	18/7326 (0.2%)
All	All	1.10	35/32364 (0.1%)	0.96	68/44032 (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	1
1	E	0	1
All	All	0	2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	478	CYS	CB-SG	9.19	1.97	1.82
1	A	478	CYS	CB-SG	8.77	1.97	1.82
1	B	620	PHE	CE1-CZ	6.48	1.49	1.37
1	B	186	TYR	CD2-CE2	-6.45	1.29	1.39
1	B	560	ALA	CA-CB	6.38	1.65	1.52
1	E	305	TYR	CG-CD1	6.26	1.47	1.39
1	B	232	VAL	CB-CG1	5.98	1.65	1.52
1	A	570	VAL	CB-CG1	5.98	1.65	1.52
1	A	122	CYS	CB-SG	5.88	1.92	1.82
1	E	460	PHE	CE1-CZ	5.78	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	498	PHE	CE1-CZ	5.76	1.48	1.37
1	E	122	CYS	CB-SG	5.66	1.91	1.82
1	E	631	PHE	CE2-CZ	5.65	1.48	1.37
1	A	620	PHE	CE2-CZ	5.64	1.48	1.37
1	D	482	SER	CB-OG	-5.59	1.34	1.42
1	F	322	GLU	CD-OE1	5.55	1.31	1.25
1	F	561	LYS	CD-CE	5.43	1.64	1.51
1	C	122	CYS	CB-SG	5.37	1.91	1.82
1	A	420	ARG	CB-CG	-5.35	1.38	1.52
1	F	199	GLU	CG-CD	5.35	1.59	1.51
1	B	122	CYS	CB-SG	5.33	1.91	1.82
1	E	300	GLU	CG-CD	5.32	1.59	1.51
1	C	272	TYR	CE1-CZ	5.30	1.45	1.38
1	A	300	GLU	CD-OE1	5.28	1.31	1.25
1	F	418	ALA	CA-CB	5.26	1.63	1.52
1	B	631	PHE	CE2-CZ	5.24	1.47	1.37
1	E	625	PHE	CE1-CZ	5.21	1.47	1.37
1	B	18	PRO	N-CD	5.20	1.55	1.47
1	E	508	VAL	CB-CG2	5.19	1.63	1.52
1	E	126	GLU	CB-CG	5.18	1.61	1.52
1	B	160	TYR	CD2-CE2	5.17	1.47	1.39
1	E	205	PHE	CE1-CZ	5.14	1.47	1.37
1	E	261	TRP	CE3-CZ3	5.06	1.47	1.38
1	F	603	GLY	N-CA	5.06	1.53	1.46
1	F	526	PHE	CD2-CE2	5.01	1.49	1.39

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	295	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	C	641	LEU	CA-CB-CG	8.63	135.16	115.30
1	E	446	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	B	463	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	E	446	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	420	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	E	213	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	F	416	ASP	CB-CG-OD1	7.34	124.91	118.30
1	C	646	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	604	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	558	LEU	CB-CG-CD1	-7.23	98.72	111.00
1	F	295	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	E	213	ARG	NE-CZ-NH2	-6.99	116.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	562	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	E	236	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	421	LEU	CB-CG-CD2	6.70	122.38	111.00
1	A	394	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	84	LEU	CA-CB-CG	6.61	130.51	115.30
1	B	416	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	463	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	369	ASP	CB-CG-OD1	6.13	123.82	118.30
1	F	178	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	D	351	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	285	ASP	CB-CG-OD1	6.05	123.74	118.30
1	F	57	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	F	562	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	182	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	610	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	352	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	17	ALA	C-N-CD	5.80	140.58	128.40
1	B	109	LEU	CA-CB-CG	5.78	128.60	115.30
