



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:40 AM UTC

PDB ID : 5JX5 / pdb_00005jx5
Title : GH6 Orpinomyces sp. Y102 enzyme
Authors : Tsai, L.C.; Huang, H.C.
Deposited on : 2016-05-12
Resolution : 1.80 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

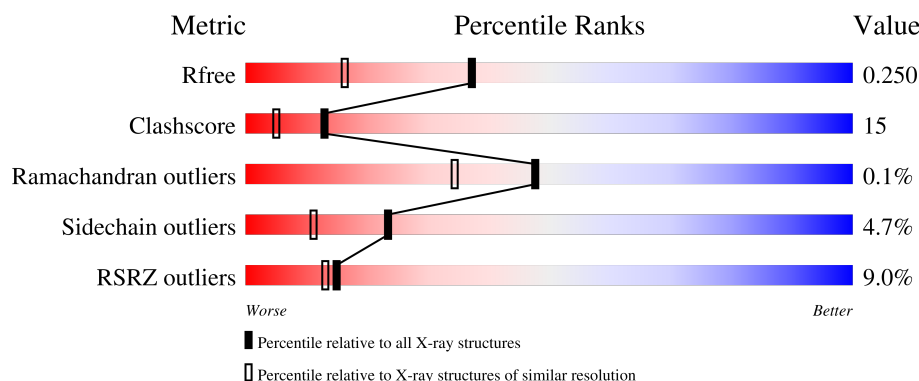
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	322	9% 76% 20% ..
1	B	322	9% 73% 24% .
1	C	322	11% 74% 20% 5% .
1	D	322	7% 74% 22% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	501	-	-	X	-
3	GOL	C	502	-	-	X	-
4	EDO	A	507	-	-	X	-
4	EDO	A	510	-	-	X	-
4	EDO	B	502	-	-	X	-
4	EDO	B	507	-	-	X	-
7	PEG	C	506	-	-	X	-
7	PEG	C	507	-	-	X	-

2 Entry composition [i](#)

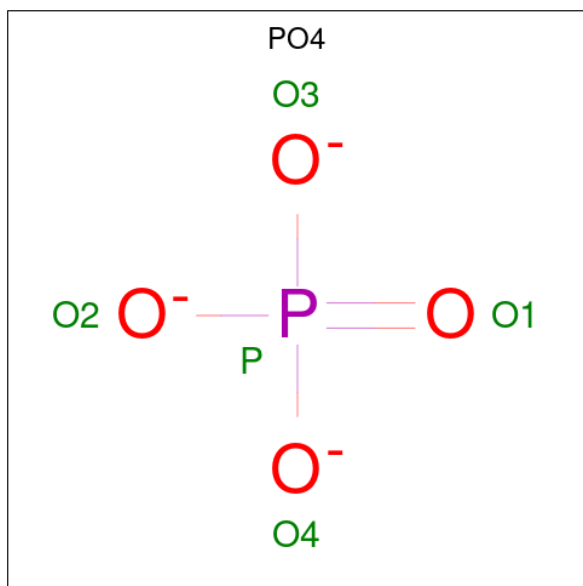
There are 9 unique types of molecules in this entry. The entry contains 11278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	5	0
			2507	1560	449	488	10			
1	B	322	Total	C	N	O	S	0	3	0
			2503	1559	448	486	10			
1	C	322	Total	C	N	O	S	0	3	0
			2501	1558	446	486	11			
1	D	322	Total	C	N	O	S	0	6	0
			2509	1562	448	489	10			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



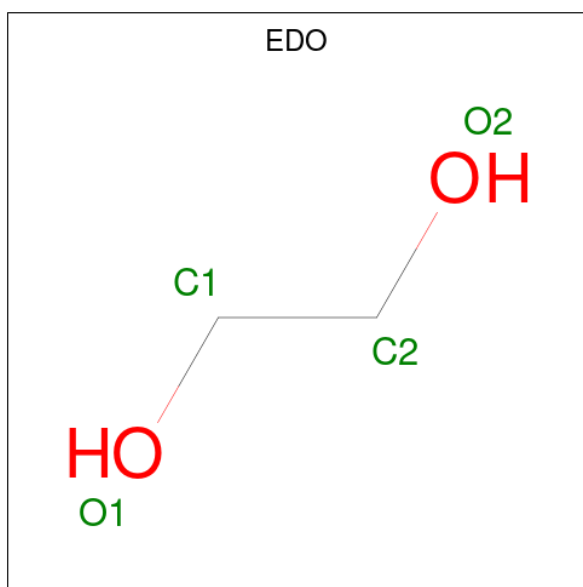
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O P	0	0
			5	4 1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



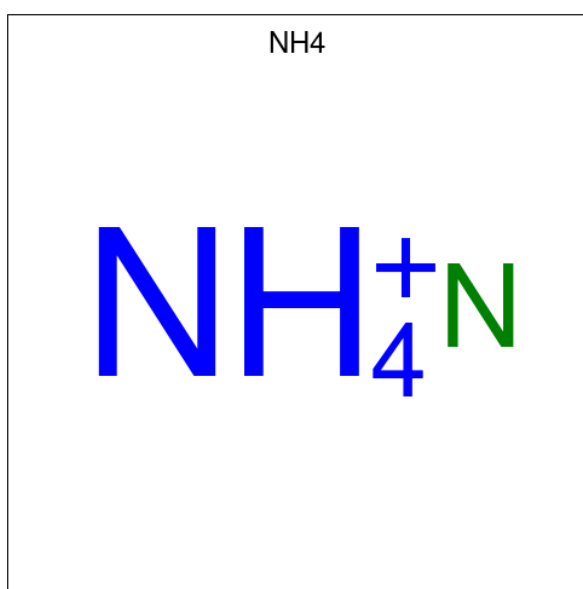
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



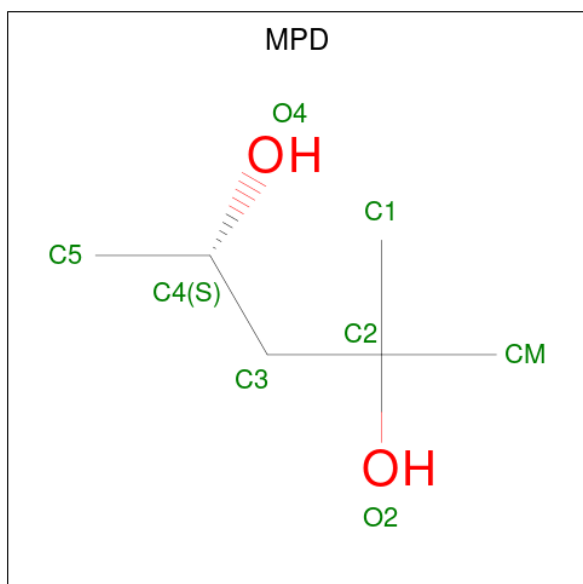
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 1 1	0	0
5	A	1	Total N 1 1	0	0
5	A	1	Total N 1 1	0	0
5	A	1	Total N 1 1	0	0
5	B	1	Total N 1 1	0	0
5	B	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0