1	E	644[A]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	644[B]	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	77	ARG	CG-CD-NE	-5.67	99.90	111.80
1	C	420	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	610	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	369	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	F	351	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	613	ASP	CB-CG-OD1	5.55	123.30	118.30
1	F	57	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	F	314	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	579	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	57	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	641	LEU	CB-CG-CD2	5.40	120.18	111.00
1	C	446	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	E	369	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	F	599	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	F	207	ASP	CB-CG-OD1	5.35	123.12	118.30
1	D	77	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	524	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	F	369	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	610	ASP	CB-CG-OD1	5.27	123.05	118.30
1	D	633	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	641	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	D	345	LEU	CA-CB-CG	5.21	127.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	416	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	604	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	254	MET	CG-SD-CE	5.14	108.42	100.20
1	F	84	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	280	ASP	CB-CG-OD1	5.13	122.91	118.30
1	E	352	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	394	LEU	CB-CG-CD2	5.11	119.69	111.00
1	D	521	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	B	446	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	D	463	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	F	633	LEU	CB-CG-CD2	5.03	119.54	111.00
1	A	599	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	F	630	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	PRO	Peptide
1	E	333	SER	Peptide

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5227	0	0	22	0
1	B	5227	0	4	19	0
1	C	5228	0	0	26	0
1	D	5223	0	7	24	0
1	E	5245	0	0	24	0
1	F	5227	0	0	27	0
2	A	30	0	40	2	0
2	B	36	0	48	3	0
2	C	36	0	48	4	0
2	D	24	0	32	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	24	0	32	4	0
2	F	30	0	40	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	1	0
5	A	8	0	9	2	0
5	B	8	0	9	2	0
5	C	8	0	9	3	0
5	D	8	0	9	1	0
5	E	8	0	9	2	0
5	F	8	0	9	1	0
6	A	529	0	0	7	0
6	B	583	0	0	8	0
6	C	499	0	0	11	0
6	D	465	0	0	4	0
6	E	462	0	0	11	0
6	F	503	0	0	9	0
All	All	34660	0	305	141	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (141) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:E:1141:HOH:O	1:F:122[B]:CYS:SG	2.05	1.14
1:B:214:LYS:O	2:B:706:GOL:H11	1.60	1.00
1:A:280:ASP:OD2	2:A:703:GOL:H12	1.66	0.96
6:C:1264:HOH:O	1:D:122[A]:CYS:SG	2.22	0.95
1:B:348:HIS:CD2	6:B:1180:HOH:O	2.29	0.86
1:F:405:TYQ:N5	5:F:708:ABN:N	2.28	0.81
1:A:405:TYQ:N5	5:A:708:ABN:N	2.31	0.78
1:A:332:LEU:O	1:A:333:SER:CB	2.31	0.78
1:A:168:LYS:O	1:A:170[B]:LEU:CD1	2.34	0.76
1:D:23:HIS:NE2	2:D:702:GOL:H11	2.01	0.75
2:C:703:GOL:H31	6:C:1152:HOH:O	1.88	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:672:VAL:CG2	6:E:1198:HOH:O	2.36	0.72
1:E:578:ASN:N	2:E:706:GOL:H11	2.04	0.71
1:E:156:TRP:CD1	5:E:707:ABN:H2	2.26	0.70
1:B:156:TRP:CD1	5:B:709:ABN:H2	2.28	0.69
1:E:658:GLN:NE2	6:E:1006:HOH:O	2.25	0.68
1:C:551:LEU:N	2:C:707:GOL:HO1	1.91	0.68
1:D:68:LYS:CE	2:D:702:GOL:H2	2.25	0.66
1:A:201:LYS:CE	6:A:1284:HOH:O	2.44	0.65
1:B:317:ALA:N	6:B:1372:HOH:O	2.31	0.63
1:E:54[B]:VAL:CG2	1:E:350:SER:CB	2.77	0.62
1:E:430:ASN:ND2	6:E:1131:HOH:O	2.33	0.61
1:A:23:HIS:CE1	2:A:703:GOL:O1	2.54	0.61
1:C:23:HIS:CE1	2:C:702:GOL:O3	2.55	0.60
2:C:707:GOL:H12	6:C:919:HOH:O	2.03	0.59
1:C:638:PRO:CD	6:D:817[B]:HOH:O	2.52	0.57
1:F:405:TYQ:OZ	4:F:707:PEO:O2	2.23	0.56
1:F:288:ASN:ND2	6:F:1270:HOH:O	2.39	0.56
1:A:68:LYS:NZ	6:A:1295:HOH:O	2.38	0.56
1:F:219:LYS:N	6:F:1213:HOH:O	2.39	0.56
1:C:211:ARG:N	6:C:985:HOH:O	2.39	0.55
1:E:71:GLY:N	6:E:948:HOH:O	2.39	0.55
1:E:23:HIS:CE1	2:E:704:GOL:O2	2.60	0.55
1:D:301:MET:CB	6:D:1245:HOH:O	2.55	0.55
1:A:420:ARG:NH1	6:A:1114:HOH:O	2.39	0.55
1:A:120:ASP:OD1	1:A:352:ARG:NH2	2.39	0.55
1:D:405:TYQ:N5	5:D:706:ABN:N	2.55	0.54
2:E:706:GOL:O3	2:E:706:GOL:O1	2.21	0.53
1:A:669:LYS:CD	6:B:1184:HOH:O	2.56	0.53
1:C:509:LYS:NZ	6:C:1167:HOH:O	2.42	0.53
1:D:481[A]:LYS:NZ	6:D:1155:HOH:O	2.42	0.53
1:E:481[B]:LYS:NZ	6:E:1000:HOH:O	2.42	0.53
1:C:344:TYR:CG	1:C:361:ASN:ND2	2.77	0.52
2:F:704:GOL:H11	6:F:1256:HOH:O	2.09	0.52
1:B:506:LYS:NZ	6:B:1173:HOH:O	2.42	0.52
1:C:92:LYS:NZ	6:C:952:HOH:O	2.42	0.52
1:C:332:LEU:O	1:C:333:SER:CB	2.58	0.52
1:A:502:LYS:NZ	6:A:1321:HOH:O	2.43	0.51
1:F:467:ARG:NE	1:F:471:ASP:OD1	2.44	0.51
1:B:74:LEU:CD1	1:B:74:LEU:C	2.79	0.51
1:E:463:ARG:NH2	6:E:954:HOH:O	2.43	0.51
1:A:670:ARG:NH1	6:A:1297:HOH:O	2.44	0.51
1:C:121:LEU:CD1	5:C:708:ABN:H4	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:168:LYS:CE	6:F:1042:HOH:O	2.60	0.50
1:D:524:ASP:OD2	6:D:900:HOH:O	2.20	0.50
1:F:148:MET:CE	1:F:148:MET:CA	2.90	0.50
1:F:26:ASP:OD1	1:F:257:ASN:ND2	2.44	0.49
1:B:214:LYS:O	2:B:706:GOL:C1	2.48	0.49
1:D:514:ASN:N	2:D:703:GOL:HO2	2.11	0.49
1:F:561:LYS:NZ	1:F:593:ASP:OD1	2.45	0.49
1:E:405:TYQ:N5	5:E:707:ABN:N	2.61	0.49
1:B:338:CYS:SG	1:B:364[B]:CYS:CB	3.01	0.48
1:E:537:LYS:NZ	6:E:1175:HOH:O	2.47	0.48
1:A:290:ARG:NH2	1:A:469:ASP:OD2	2.46	0.48
1:F:265:LYS:NZ	2:F:702:GOL:H12	2.29	0.48
1:F:644:ARG:NH1	6:F:923:HOH:O	2.47	0.48
1:C:527:ASN:ND2	1:C:527:ASN:C	2.67	0.48
1:B:235:MET:N	6:B:829:HOH:O	2.46	0.48
1:A:34:LYS:NZ	1:A:355:ASP:OD1	2.47	0.48
1:F:545:SER:OG	1:F:618:HIS:NE2	2.47	0.48
1:E:58:GLU:OE2	1:E:295:ARG:NH2	2.47	0.47
1:F:214:LYS:O	2:F:705:GOL:O3	2.18	0.47
1:E:552:LEU:O	1:F:482:SER:OG	2.32	0.47
1:C:156:TRP:CD1	5:C:708:ABN:H2	2.50	0.47
1:C:405:TYQ:N5	5:C:708:ABN:N	2.62	0.47
1:D:364[B]:CYS:SG	1:D:365:ILE:N	2.88	0.47
1:A:178:ARG:NH1	6:A:929:HOH:O	2.47	0.47
1:D:199:GLU:OE2	1:D:352:ARG:NH2	2.49	0.46
1:D:535:SER:OG	1:D:647:HIS:ND1	2.48	0.46
1:F:579:ARG:NH1	6:F:929:HOH:O	2.47	0.46
1:C:507:THR:O	1:C:508:VAL:C	2.53	0.46
1:F:338:CYS:CB	1:F:364[B]:CYS:SG	3.03	0.46
1:C:494:TYR:OH	1:D:162:GLU:OE2	2.33	0.46
1:A:405:TYQ:OZ	4:A:707:PEO:O2	2.33	0.46
1:B:502:LYS:NZ	6:B:1328:HOH:O	2.49	0.46
1:D:121:LEU:CD1	1:D:155:PRO:O	2.63	0.45
1:E:337:ASP:N	6:E:1122:HOH:O	2.50	0.45
1:F:437:ASP:N	6:F:980:HOH:O	2.50	0.45