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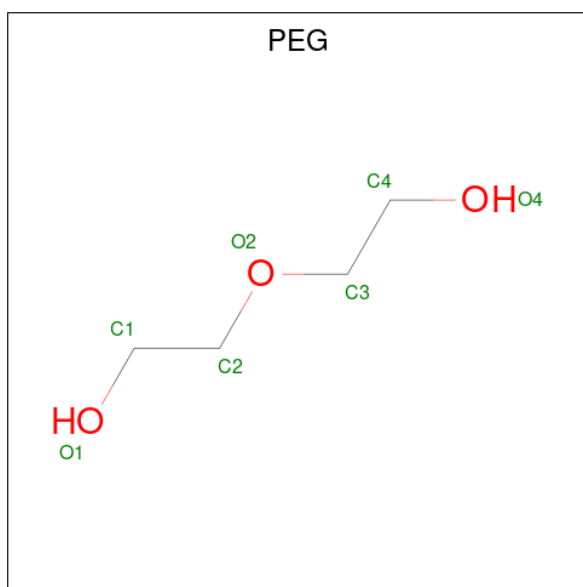
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	D	1	Total N 1 1	0	0
5	D	1	Total N 1 1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



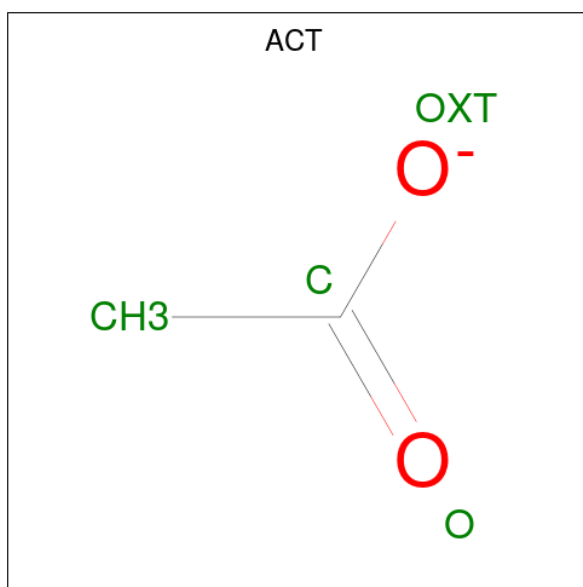
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 8 6 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		

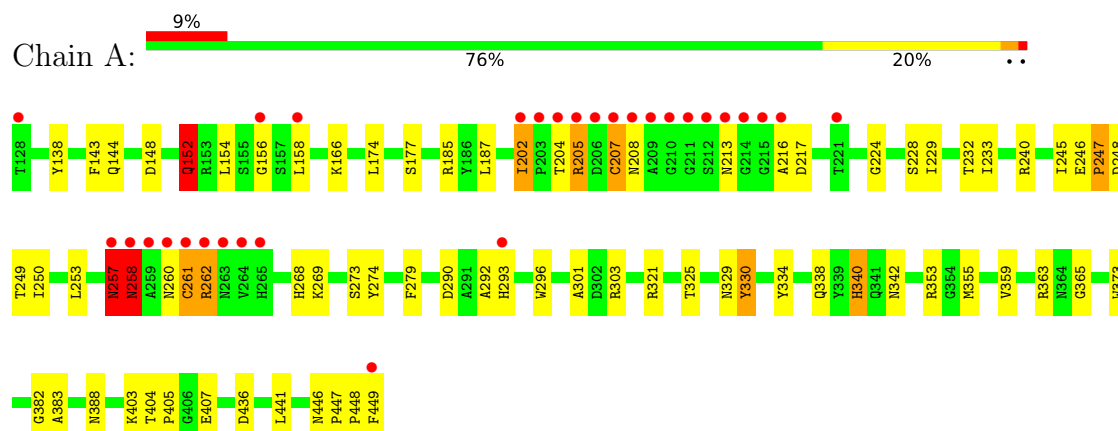
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	275	Total 275	O 275	0	0
9	B	274	Total 274	O 274	0	0
9	C	273	Total 273	O 273	0	0
9	D	271	Total 271	O 271	0	0

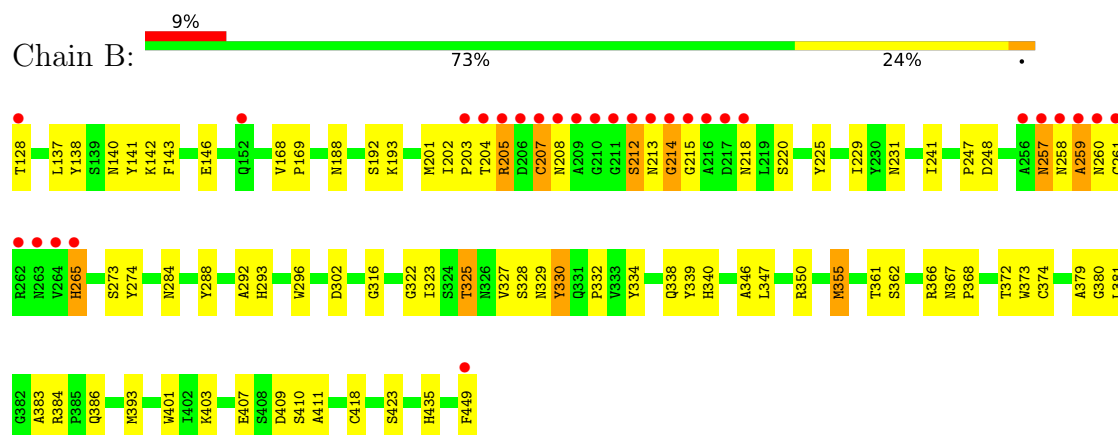
3 Residue-property plots [i](#)

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.