1:D:280:ASP:OD2	2:D:702:GOL:H12	2.16	0.45
1:F:607:GLU:OE1	6:F:1007:HOH:O	2.21	0.45
1:E:332:LEU:O	1:E:333:SER:O	2.34	0.45
1:E:333:SER:CB	6:E:1121:HOH:O	2.65	0.44
2:B:703:GOL:H32	6:B:1232:HOH:O	2.16	0.44
1:A:315:LYS:NZ	1:A:454:HIS:ND1	2.65	0.44
1:C:424:ARG:NE	6:C:1152:HOH:O	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:305:TYR:OH	1:D:405:TYQ:OH	2.35	0.44
1:F:199:GLU:OE2	1:F:352:ARG:NH2	2.50	0.44
1:C:415:GLN:N	6:C:869:HOH:O	2.51	0.44
1:B:218:HIS:CD2	1:B:450:ASN:ND2	2.86	0.44
1:C:337:ASP:OD2	1:D:375:LYS:NZ	2.51	0.44
1:A:168:LYS:C	1:A:170[B]:LEU:CD1	2.85	0.44
1:E:527:ASN:C	1:E:527:ASN:ND2	2.71	0.44
1:D:443:TRP:O	1:D:455:ASN:N	2.51	0.43
1:F:119:GLU:OE1	1:F:352:ARG:N	2.51	0.43
1:B:604:ASP:OD1	1:B:604:ASP:C	2.55	0.43
1:D:344:TYR:CB	1:D:361:ASN:ND2	2.81	0.43
1:E:265:LYS:CE	2:E:704:GOL:H12	2.49	0.43
1:C:34:LYS:NZ	1:C:355:ASP:OD1	2.51	0.43
1:B:338:CYS:CB	1:B:364[B]:CYS:SG	3.06	0.43
1:D:261:TRP:O	1:D:264:PHE:N	2.52	0.43
1:C:481:LYS:CE	6:C:1297:HOH:O	2.67	0.43
1:F:290:ARG:NH2	1:F:469:ASP:OD2	2.52	0.42
1:F:171:GLN:NE2	1:F:198:THR:OG1	2.52	0.42
1:A:156:TRP:CD1	5:A:708:ABN:H6	2.55	0.42
1:C:344:TYR:CB	1:C:361:ASN:ND2	2.83	0.42
1:D:364[B]:CYS:SG	1:D:366:HIS:CD2	3.13	0.42
1:A:366:HIS:CD2	6:A:1300:HOH:O	2.72	0.42
1:B:20:ARG:NH2	6:B:985:HOH:O	2.51	0.42
1:C:554:LYS:NZ	1:D:483:SER:O	2.52	0.42
1:B:366:HIS:CE1	1:B:368:GLU:CG	3.02	0.42
1:B:156:TRP:CG	5:B:709:ABN:H2	2.55	0.42
1:D:448:TYR:O	1:D:449:PRO:C	2.57	0.42
1:F:524:ASP:OD1	1:F:542:LYS:NZ	2.52	0.42
1:C:644:ARG:CD	6:C:1280:HOH:O	2.67	0.42
1:E:587:VAL:O	1:E:588:PRO:C	2.58	0.42
1:E:305:TYR:OH	1:E:405:TYQ:OH	2.37	0.41
1:E:162:GLU:OE2	1:F:494:TYR:OH	2.37	0.41
1:F:61:ARG:NH2	6:F:1262:HOH:O	2.53	0.41
1:C:446:ARG:NE	6:C:832:HOH:O	2.53	0.41
1:C:569:SER:O	1:C:619:THR:N	2.54	0.41
1:D:419:ILE:O	1:D:643:LEU:N	2.53	0.41
1:B:121:LEU:CD1	1:B:328[B]:MET:CE	2.98	0.41
1:F:55:THR:O	1:F:80:TYR:N	2.54	0.41
1:B:228:MET:O	1:B:232:VAL:N	2.53	0.41
1:C:376:HIS:ND1	1:D:406:GLU:OE2	2.54	0.41
1:A:591:SER:OG	1:A:593:ASP:OD2	2.39	0.40
1:E:644[A]:ARG:NH2	6:E:1022:HOH:O	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:381:ASP:OD2	1:E:385:THR:OG1	2.39	0.40
1:B:349:PHE:O	1:B:357:ILE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	662/692 (96%)	635 (96%)	25 (4%)	2 (0%)	50	54
1	B	660/692 (95%)	631 (96%)	29 (4%)	0	100	100
1	C	663/692 (96%)	634 (96%)	25 (4%)	4 (1%)	33	33
1	D	660/692 (95%)	633 (96%)	27 (4%)	0	100	100
1	E	664/692 (96%)	637 (96%)	26 (4%)	1 (0%)	56	63
1	F	660/692 (95%)	629 (95%)	30 (4%)	1 (0%)	56	63
All	All	3969/4152 (96%)	3799 (96%)	162 (4%)	8 (0%)	56	63

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	E	333	SER
1	F	333	SER
1	A	22	ALA
1	C	333	SER
1	C	155	PRO
1	C	114	PRO
1	C	468	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	574/593 (97%)	550 (96%)	24 (4%)	40	46
1	B	572/593 (96%)	551 (96%)	21 (4%)	45	53
1	C	574/593 (97%)	550 (96%)	24 (4%)	40	46
1	D	572/593 (96%)	550 (96%)	22 (4%)	44	52
1	E	577/593 (97%)	552 (96%)	25 (4%)	40	45
1	F	573/593 (97%)	547 (96%)	26 (4%)	38	42
All	All	3442/3558 (97%)	3300 (96%)	142 (4%)	43	47

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	126[A]	GLU
1	A	126[B]	GLU
1	A	146	ASN
1	A	187	SER
1	A	313	GLN
1	A	329	THR
1	A	334	LEU
1	A	360	LYS