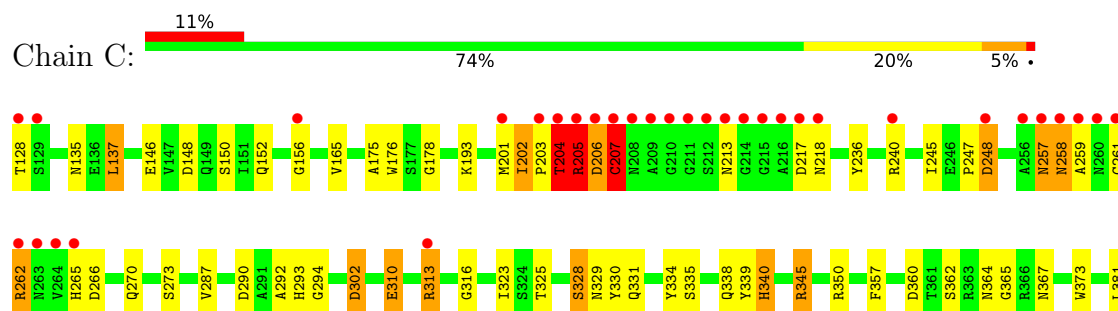
• Molecule 1: Glucanase



• Molecule 1: Glucanase

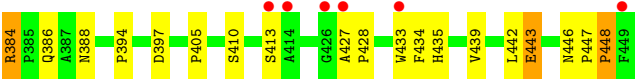
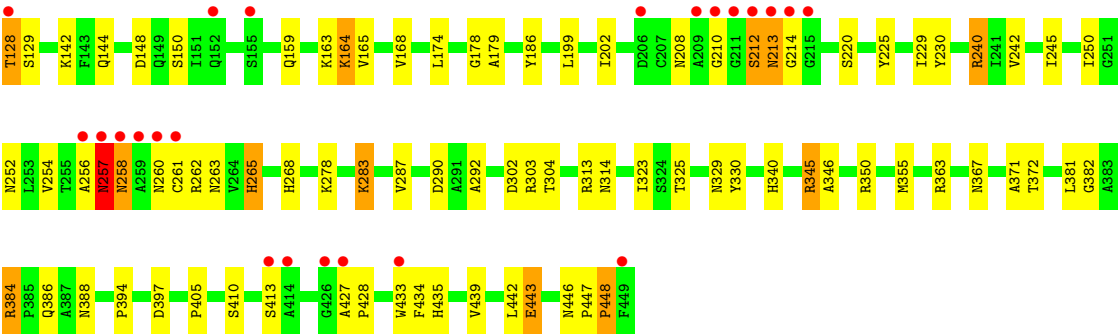
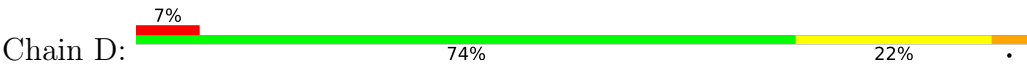


• Molecule 1: Glucanase





● Molecule 1: Glucanase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	309.86Å 87.35Å 82.55Å 90.00° 93.95° 90.00°	Depositor
Resolution (Å)	27.76 – 1.80 27.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (27.76-1.80) 98.4 (27.76-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.239 (Not available) , 0.250	Depositor DCC
R_{free} test set	10048 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.2	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	0.95	EDS
Total number of atoms	11278	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, NH4, GOL, ACT, MPD, PO4

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	1.75	27/2592 (1.0%)	1.39	12/3523 (0.3%)
1	B	1.71	34/2577 (1.3%)	1.42	23/3503 (0.7%)
1	C	1.63	21/2574 (0.8%)	1.34	11/3498 (0.3%)
1	D	1.65	26/2598 (1.0%)	1.41	21/3532 (0.6%)
All	All	1.69	108/10341 (1.0%)	1.39	67/14056 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	382	GLY	C-O	9.01	1.32	1.23
1	B	366	ARG	N-CA	8.98	1.57	1.45
1	B	372	THR	CA-C	8.76	1.64	1.52
1	D	168	VAL	CA-C	8.49	1.59	1.53
1	D	388	ASN	N-CA	8.42	1.52	1.46
1	C	340	HIS	ND1-CE1	8.25	1.40	1.32
1	A	382	GLY	C-O	-8.02	1.16	1.24
1	D	229	ILE	CA-C	-8.01	1.42	1.52
1	D	278	LYS	C-O	7.92	1.30	1.23
1	D	388	ASN	CA-CB	7.84	1.59	1.52
1	D	268	HIS	CE1-NE2	7.67	1.40	1.32
1	C	175	ALA	N-CA	7.63	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	LYS	CA-C	7.26	1.62	1.52
1	C	287	VAL	CA-C	7.25	1.61	1.52
1	D	144	GLN	N-CA	7.20	1.54	1.46
1	B	347	LEU	N-CA	7.17	1.54	1.46
1	B	231	ASN	N-CA	7.15	1.55	1.46
1	B	346	ALA	CA-C	7.02	1.61	1.52
1	B	288	TYR	N-CA	6.95	1.54	1.46
1	A	405	PRO	C-O	-6.94	1.16	1.23
1	D	394	PRO	N-CA	-6.86	1.38	1.47
1	A	334	TYR	N-CA	6.82	1.54	1.46
1	B	373	TRP	N-CA	6.82	1.55	1.46
1	B	229	ILE	CA-CB	6.79	1.62	1.54
1	B	380	GLY	N-CA	6.78	1.52	1.45
1	D	292	ALA	C-O	-6.76	1.17	1.24
1	B	435	HIS	CG-ND1	-6.68	1.30	1.38
1	B	292	ALA	C-O	-6.63	1.18	1.24
1	D	148	ASP	N-CA	6.60	1.54	1.46
1	A	292	ALA	C-O	-6.49	1.17	1.24
1	B	274	TYR	N-CA	6.49	1.54	1.46
1	B	409	ASP	C-O	-6.48	1.16	1.24
1	D	174	LEU	CA-C	-6.34	1.44	1.53
1	C	340	HIS	N-CA	6.30	1.53	1.46
1	A	388	ASN	C-O	-6.21	1.21	1.23
1	A	359	VAL	CA-CB	6.20	1.63	1.54
1	B	401	TRP	NE1-CE2	-6.18	1.30	1.37
1	D	225	TYR	N-CA	6.17	1.53	1.46
1	C	292	ALA	C-O	-6.15	1.17	1.24
1	B	323	ILE	C-O	-6.10	1.18	1.24
1	B	339	TYR	CA-C	6.05	1.60	1.52
1	B	401	TRP	C-O	6.04	1.31	1.23
1	C	400	VAL	N-CA	6.03	1.53	1.46
1	A	365	GLY	N-CA	5.98	1.53	1.45
1	D	443	GLU	N-CA	5.93	1.53	1.46
1	B	325	THR	N-CA	5.92	1.53	1.45
1	C	328	SER	CA-C	5.91	1.60	1.52
1	D	323	ILE	C-O	-5.89	1.18	1.24
1	C	410	SER	C-O	-5.89	1.17	1.23
1	A	404	THR	C-O	-5.89	1.17	1.24
1	C	293	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	342	ASN	N-CA	-5.83	1.39	1.46
1	B	193	LYS	N-CA	5.82	1.53	1.45
1	A	245	ILE	CA-C	-5.82	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	ASN	CA-C	5.82	1.61	1.52
1	A	232	THR	N-CA	5.76	1.53	1.46
1	A	229	ILE	CA-CB	5.74	1.61	1.54
1	B	435	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	188	ASN	N-CA	5.68	1.53	1.46
1	A	174	LEU	CA-C	-5.67	1.46	1.53
1	A	202	ILE	CA-C	5.62	1.58	1.52
1	D	405	PRO	C-O	-5.62	1.17	1.23
1	D	230	TYR	CA-C	5.61	1.59	1.52
1	C	293	HIS	CG-ND1	-5.60	1.32	1.38
1	D	179	ALA	CA-C	-5.59	1.45	1.52
1	B	393	MET	CA-C	5.55	1.59	1.52
1	A	148	ASP	N-CA	5.52	1.53	1.46
1	D	245	ILE	N-CA	5.52	1.52	1.46
1	A	273	SER	C-O	-5.51	1.17	1.24
1	A	301	ALA	N-CA	-5.50	1.39	1.46
1	D	142	LYS	CA-CB	5.49	1.62	1.53
1	A	279	PHE	N-CA	5.48	1.53	1.46
1	B	137	LEU	CA-CB	5.44	1.61	1.53
1	B	316	GLY	N-CA	5.42	1.53	1.45
1	D	186	TYR	CA-CB	5.42	1.61	1.53
1	B	386	GLN	CA-C	-5.41	1.45	1.52
1	C	137	LEU	CA-CB	5.39	1.61	1.53
1	C	236	TYR	C-O	-5.39	1.17	1.24
1	A	187	LEU	N-CA	-5.38	1.39	1.46
1	A	446	ASN	C-O	-5.38	1.17	1.24
1	B	293	HIS	CD2-NE2	-5.34	1.31	1.37
1	A	202	ILE	C-N	5.34	1.40	1.33
1	C	331	GLN	N-CA	5.33	1.53	1.45
1	C	401	TRP	C-O	5.32	1.30	1.23
1	B	192	SER	CA-C	5.31	1.60	1.52
1	A	321	ARG	C-O	-5.30	1.17	1.24
1	B	411	ALA	C-O	-5.29	1.17	1.23
1	D	397	ASP	C-O	-5.26	1.18	1.24
1	D	199	LEU	C-O	5.26	1.30	1.24
1	A	247	PRO	CA-C	-5.26	1.46	1.52
1	A	143	PHE	CA-CB	5.26	1.61	1.53
1	C	340	HIS	CG-ND1	-5.24	1.32	1.38
1	B	355	MET	C-O	5.23	1.30	1.23
1	C	365	GLY	CA-C	5.22	1.58	1.51
1	C	387	ALA	CA-C	5.16	1.59	1.52
1	C	373	TRP	NE1-CE2	-5.14	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	TYR	CA-CB	5.13	1.62	1.53
1	A	340	HIS	CB-CG	5.11	1.57	1.50
1	C	290	ASP	C-O	-5.11	1.17	1.23
1	A	383	ALA	C-O	-5.10	1.17	1.23
1	A	441	LEU	CA-CB	5.10	1.61	1.53
1	D	381	LEU	C-O	5.09	1.29	1.23
1	B	423	SER	C-O	5.07	1.30	1.24
1	D	287	VAL	N-CA	5.07	1.52	1.46
1	D	159	GLN	C-O	-5.07	1.18	1.24
1	C	316	GLY	C-O	-5.05	1.17	1.24
1	C	360	ASP	C-O	5.04	1.29	1.24
1	B	361	THR	N-CA	5.02	1.51	1.46

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	258	ASN	N-CA-C	11.38	123.76	111.36
1	C	411	ALA	N-CA-C	-9.31	96.70	110.48
1	B	214	GLY	N-CA-C	9.17	127.51	111.46
1	B	207	CYS	N-CA-C	8.57	122.97	108.23
1	C	217	ASP	N-CA-C	8.22	122.03	108.96
1	B	379	ALA	CA-C-N	-7.82	113.30	121.35
1	B	379	ALA	C-N-CA	-7.82	113.30	121.35
1	A	373	TRP	N-CA-C	7.76	120.82	111.82
1	A	233	ILE	N-CA-C	7.62	119.30	110.62
1	B	168	VAL	N-CA-C	-6.91	102.69	108.63
1	A	330	TYR	N-CA-CB	-6.75	100.29	111.49
1	C	339	TYR	N-CA-C	-6.46	104.32	111.36
1	D	163	LYS	N-CA-C	6.32	118.98	111.71
1	D	367	ASN	CA-C-N	-6.28	113.48	119.76
1	D	367	ASN	C-N-CA	-6.28	113.48	119.76
1	D	202	ILE	CA-C-N	-6.03	113.55	119.64
1	D	202	ILE	C-N-CA	-6.03	113.55	119.64
1	A	138	TYR	N-CA-C	6.00	119.03	110.10
1	B	273	SER	O-C-N	5.98	128.46	122.12
1	D	254	VAL	N-CA-C	5.98	116.15	110.53
1	B	140	ASN	N-CA-C	5.96	119.34	110.52
1	D	435	HIS	N-CA-C	5.95	117.56	111.14
1	D	443	GLU	N-CA-C	-5.83	105.00	111.71
1	C	207	CYS	N-CA-C	5.79	120.50	112.45
1	B	143	PHE	N-CA-C	-5.75	104.62	111.69
1	C	258	ASN	CB-CA-C	-5.74	100.22	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	GLY	N-CA-C	5.73	120.07	111.42
1	B	169	PRO	CB-CA-C	-5.70	103.62	111.21
1	D	178	GLY	N-CA-C	5.66	120.90	114.67
1	D	257	ASN	CA-C-N	5.64	128.30	120.29
1	D	257	ASN	C-N-CA	5.64	128.30	120.29
1	D	304	THR	N-CA-C	-5.63	105.22	111.36
1	B	330	TYR	N-CA-CB	-5.63	102.15	111.49
1	D	314	ASN	N-CA-C	5.62	119.76	113.02
1	B	168	VAL	CB-CA-C	-5.61	105.72	110.94
1	D	265	HIS	N-CA-C	5.61	117.39	111.28
1	B	138	TYR	N-CA-C	5.59	118.34	109.96
1	A	166	LYS	N-CA-C	5.57	117.79	111.11
1	C	135	ASN	N-CA-C	-5.52	99.05	110.80
1	B	207	CYS	CB-CA-C	-5.50	101.76	111.05
1	B	374	CYS	N-CA-C	5.47	117.22	108.41
1	C	204	THR	N-CA-C	5.43	122.37	110.80
1	A	217	ASP	N-CA-CB	5.40	119.68	110.50
1	D	168	VAL	N-CA-C	-5.39	103.99	108.63
1	A	363	ARG	CA-CB-CG	-5.31	103.47	114.10
1	D	363	ARG	CA-C-N	-5.28	114.19	122.79
1	D	363	ARG	C-N-CA	-5.28	114.19	122.79
1	A	152[A]	GLN	N-CA-C	-5.27	106.69	113.01
1	A	152[B]	GLN	N-CA-C	-5.27	106.69	113.01
1	C	248	ASP	CB-CA-C	-5.24	104.84	111.86
1	B	327	VAL	N-CA-C	5.23	115.99	108.93
1	A	258	ASN	N-CA-CB	-5.22	103.79	111.51
1	B	241	ILE	CA-C-N	-5.19	116.76	123.19
1	B	241	ILE	C-N-CA	-5.19	116.76	123.19
1	B	292	ALA	CB-CA-C	-5.16	110.65	116.63
1	C	245	ILE	N-CA-C	5.14	115.75	107.73
1	B	368	PRO	CB-CA-C	-5.13	103.30	110.63
1	D	346	ALA	N-CA-C	5.12	116.86	111.28
1	B	259	ALA	CB-CA-C	-5.11	102.31	110.79
1	D	242	VAL	N-CA-C	-5.11	101.02	108.17
1	C	398	ALA	CB-CA-C	-5.10	101.78	109.99
1	B	215	GLY	N-CA-C	5.09	125.24	113.18
1	B	373	TRP	N-CA-C	-5.07	107.27	113.50
1	D	142	LYS	N-CA-C	5.05	116.59	111.14
1	A	388	ASN	CA-C-N	-5.04	114.55	119.64
1	A	388	ASN	C-N-CA	-5.04	114.55	119.64
1	C	302	ASP	N-CA-C	5.01	116.44	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	ALA	Peptide
1	A	257	ASN	Peptide
1	C	207	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2507	0	2391	79	0
1	B	2503	0	2390	83	0
1	C	2501	0	2396	69	0
1	D	2509	0	2400	55	0
2	A	5	0	0	1	0
3	A	12	0	16	4	0
3	B	6	0	8	2	0
3	C	12	0	16	13	0
3	D	12	0	16	3	0
4	A	40	0	60	36	0
4	B	12	0	18	19	0
4	C	12	0	18	3	0
4	D	8	0	12	2	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	5	0	0	0	0
5	D	2	0	0	0	0
6	B	8	0	14	2	0
7	C	14	0	20	11	0
7	D	7	0	10	2	0
8	C	4	0	3	1	0
9	A	275	0	0	17	0
9	B	274	0	0	12	0
9	C	273	0	0	11	0
9	D	271	0	0	5	0
All	All	11278	0	9788	300	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 15.