1	A	364	CYS
1	A	369	ASP
1	A	382	ASN
1	A	394	LEU
1	A	397[A]	SER
1	A	397[B]	SER
1	A	406	GLU
1	A	439	GLU
1	A	452	ASN
1	A	481[A]	LYS
1	A	481[B]	LYS
1	A	527	ASN
1	A	531	VAL
1	A	558	LEU
1	A	622	ILE
1	B	68	LYS
1	B	84	LEU
1	B	106	THR

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Mol	Chain	Res	Type
1	B	109	LEU
1	B	201	LYS
1	B	213	ARG
1	B	217	LYS
1	B	238	GLU
1	B	265	LYS
1	B	313	GLN
1	B	329	THR
1	B	332	LEU
1	B	352	ARG
1	B	359	VAL
1	B	369	ASP
1	B	421	LEU
1	B	452	ASN
1	B	527	ASN
1	B	576[A]	LYS
1	B	576[B]	LYS
1	B	633	LEU
1	C	20	ARG
1	C	102[A]	SER
1	C	102[B]	SER
1	C	125	GLU
1	C	146	ASN
1	C	157[A]	THR
1	C	157[B]	THR
1	C	202	LYS
1	C	213	ARG
1	C	313	GLN
1	C	329	THR
1	C	333	SER
1	C	334	LEU
1	C	360	LYS
1	C	364	CYS
1	C	382	ASN
1	C	394	LEU
1	C	425	LEU
1	C	452	ASN
1	C	527	ASN
1	C	531	VAL
1	C	558	LEU
1	C	641	LEU
1	C	670	ARG

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Mol	Chain	Res	Type
1	D	20	ARG
1	D	48	LYS
1	D	77	ARG
1	D	109	LEU
1	D	118	VAL
1	D	125	GLU
1	D	136	GLU
1	D	143	ILE
1	D	248	GLU
1	D	313	GLN
1	D	334	LEU
1	D	352	ARG
1	D	397[A]	SER
1	D	397[B]	SER
1	D	421	LEU
1	D	430	ASN
1	D	452	ASN
1	D	482	SER
1	D	527	ASN
1	D	558	LEU
1	D	633	LEU
1	D	642	MET
1	E	34	LYS
1	E	57	ARG
1	E	101	LEU
1	E	146	ASN
1	E	217	LYS
1	E	231	LYS
1	E	251	SER
1	E	254	MET
1	E	291	PRO
1	E	313	GLN
1	E	329	THR
1	E	360	LYS
1	E	364	CYS
1	E	382	ASN
1	E	394	LEU
1	E	452	ASN
1	E	517	SER
1	E	527	ASN
1	E	558	LEU
1	E	567[A]	SER

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Mol	Chain	Res	Type
1	E	567[B]	SER
1	E	642	MET
1	E	644[A]	ARG
1	E	644[B]	ARG
1	E	672	VAL
1	F	20	ARG
1	F	48	LYS
1	F	84	LEU
1	F	109	LEU
1	F	122[A]	CYS
1	F	122[B]	CYS
1	F	126	GLU
1	F	148	MET
1	F	202	LYS
1	F	213	ARG
1	F	226	LYS
1	F	253	LYS
1	F	288	ASN
1	F	313	GLN
1	F	329	THR
1	F	338	CYS
1	F	357	ILE
1	F	359	VAL
1	F	369	ASP
1	F	452	ASN
1	F	527	ASN
1	F	554	LYS
1	F	576[A]	LYS
1	F	576[B]	LYS
1	F	628	PRO
1	F	633	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TYQ	A	405	1	14,14,15	5.82	3 (21%)	17,19,21	1.70	3 (17%)
1	TYQ	B	405	1	14,14,15	6.81	4 (28%)	17,19,21	3.28	10 (58%)
1	TYQ	C	405	1	14,14,15	5.51	3 (21%)	17,19,21	1.73	3 (17%)
1	TYQ	D	405	1	14,14,15	6.25	3 (21%)	17,19,21	1.99	6 (35%)
1	TYQ	E	405	1	14,14,15	5.59	5 (35%)	17,19,21	1.40	3 (17%)
1	TYQ	F	405	1	14,14,15	6.57	3 (21%)	17,19,21	2.02	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYQ	A	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	B	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	C	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	D	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	E	405	1	-	0/4/6/8	0/1/1/1
1	TYQ	F	405	1	-	0/4/6/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	TYQ	O-C	23.38	1.27	1.11
1	F	405	TYQ	O-C	21.91	1.26	1.11
1	D	405	TYQ	O-C	21.65	1.26	1.11
1	E	405	TYQ	O-C	19.27	1.24	1.11
1	A	405	TYQ	O-C	19.02	1.24	1.11
1	C	405	TYQ	O-C	17.90	1.23	1.11
1	F	405	TYQ	CE2-CZ	9.38	1.54	1.40
1	C	405	TYQ	CE2-CZ	7.47	1.51	1.40
1	A	405	TYQ	CE2-CZ	7.32	1.51	1.40
1	A	405	TYQ	CD1-CG	6.97	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405	TYQ	CD1-CG	6.44	1.49	1.39
1	B	405	TYQ	CD1-CG	6.33	1.49	1.39
1	B	405	TYQ	CE2-CZ	6.21	1.49	1.40
1	E	405	TYQ	CE2-CZ	6.04	1.49	1.40
1	D	405	TYQ	CD1-CG	6.00	1.48	1.39