All (300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:HG22	1:B:213:ASN:CB	1.65	1.23
1:A:248:ASP:HA	9:A:665:HOH:O	1.47	1.15
1:D:240:ARG:HG3	1:D:240:ARG:HH11	1.12	1.13
1:B:204:THR:HG22	1:B:213:ASN:HB3	1.24	1.11
1:A:250:ILE:H	4:A:507:EDO:C1	1.64	1.10
3:C:501:GOL:H31	9:C:769:HOH:O	1.54	1.05
1:D:208:ASN:O	1:D:210:GLY:HA3	1.58	1.04
1:B:257:ASN:ND2	1:B:258:ASN:N	2.11	0.98
1:A:250:ILE:H	4:A:507:EDO:H12	1.29	0.97
1:B:407:GLU:OE1	3:B:501:GOL:H11	1.65	0.95
1:B:338:GLN:CB	4:B:507:EDO:H12	1.97	0.95
1:B:257:ASN:ND2	1:B:259:ALA:H	1.64	0.94
1:B:257:ASN:HD22	1:B:259:ALA:H	1.13	0.93
1:B:204:THR:CG2	1:B:213:ASN:HB3	1.99	0.93
1:B:257:ASN:HD22	1:B:258:ASN:N	1.68	0.92
4:B:502:EDO:H22	9:B:699:HOH:O	1.70	0.90
1:C:205:ARG:HG3	1:C:205:ARG:HH11	1.37	0.89
1:A:248:ASP:N	4:A:507:EDO:H21	1.88	0.88
1:B:204:THR:HG22	1:B:213:ASN:HB2	1.53	0.88
7:D:505:PEG:H41	9:D:614:HOH:O	1.72	0.88
1:D:252:ASN:O	1:D:256:ALA:HB2	1.72	0.88
1:D:220[A]:SER:OG	3:D:501:GOL:C3	2.21	0.88
1:B:204:THR:CG2	1:B:213:ASN:CB	2.51	0.88
1:B:201:MET:HG2	9:B:841:HOH:O	1.71	0.87
1:A:250:ILE:H	4:A:507:EDO:H11	1.39	0.86
1:C:387:ALA:H	7:C:506:PEG:C4	1.89	0.85
4:B:507:EDO:H11	1:C:335:SER:HB2	1.57	0.85
1:B:205:ARG:HD2	9:B:673:HOH:O	1.75	0.84
1:A:224:GLY:HA2	4:A:512:EDO:H22	1.59	0.84
1:B:384:ARG:HB3	4:B:503:EDO:H21	1.60	0.84
1:C:257:ASN:HD22	1:C:258:ASN:N	1.76	0.84
1:D:220[A]:SER:OG	3:D:501:GOL:H31	1.77	0.83
4:A:505:EDO:H11	1:C:156:GLY:HA3	1.61	0.82
1:D:427:ALA:HB2	1:D:434:PHE:CE2	2.14	0.82
9:B:790:HOH:O	1:C:345:ARG:HD2	1.78	0.82
1:A:290:ASP:OD2	4:A:507:EDO:H22	1.79	0.82
1:B:329:ASN:HD22	1:B:330:TYR:H	1.25	0.81
1:B:338:GLN:HB2	4:B:507:EDO:H12	1.61	0.81
1:A:338:GLN:CD	9:A:644:HOH:O	2.24	0.81
1:A:144:GLN:OE1	3:A:503:GOL:H31	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:O	1:D:210:GLY:CA	2.29	0.80
1:C:137:LEU:HG	7:C:506:PEG:H11	1.64	0.80
1:C:273:SER:HB2	4:C:504:EDO:H21	1.64	0.80
1:B:204:THR:CG2	1:B:214:GLY:H	1.96	0.79
1:B:205:ARG:NH1	1:B:205:ARG:HB2	1.98	0.79
1:B:329:ASN:ND2	1:B:330:TYR:H	1.79	0.79
1:D:384:ARG:HD3	1:D:384:ARG:N	1.97	0.77
1:A:250:ILE:HB	4:A:507:EDO:H11	1.64	0.77
1:A:262:ARG:HA	1:A:262:ARG:HE	1.50	0.77
1:B:334:TYR:HB3	3:C:502:GOL:H11	1.67	0.77
1:A:329:ASN:HD22	1:A:330:TYR:H	1.31	0.77
1:C:205:ARG:HH11	1:C:205:ARG:CG	1.96	0.77
1:A:224:GLY:CA	4:A:512:EDO:H22	2.15	0.76
7:C:506:PEG:H12	9:C:640:HOH:O	1.86	0.76
1:B:257:ASN:HD22	1:B:257:ASN:C	1.93	0.76
1:A:329:ASN:ND2	1:A:330:TYR:H	1.84	0.74
1:A:204:THR:O	1:A:268:HIS:HE1	1.70	0.73
1:C:257:ASN:HD22	1:C:259:ALA:H	1.36	0.73
1:B:204:THR:HA	1:B:213:ASN:CG	2.13	0.73
1:C:206:ASP:OD1	1:C:206:ASP:C	2.31	0.73
1:B:338:GLN:HG3	4:B:507:EDO:O2	1.89	0.73
1:A:338:GLN:NE2	9:A:601:HOH:O	2.20	0.73
1:C:329:ASN:HD22	1:C:330:TYR:H	1.37	0.72
7:C:507:PEG:H11	9:C:677:HOH:O	1.88	0.72
1:B:204:THR:HG22	1:B:214:GLY:N	2.05	0.72
1:C:387:ALA:H	7:C:506:PEG:H41	1.55	0.72
1:C:364:ASN:O	3:C:501:GOL:H11	1.90	0.71
1:B:205:ARG:NH1	1:B:205:ARG:H	1.88	0.71
1:C:329:ASN:ND2	1:C:330:TYR:H	1.88	0.71
4:B:503:EDO:H11	9:B:836:HOH:O	1.91	0.71
1:B:204:THR:CG2	1:B:213:ASN:HB2	2.20	0.71
1:B:257:ASN:HD22	1:B:259:ALA:N	1.87	0.70
1:A:250:ILE:CB	4:A:507:EDO:H11	2.20	0.70
1:C:310:GLU:HG2	1:C:313:ARG:NH1	2.06	0.70
1:C:302:ASP:HB3	1:C:350:ARG:NH2	2.07	0.70
1:B:257:ASN:ND2	1:B:259:ALA:N	2.39	0.70
1:B:204:THR:HG22	1:B:214:GLY:H	1.55	0.70
1:D:240:ARG:HH11	1:D:240:ARG:CG	2.00	0.69
1:A:250:ILE:N	4:A:507:EDO:H12	2.05	0.69
1:C:384:ARG:HD3	1:C:384:ARG:N	2.06	0.69
1:D:220[A]:SER:OG	3:D:501:GOL:H32	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:505:EDO:H11	1:C:156:GLY:CA	2.22	0.69
1:B:302:ASP:HB3	1:B:350:ARG:NH2	2.08	0.69
1:B:383:ALA:HB1	4:B:502:EDO:H21	1.74	0.69
1:D:212:SER:HA	1:D:214:GLY:H	1.57	0.68
1:B:205:ARG:N	1:B:205:ARG:HH11	1.91	0.68
6:B:504:MPD:C5	9:B:834:HOH:O	2.42	0.67
1:A:248:ASP:H	4:A:507:EDO:H21	1.58	0.67
1:C:257:ASN:ND2	1:C:258:ASN:N	2.42	0.66
1:A:247:PRO:O	1:A:248:ASP:HB2	1.96	0.66
1:A:290:ASP:HB3	4:A:507:EDO:H22	1.78	0.66
1:D:329:ASN:ND2	1:D:330:TYR:H	1.92	0.65
1:B:204:THR:CG2	1:B:214:GLY:N	2.59	0.65
1:B:257:ASN:ND2	1:B:258:ASN:H	1.92	0.64
1:D:256:ALA:HB1	1:D:265:HIS:HE1	1.62	0.64
4:A:509:EDO:H11	9:A:677:HOH:O	1.97	0.64
1:D:213:ASN:O	1:D:213:ASN:ND2	2.30	0.64
1:A:325:THR:OG1	1:A:340:HIS:HE1	1.80	0.64
1:B:384:ARG:CB	4:B:503:EDO:H21	2.28	0.64
1:B:260:ASN:OD1	1:B:260:ASN:O	2.16	0.64
1:A:403:LYS:NZ	3:A:502:GOL:H31	2.13	0.64
1:D:164:LYS:HE3	9:D:828:HOH:O	1.98	0.63
1:A:154:LEU:HD23	4:A:510:EDO:H11	1.78	0.63
1:D:240:ARG:HG3	1:D:240:ARG:NH1	1.91	0.63
1:B:214:GLY:C	1:B:218:ASN:HD21	2.07	0.63
1:C:257:ASN:O	1:C:258:ASN:CB	2.47	0.62
1:D:302:ASP:CG	1:D:350:ARG:HH21	2.07	0.62
1:C:205:ARG:CG	1:C:205:ARG:NH1	2.61	0.62
1:B:338:GLN:NE2	9:B:602:HOH:O	2.31	0.62
1:A:257:ASN:HA	1:A:258:ASN:OD1	1.99	0.62
1:C:257:ASN:O	1:C:258:ASN:HB2	1.98	0.62
1:B:204:THR:CB	1:B:213:ASN:HB2	2.30	0.62
1:D:303:ARG:HG3	1:D:303:ARG:HH11	1.64	0.61
1:B:204:THR:HA	1:B:213:ASN:CB	2.30	0.61
1:B:205:ARG:HB2	1:B:205:ARG:CZ	2.30	0.61
1:B:260:ASN:O	1:B:260:ASN:CG	2.44	0.61
1:C:334:TYR:HB3	3:C:502:GOL:H31	1.82	0.61
1:A:353:ARG:HD2	9:A:652:HOH:O	2.00	0.61
1:B:338:GLN:HB3	4:B:507:EDO:H12	1.81	0.61
1:B:449:PHE:C	9:B:820:HOH:O	2.45	0.60
1:D:252:ASN:O	1:D:256:ALA:CB	2.49	0.60
1:A:250:ILE:N	4:A:507:EDO:H11	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152[A]:GLN:NE2	9:A:606:HOH:O	2.33	0.60
1:D:329:ASN:HD22	1:D:330:TYR:H	1.48	0.60
1:B:204:THR:CA	1:B:213:ASN:CB	2.79	0.60
1:C:261:CYS:SG	1:C:265:HIS:CE1	2.95	0.59
1:C:383:ALA:HB1	7:C:507:PEG:H12	1.85	0.59
1:B:258:ASN:HA	1:B:261:CYS:HB2	1.85	0.58
1:C:334:TYR:CB	3:C:502:GOL:H31	2.34	0.57
1:C:150:SER:OG	1:C:435:HIS:HD2	1.87	0.57
1:D:128:THR:CG2	1:D:129:SER:N	2.68	0.57
1:A:407:GLU:OE1	3:A:502:GOL:H32	2.05	0.57
7:C:507:PEG:C1	9:C:677:HOH:O	2.50	0.57
1:A:154:LEU:HD23	4:A:510:EDO:C1	2.34	0.57
1:B:205:ARG:H	1:B:205:ARG:HH11	1.51	0.57
1:D:256:ALA:CB	1:D:265:HIS:HE1	2.18	0.57
1:B:203:PRO:O	1:B:204:THR:OG1	2.22	0.56
1:C:435:HIS:HE1	9:C:828:HOH:O	1.86	0.56
1:A:290:ASP:OD2	4:A:507:EDO:C2	2.52	0.56
1:B:338:GLN:CG	4:B:507:EDO:O2	2.52	0.56
1:C:387:ALA:CB	7:C:506:PEG:H41	2.36	0.56
3:C:501:GOL:C3	9:C:769:HOH:O	2.30	0.56
1:A:403:LYS:HZ1	3:A:502:GOL:H31	1.69	0.56
1:D:164:LYS:HE2	1:D:164:LYS:HA	1.88	0.56
1:A:253:LEU:HD22	1:A:269[B]:LYS:HE3	1.88	0.56
1:B:204:THR:HG21	1:B:214:GLY:H	1.70	0.56
1:B:332:PRO:CB	3:C:502:GOL:H2	2.36	0.56
1:A:268:HIS:HD2	9:A:788:HOH:O	1.89	0.55
1:C:165:VAL:HG21	1:C:442:LEU:HD11	1.88	0.55
1:A:436:ASP:HB3	4:A:505:EDO:H22	1.88	0.55
1:B:367:ASN:HD21	3:C:502:GOL:C3	2.20	0.55
1:C:310:GLU:HG2	1:C:313:ARG:HH11	1.71	0.55
1:C:325:THR:OG1	1:C:340:HIS:HE1	1.89	0.54
1:D:302:ASP:OD2	1:D:350:ARG:NH2	2.40	0.54