1	D	405	TYQ	CE2-CZ	5.95	1.49	1.40
1	F	405	TYQ	CD1-CG	5.66	1.48	1.39
1	B	405	TYQ	CE1-CZ	3.93	1.44	1.38
1	E	405	TYQ	CD1-CG	3.17	1.44	1.39
1	E	405	TYQ	CA-C	3.02	1.54	1.48
1	E	405	TYQ	CE1-CZ	2.23	1.42	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	TYQ	CD2-CG-CD1	7.25	124.45	118.23
1	B	405	TYQ	CB-CG-CD1	-5.86	114.49	120.78
1	B	405	TYQ	CE1-CD1-CG	-4.98	116.97	120.85
1	D	405	TYQ	CE1-CD1-CG	-4.64	117.25	120.85
1	F	405	TYQ	OH-CZ-CE2	4.26	123.86	116.28
1	C	405	TYQ	CD2-CG-CD1	4.26	121.88	118.23
1	B	405	TYQ	CE1-CZ-CE2	3.91	122.51	119.61
1	A	405	TYQ	CD2-CG-CD1	3.67	121.37	118.23
1	F	405	TYQ	CD2-CG-CD1	3.64	121.35	118.23
1	A	405	TYQ	CE1-CZ-CE2	3.54	122.23	119.61
1	F	405	TYQ	CZ-CE2-N5	3.53	125.02	118.60
1	B	405	TYQ	C-CA-N	3.41	117.24	113.83
1	A	405	TYQ	CE2-CD2-CG	-3.39	118.49	122.38
1	D	405	TYQ	CD2-CG-CD1	3.35	121.10	118.23
1	B	405	TYQ	CE2-CD2-CG	-3.31	118.59	122.38
1	F	405	TYQ	CE2-CD2-CG	-3.15	118.77	122.38
1	C	405	TYQ	CE2-CD2-CG	-3.04	118.89	122.38
1	D	405	TYQ	CZ-CE1-CD1	2.84	122.85	120.03
1	B	405	TYQ	CD2-CE2-N5	2.81	126.09	120.19
1	C	405	TYQ	CB-CG-CD1	-2.75	117.83	120.78
1	B	405	TYQ	OH-CZ-CE2	-2.68	111.52	116.28
1	F	405	TYQ	CD2-CE2-N5	-2.64	114.67	120.19
1	D	405	TYQ	OH-CZ-CE2	2.48	120.69	116.28
1	B	405	TYQ	OH-CZ-CE1	2.48	125.96	119.42
1	E	405	TYQ	C-CA-N	2.44	116.27	113.83
1	E	405	TYQ	CE1-CZ-CE2	-2.32	117.90	119.61
1	E	405	TYQ	OH-CZ-CE1	2.31	125.51	119.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	TYQ	C-CA-N	2.30	116.13	113.83
1	B	405	TYQ	OZ-CD1-CE1	2.24	125.33	119.42
1	D	405	TYQ	CZ-CE2-N5	2.00	122.25	118.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 46 ligands modelled in this entry, 6 are monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	701	-	5,5,5	0.40	0	5,5,5	0.47	0
2	GOL	A	703	-	5,5,5	0.41	0	5,5,5	0.76	0
2	GOL	A	704	-	5,5,5	0.43	0	5,5,5	0.26	0
2	GOL	A	705	-	5,5,5	0.40	0	5,5,5	0.45	0
2	GOL	A	706	-	5,5,5	0.35	0	5,5,5	0.57	0
4	PEO	A	707	-	1,1,1	0.87	0	0,0,0	0.00	-
5	ABN	A	708	-	8,8,8	0.63	0	9,9,9	0.71	0
2	GOL	B	701	-	5,5,5	0.48	0	5,5,5	0.82	0
2	GOL	B	703	-	5,5,5	0.77	0	5,5,5	0.74	0
2	GOL	B	704	-	5,5,5	0.44	0	5,5,5	1.12	0
2	GOL	B	705	-	5,5,5	0.52	0	5,5,5	1.08	0
2	GOL	B	706	-	5,5,5	0.36	0	5,5,5	0.85	0
2	GOL	B	707	-	5,5,5	0.35	0	5,5,5	0.91	0
4	PEO	B	708	3	1,1,1	0.40	0	0,0,0	0.00	-
5	ABN	B	709	-	8,8,8	1.13	1 (12%)	9,9,9	1.60	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	702	-	5,5,5	0.25	0	5,5,5	0.41	0
2	GOL	C	703	-	5,5,5	0.30	0	5,5,5	0.90	0
2	GOL	C	704	-	5,5,5	0.55	0	5,5,5	0.56	0
2	GOL	C	705	-	5,5,5	0.58	0	5,5,5	0.67	0
2	GOL	C	706	-	5,5,5	0.47	0	5,5,5	0.69	0
2	GOL	C	707	-	5,5,5	0.52	0	5,5,5	1.40	0
5	ABN	C	708	-	8,8,8	1.04	0	9,9,9	0.46	0
2	GOL	D	702	-	5,5,5	0.38	0	5,5,5	0.74	0
2	GOL	D	703	-	5,5,5	0.77	0	5,5,5	0.56	0
2	GOL	D	704	-	5,5,5	0.31	0	5,5,5	0.52	0
2	GOL	D	705	-	5,5,5	0.45	0	5,5,5	0.58	0
5	ABN	D	706	-	8,8,8	1.08	0	9,9,9	1.00	1 (11%)
2	GOL	E	702	-	5,5,5	0.44	0	5,5,5	0.56	0
2	GOL	E	703	-	5,5,5	0.25	0	5,5,5	0.97	0
2	GOL	E	704	-	5,5,5	0.23	0	5,5,5	0.79	0
4	PEO	E	705	-	1,1,1	0.20	0	0,0,0	0.00	-
2	GOL	E	706	-	5,5,5	0.43	0	5,5,5	0.96	0
5	ABN	E	707	-	8,8,8	0.51	0	9,9,9	0.39	0
2	GOL	F	702	-	5,5,5	0.58	0	5,5,5	0.94	0
2	GOL	F	703	-	5,5,5	0.67	0	5,5,5	0.62	0
2	GOL	F	704	-	5,5,5	0.29	0	5,5,5	0.72	0