1:A:290:ASP:CB	4:A:507:EDO:H22	2.37	0.54
1:A:250:ILE:N	4:A:507:EDO:C1	2.50	0.54
1:B:355:MET:HA	1:B:355:MET:HE2	1.89	0.54
1:B:204:THR:CA	1:B:213:ASN:HB2	2.37	0.54
1:B:367:ASN:HD21	3:C:502:GOL:H32	1.73	0.54
1:C:257:ASN:ND2	1:C:258:ASN:H	2.05	0.54
1:D:283:LYS:H	1:D:283:LYS:HZ2	1.54	0.54
1:A:269[A]:LYS:HE2	9:A:840:HOH:O	2.08	0.53
1:C:204:THR:C	1:C:206:ASP:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:TYR:HA	4:A:504:EDO:H11	1.91	0.53
1:C:447:PRO:HG2	7:C:507:PEG:H21	1.91	0.53
1:D:256:ALA:CB	1:D:265:HIS:CE1	2.91	0.52
1:B:257:ASN:O	1:B:258:ASN:CB	2.58	0.52
1:D:165:VAL:HG21	1:D:442:LEU:CD1	2.39	0.52
1:D:263:ASN:HD21	4:D:503:EDO:H21	1.74	0.52
1:A:249:THR:H	4:A:507:EDO:H21	1.75	0.52
1:C:364:ASN:O	3:C:501:GOL:C1	2.56	0.52
1:D:263:ASN:HD21	4:D:503:EDO:C2	2.23	0.52
4:B:507:EDO:H22	1:C:294:GLY:HA3	1.92	0.51
1:D:212:SER:HA	1:D:214:GLY:N	2.25	0.51
1:B:296:TRP:HZ3	9:B:823:HOH:O	1.91	0.51
1:B:325:THR:OG1	1:B:340:HIS:HE1	1.94	0.51
1:A:208:ASN:OD1	1:A:208:ASN:O	2.29	0.51
1:B:261:CYS:HB3	1:B:265[B]:HIS:CE1	2.45	0.51
1:A:250:ILE:CG1	4:A:507:EDO:H11	2.41	0.50
6:B:504:MPD:H52	9:B:834:HOH:O	2.08	0.50
1:C:262:ARG:O	1:C:266:ASP:OD2	2.29	0.50
1:B:212:SER:C	1:B:213:ASN:HD22	2.19	0.50
1:C:206:ASP:OD1	1:C:207:CYS:N	2.45	0.50
1:A:156:GLY:HA3	9:C:669:HOH:O	2.11	0.50
1:A:262:ARG:HA	1:A:262:ARG:NE	2.24	0.50
1:A:258:ASN:ND2	1:A:262:ARG:NH2	2.59	0.50
1:C:257:ASN:ND2	1:C:259:ALA:H	2.06	0.50
1:D:303:ARG:HH11	1:D:303:ARG:CG	2.25	0.50
1:B:205:ARG:HG2	9:B:613:HOH:O	2.12	0.50
1:C:165:VAL:HG21	1:C:442:LEU:CD1	2.41	0.50
1:A:249:THR:HB	4:A:507:EDO:H12	1.94	0.49
1:D:250[A]:ILE:HD12	1:D:290:ASP:O	2.13	0.49
1:C:148:ASP:O	1:C:152:GLN:HG2	2.12	0.49
1:C:176:TRP:CZ2	1:C:178:GLY:HA3	2.47	0.49
1:B:367:ASN:ND2	3:C:502:GOL:H32	2.27	0.49
1:C:362:SER:O	1:C:381:LEU:HA	2.12	0.49
1:D:257:ASN:C	1:D:257:ASN:HD22	2.20	0.49
1:A:355:MET:HE2	1:A:355:MET:HA	1.95	0.48
1:D:262:ARG:NH2	9:D:605:HOH:O	2.40	0.48
1:B:247:PRO:O	1:B:248:ASP:HB2	2.14	0.48
1:B:338:GLN:HE21	4:B:507:EDO:H21	1.78	0.48
1:D:257:ASN:ND2	1:D:257:ASN:H	2.11	0.48
1:A:293:HIS:CE1	1:A:296:TRP:N	2.81	0.48
1:B:204:THR:OG1	1:B:204:THR:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLN:CG	9:A:644:HOH:O	2.60	0.48
1:A:248:ASP:H	4:A:507:EDO:C2	2.26	0.48
1:D:258:ASN:O	1:D:261:CYS:N	2.47	0.48
1:D:325:THR:OG1	1:D:340:HIS:HE1	1.97	0.47
1:D:448[A]:PRO:HB3	9:D:823:HOH:O	2.12	0.47
1:A:207:CYS:HB3	1:A:261:CYS:CA	2.44	0.47
1:C:257:ASN:HD22	1:C:259:ALA:N	2.07	0.47
1:B:338:GLN:NE2	4:B:507:EDO:O2	2.47	0.47
1:A:290:ASP:CG	4:A:507:EDO:H22	2.37	0.47
1:A:204:THR:O	1:A:268:HIS:CE1	2.60	0.47
1:C:338:GLN:NE2	9:C:603:HOH:O	2.30	0.47
1:D:128:THR:HG22	1:D:129:SER:N	2.30	0.47
1:D:303:ARG:CG	1:D:303:ARG:NH1	2.77	0.47
1:D:428:PRO:HG3	1:D:433:TRP:O	2.14	0.47
1:A:205:ARG:HG3	1:A:205:ARG:HH11	1.79	0.47
1:B:384:ARG:H	4:B:502:EDO:C2	2.28	0.47
1:A:447:PRO:HA	1:A:448:PRO:HD3	1.77	0.47
1:A:258:ASN:O	1:A:262:ARG:HB2	2.15	0.46
1:A:258:ASN:CB	1:A:262:ARG:HH21	2.28	0.46
1:A:338:GLN:HG3	9:A:644:HOH:O	2.14	0.46
1:B:383:ALA:CB	4:B:502:EDO:H21	2.43	0.46
1:C:302:ASP:HB3	9:C:605:HOH:O	2.15	0.46
1:D:446:ASN:HA	1:D:447:PRO:C	2.40	0.46
1:A:257:ASN:ND2	1:A:257:ASN:H	2.13	0.46
1:C:202:ILE:O	1:C:202:ILE:CG2	2.62	0.46
1:A:154:LEU:CD2	4:A:510:EDO:C1	2.93	0.46
1:A:249:THR:H	4:A:507:EDO:H12	1.81	0.46
1:C:350:ARG:NH2	9:C:605:HOH:O	2.38	0.46
4:A:509:EDO:H21	9:A:677:HOH:O	2.16	0.45
1:A:205:ARG:HH11	1:A:205:ARG:CG	2.29	0.45
1:B:204:THR:HA	1:B:213:ASN:HB2	1.97	0.45
1:D:257:ASN:ND2	1:D:257:ASN:O	2.49	0.45
1:D:439:VAL:O	1:D:443:GLU:HG3	2.17	0.45
1:C:176:TRP:CH2	1:C:178:GLY:HA3	2.50	0.45
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.88	0.45
1:C:137:LEU:CG	7:C:506:PEG:H11	2.42	0.45
1:D:384:ARG:HD3	1:D:384:ARG:H	1.75	0.45
1:D:427:ALA:CB	1:D:434:PHE:CE2	2.92	0.45
1:C:248:ASP:OD2	8:C:513:ACT:OXT	2.34	0.45
1:B:338:GLN:HE21	4:B:507:EDO:C2	2.30	0.44
1:C:334:TYR:HB3	3:C:502:GOL:O1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD21	4:A:510:EDO:H12	1.99	0.44
1:A:250:ILE:HG12	4:A:507:EDO:H11	1.98	0.44
1:B:403:LYS:NZ	3:B:501:GOL:H12	2.32	0.44
1:D:257:ASN:ND2	1:D:257:ASN:N	2.66	0.44
1:D:165:VAL:HG21	1:D:442:LEU:HD11	2.00	0.43
1:A:249:THR:N	4:A:507:EDO:H12	2.33	0.43
1:B:329:ASN:HD22	1:B:330:TYR:N	2.04	0.43
1:D:447:PRO:HG2	7:D:505:PEG:O2	2.17	0.43
1:B:201:MET:HE2	1:B:225:TYR:CG	2.53	0.43
1:C:203:PRO:C	1:C:204:THR:OG1	2.62	0.43
1:A:158:LEU:HB2	9:A:604:HOH:O	2.18	0.43
1:C:146:GLU:OE2	1:C:407:GLU:OE2	2.36	0.43
1:B:302:ASP:CG	1:B:350:ARG:HH22	2.26	0.43
1:C:367:ASN:OD1	3:C:501:GOL:O1	2.37	0.43
1:D:355:MET:HE2	1:D:355:MET:HA	2.01	0.43
1:A:154:LEU:CD2	4:A:510:EDO:H12	2.49	0.42
1:A:185:ARG:HB3	9:A:622:HOH:O	2.19	0.42
7:C:506:PEG:C1	9:C:640:HOH:O	2.57	0.42
1:A:207:CYS:HB3	1:A:261:CYS:HA	2.00	0.42
1:B:205:ARG:NH1	1:B:205:ARG:CB	2.76	0.42
1:C:247:PRO:O	1:C:248:ASP:HB2	2.19	0.42
1:C:203:PRO:CB	1:C:218:ASN:HB3	2.49	0.42
1:A:240:ARG:NH2	9:A:617:HOH:O	2.52	0.42
1:B:410[A]:SER:HB3	1:B:418:CYS:SG	2.60	0.42
1:C:148:ASP:OD1	4:C:505:EDO:C2	2.68	0.42
1:D:258:ASN:O	1:D:261:CYS:HB2	2.20	0.42
1:A:303:ARG:HH22	2:A:501:PO4:P	2.43	0.41
1:A:207:CYS:O	1:A:208:ASN:HB3	2.21	0.41
1:A:449:PHE:C	9:A:714:HOH:O	2.63	0.41
1:A:205:ARG:O	9:A:602:HOH:O	2.22	0.41
9:A:768:HOH:O	1:D:345:ARG:HG2	2.20	0.41
4:B:502:EDO:C2	9:B:699:HOH:O	2.46	0.41
1:B:362:SER:O	1:B:381:LEU:HA	2.20	0.41
1:C:202:ILE:HA	1:C:203:PRO:HD3	1.90	0.41
1:C:412:SER:HA	1:C:418:CYS:HB3	2.01	0.41
1:A:202:ILE:HG13	1:A:246:GLU:CD	2.46	0.41
1:C:266:ASP:O	1:C:270:GLN:HG3	2.20	0.41
1:A:228:SER:HA	4:A:511:EDO:H21	2.03	0.41
1:B:328:SER:HA	1:B:403:LYS:HB2	2.03	0.41
1:C:323:ILE:HB	1:C:357:PHE:CD2	2.55	0.41
1:B:146:GLU:OE2	1:B:407:GLU:OE2	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASP:CB	1:B:350:ARG:NH2	2.82	0.40
1:C:204:THR:C	1:C:206:ASP:N	2.79	0.40
1:C:273:SER:CB	4:C:504:EDO:H21	2.43	0.40
1:D:386:GLN:NE2	9:D:614:HOH:O	2.52	0.40
1:D:213:ASN:O	1:D:213:ASN:CG	2.64	0.40
1:D:371:ALA:O	1:D:372:THR:C	2.65	0.40
1:C:328:SER:HA	1:C:403:LYS:HB2	2.04	0.40
1:C:447:PRO:HA	1:C:448:PRO:HD3	1.96	0.40
1:B:205:ARG:HH11	1:B:205:ARG:CB	2.34	0.40
1:B:383:ALA:CA	4:B:502:EDO:H21	2.51	0.40
1:C:218:ASN:HD22	1:C:218:ASN:HA	1.67	0.40
1:A:207:CYS:O	1:A:208:ASN:CB	2.70	0.40
1:A:262:ARG:NE	1:A:262:ARG:CA	2.84	0.40
1:B:204:THR:HA	1:B:213:ASN:OD1	2.22	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	325/322 (101%)	313 (96%)	12 (4%)	0	100	100
1	B	323/322 (100%)	306 (95%)	17 (5%)	0	100	100
1	C	323/322 (100%)	309 (96%)	13 (4%)	1 (0%)	36	25
1	D	326/322 (101%)	315 (97%)	11 (3%)	0	100	100
All	All	1297/1288 (101%)	1243 (96%)	53 (4%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	205	ARG

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	271/266 (102%)	260 (96%)	11 (4%)	27	15
1	B	269/266 (101%)	259 (96%)	10 (4%)	30	18
1	C	269/266 (101%)	252 (94%)	17 (6%)	16	6
1	D	272/266 (102%)	255 (94%)	17 (6%)	16	6
All	All	1081/1064 (102%)	1026 (95%)	55 (5%)	23	9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152[A]	GLN
1	A	152[B]	GLN
1	A	177	SER
1	A	205	ARG
1	A	207	CYS
1	A	213	ASN
1	A	257	ASN
1	A	258	ASN
1	A	260	ASN
1	A	261	CYS
1	A	262	ARG
1	B	128	THR
1	B	202	ILE
1	B	205	ARG
1	B	207	CYS
1	B	208	ASN
1	B	212	SER
1	B	220	SER
1	B	257	ASN
1	B	265[A]	HIS
1	B	265[B]	HIS
1	C	128	THR
1	C	193	LYS
1	C	201[A]	MET

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Mol	Chain	Res	Type
1	C	201[B]	MET
1	C	202	ILE
1	C	204	THR
1	C	205	ARG
1	C	206	ASP
1	C	207	CYS
1	C	213	ASN
1	C	240	ARG
1	C	257	ASN
1	C	262	ARG
1	C	310	GLU
1	C	313	ARG
1	C	345	ARG
1	C	384	ARG
1	D	128	THR
1	D	150	SER
1	D	164	LYS
1	D	212	SER
1	D	213	ASN
1	D	240	ARG
1	D	257	ASN
1	D	260	ASN
1	D	283	LYS
1	D	313[A]	ARG
1	D	313[B]	ARG
1	D	345	ARG
1	D	384	ARG
1	D	410	SER
1	D	413	SER
1	D	448[A]	PRO
1	D	448[B]	PRO