2	GOL	F	705	-	5,5,5	0.36	0	5,5,5	1.10	0
2	GOL	F	706	-	5,5,5	0.43	0	5,5,5	0.74	0
4	PEO	F	707	-	1,1,1	0.28	0	0,0,0	0.00	-
5	ABN	F	708	-	8,8,8	0.57	0	9,9,9	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	701	-	-	0/4/4/4	0/0/0/0
2	GOL	A	703	-	-	0/4/4/4	0/0/0/0
2	GOL	A	704	-	-	0/4/4/4	0/0/0/0
2	GOL	A	705	-	-	0/4/4/4	0/0/0/0
2	GOL	A	706	-	-	0/4/4/4	0/0/0/0
4	PEO	A	707	-	-	0/0/0/0	0/0/0/0
5	ABN	A	708	-	-	0/2/2/2	0/1/1/1
2	GOL	B	701	-	-	0/4/4/4	0/0/0/0
2	GOL	B	703	-	-	0/4/4/4	0/0/0/0
2	GOL	B	704	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	705	-	-	0/4/4/4	0/0/0/0
2	GOL	B	706	-	-	0/4/4/4	0/0/0/0
2	GOL	B	707	-	-	0/4/4/4	0/0/0/0
4	PEO	B	708	3	-	0/0/0/0	0/0/0/0
5	ABN	B	709	-	-	0/2/2/2	0/1/1/1
2	GOL	C	702	-	-	0/4/4/4	0/0/0/0
2	GOL	C	703	-	-	0/4/4/4	0/0/0/0
2	GOL	C	704	-	-	0/4/4/4	0/0/0/0
2	GOL	C	705	-	-	0/4/4/4	0/0/0/0
2	GOL	C	706	-	-	0/4/4/4	0/0/0/0
2	GOL	C	707	-	-	0/4/4/4	0/0/0/0
5	ABN	C	708	-	-	0/2/2/2	0/1/1/1
2	GOL	D	702	-	-	0/4/4/4	0/0/0/0
2	GOL	D	703	-	-	0/4/4/4	0/0/0/0
2	GOL	D	704	-	-	0/4/4/4	0/0/0/0
2	GOL	D	705	-	-	0/4/4/4	0/0/0/0
5	ABN	D	706	-	-	0/2/2/2	0/1/1/1
2	GOL	E	702	-	-	0/4/4/4	0/0/0/0
2	GOL	E	703	-	-	0/4/4/4	0/0/0/0
2	GOL	E	704	-	-	0/4/4/4	0/0/0/0
4	PEO	E	705	-	-	0/0/0/0	0/0/0/0
2	GOL	E	706	-	-	0/4/4/4	0/0/0/0
5	ABN	E	707	-	-	0/2/2/2	0/1/1/1
2	GOL	F	702	-	-	0/4/4/4	0/0/0/0
2	GOL	F	703	-	-	0/4/4/4	0/0/0/0
2	GOL	F	704	-	-	0/4/4/4	0/0/0/0
2	GOL	F	705	-	-	0/4/4/4	0/0/0/0
2	GOL	F	706	-	-	0/4/4/4	0/0/0/0
4	PEO	F	707	-	-	0/0/0/0	0/0/0/0
5	ABN	F	708	-	-	0/2/2/2	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	709	ABN	C3-C2	2.04	1.43	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	709	ABN	C3-C2-C1	2.76	125.25	120.64
5	B	709	ABN	C4-C5-C6	2.46	124.27	120.17
5	D	706	ABN	C4-C5-C6	-2.10	116.67	120.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	654/692 (94%)	-0.11	16 (2%) 56 63	15, 31, 53, 86	0
1	B	655/692 (94%)	-0.26	7 (1%) 77 83	15, 27, 45, 67	0
1	C	655/692 (94%)	-0.15	17 (2%) 53 60	20, 32, 54, 84	0
1	D	655/692 (94%)	0.12	29 (4%) 33 37	22, 37, 60, 89	0
1	E	654/692 (94%)	-0.03	18 (2%) 50 57	18, 33, 54, 83	0
1	F	655/692 (94%)	-0.13	13 (1%) 62 68	15, 31, 54, 76	0
All	All	3928/4152 (94%)	-0.09	100 (2%) 54 62	15, 32, 55, 89	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	PRO	7.2
1	E	334	LEU	6.8
1	A	18	PRO	6.8
1	A	19	ALA	6.7
1	F	672	VAL	5.8
1	B	17	ALA	5.5
1	E	672	VAL	5.4
1	E	20	ARG	5.3
1	E	21	PRO	4.6
1	D	46	GLY	4.5
1	F	19	ALA	4.5
1	E	19	ALA	4.4
1	D	21	PRO	4.3
1	D	19	ALA	4.3
1	F	334	LEU	4.2
1	D	672	VAL	4.0
1	C	334	LEU	3.9
1	E	671	ALA	3.8
1	E	46	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	3.7
1	A	22	ALA	3.5
1	D	423	ILE	3.4
1	C	242	ILE	3.4
1	C	247	PRO	3.3
1	D	22	ALA	3.3
1	D	20	ARG	3.3
1	D	409	LEU	3.2
1	D	122[A]	CYS	3.2
1	F	20	ARG	3.2
1	E	48	LYS	3.1
1	A	671	ALA	3.1
1	C	671	ALA	3.1
1	D	671	ALA	3.1
1	E	101	LEU	3.0
1	C	237	PRO	3.0
1	C	670	ARG	3.0
1	D	142	GLY	3.0
1	D	247	PRO	2.9
1	E	423	ILE	2.9
1	C	672	VAL	2.9
1	F	335	GLY	2.9
1	F	18	PRO	2.9
1	D	135	ILE	2.8
1	A	421	LEU	2.8
1	B	437	ASP	2.8
1	D	45	ALA	2.8
1	C	638	PRO	2.8
1	A	101	LEU	2.6
1	D	638	PRO	2.6
1	A	334	LEU	2.6
1	A	99	ALA	2.6
1	D	143	ILE	2.6
1	A	423	ILE	2.6
1	D	639	ILE	2.6
1	D	146	ASN	2.6
1	D	245	THR	2.6
1	D	335	GLY	2.5
1	E	45	ALA	2.5
1	C	18	PRO	2.5
1	D	421	LEU	2.5
1	D	42	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	336	CYS	2.5
1	F	437	ASP	2.5
1	A	407	TYR	2.4
1	A	45	ALA	2.4
1	C	544	VAL	2.4
1	E	44	PHE	2.4
1	A	46	GLY	2.3
1	A	333	SER	2.3
1	B	18	PRO	2.3
1	B	340	GLY	2.3
1	D	121	LEU	2.3
1	E	408	CYS	2.3
1	A	21	PRO	2.3
1	C	640	THR	2.3
1	C	423	ILE	2.3
1	E	22	ALA	2.3
1	F	21	PRO	2.2
1	F	671	ALA	2.2
1	C	233	GLY	2.2
1	E	43	TYR	2.2
1	D	44	PHE	2.2
1	F	46	GLY	2.2
1	E	100	SER	2.2
1	F	48	LYS	2.2
1	F	639	ILE	2.2
1	C	621	GLY	2.2
1	A	48	LYS	2.2
1	C	634[A]	MET	2.2
1	C	437[A]	ASP	2.1
1	D	426	THR	2.1
1	B	19	ALA	2.1
1	C	245	THR	2.1
1	F	670	ARG	2.1
1	D	622	ILE	2.0
1	E	320	ILE	2.0
1	B	22	ALA	2.0
1	E	336[A]	CYS	2.0
1	D	340	GLY	2.0
1	D	408	CYS	2.0

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

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, 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.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	TYQ	F	405	14/15	0.16	1.15	28,36,44,46	0
1	TYQ	D	405	14/15	0.19	0.77	38,42,46,47	0
1	TYQ	B	405	14/15	0.14	0.77	22,26,33,36	0
1	TYQ	E	405	14/15	0.17	0.72	23,29,40,42	0
1	TYQ	A	405	14/15	0.18	0.60	23,31,35,35	0
1	TYQ	C	405	14/15	0.17	0.53	28,35,42,43	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	706	6/6	0.34	15.51	56,61,66,69	0
2	GOL	F	706	6/6	0.27	15.02	57,57,60,60	0
2	GOL	B	704	6/6	0.26	13.83	41,49,51,55	0
2	GOL	E	703	6/6	0.25	12.73	64,65,66,67	0
2	GOL	B	705	6/6	0.31	11.05	62,64,67,70	0
2	GOL	D	703	6/6	0.21	10.93	51,54,56,57	0
2	GOL	F	702	6/6	0.27	8.08	44,51,52,55	0
2	GOL	E	704	6/6	0.26	5.05	66,69,70,71	0
4	PEO	F	707	2/2	0.20	4.32	28,28,28,36	0
2	GOL	C	706	6/6	0.24	4.25	62,64,67,68	0
2	GOL	D	704	6/6	0.24	4.00	52,58,61,63	0
2	GOL	C	707	6/6	0.17	3.96	45,55,56,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	D	705	6/6	0.29	3.42	70,72,73,74	0
2	GOL	C	703	6/6	0.27	3.39	46,49,50,53	0
2	GOL	C	704	6/6	0.23	3.35	52,56,56,60	0
4	PEO	B	708	2/2	0.19	2.74	24,24,24,26	0
2	GOL	D	702	6/6	0.19	2.48	57,60,61,62	0
2	GOL	E	702	6/6	0.25	2.39	55,58,60,60	0
2	GOL	F	703	6/6	0.20	2.37	62,65,65,66	0
2	GOL	A	705	6/6	0.25	2.26	50,52,53,54	0
2	GOL	B	701	6/6	0.18	2.17	27,33,35,36	0
2	GOL	A	703	6/6	0.21	2.05	51,56,57,60	0
2	GOL	F	704	6/6	0.21	2.03	46,52,53,56	0
5	ABN	B	709	8/8	0.20	1.98	40,42,44,44	0
4	PEO	E	705	2/2	0.25	1.96	30,30,30,35	0
2	GOL	B	703	6/6	0.18	1.82	46,49,50,50	0
2	GOL	B	706	6/6	0.18	1.80	50,52,54,57	0
4	PEO	A	707	2/2	0.20	1.55	26,26,26,31	0
2	GOL	A	704	6/6	0.20	1.45	59,64,67,67	0
2	GOL	E	706	6/6	0.17	1.36	52,55,56,57	0
2	GOL	F	705	6/6	0.24	1.24	61,65,66,68	0
5	ABN	C	708	8/8	0.17	1.07	38,39,41,42	0
2	GOL	C	702	6/6	0.14	0.98	49,57,59,61	0
2	GOL	B	707	6/6	0.16	0.80	50,52,53,55	0
5	ABN	D	706	8/8	0.17	0.36	36,37,37,38	0
5	ABN	A	708	8/8	0.15	0.32	31,32,34,37	0
5	ABN	E	707	8/8	0.16	0.16	32,33,34,35	0
5	ABN	F	708	8/8	0.14	0.15	38,41,42,42	0
2	GOL	C	705	6/6	0.16	0.08	62,64,65,66	0
2	GOL	A	701	6/6	0.10	-0.45	32,34,37,42	0
3	CU	A	702	1/1	0.12	-0.70	28,28,28,28	0
3	CU	C	701	1/1	0.11	-1.22	33,33,33,33	0
3	CU	F	701	1/1	0.11	-1.27	31,31,31,31	0
3	CU	E	701	1/1	0.11	-1.38	28,28,28,28	0
3	CU	B	702	1/1	0.11	-1.41	26,26,26,26	0
3	CU	D	701	1/1	0.12	-1.71	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.