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

Mol	Chain	Res	Type
1	A	159	GLN
1	A	208	ASN
1	A	213	ASN
1	A	218	ASN
1	A	257	ASN
1	A	268	HIS
1	A	329	ASN

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Mol	Chain	Res	Type
1	A	331	GLN
1	A	338	GLN
1	A	340	HIS
1	A	420	ASN
1	B	218	ASN
1	B	257	ASN
1	B	258	ASN
1	B	329	ASN
1	B	331	GLN
1	B	338	GLN
1	B	340	HIS
1	B	367	ASN
1	B	420	ASN
1	C	152	GLN
1	C	218	ASN
1	C	257	ASN
1	C	265	HIS
1	C	329	ASN
1	C	331	GLN
1	C	340	HIS
1	C	386	GLN
1	C	420	ASN
1	C	435	HIS
1	D	213	ASN
1	D	223	GLN
1	D	257	ASN
1	D	258	ASN
1	D	263	ASN
1	D	329	ASN
1	D	340	HIS
1	D	386	GLN
1	D	392	ASN
1	D	420	ASN

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, 13 are modelled with single atom - leaving 31 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
4	EDO	C	503	-	3,3,3	0.76	0	2,2,2	0.08	0
3	GOL	B	501	-	5,5,5	0.60	0	5,5,5	0.99	0
4	EDO	A	512	-	3,3,3	0.27	0	2,2,2	1.50	1 (50%)
7	PEG	D	505	-	6,6,6	0.95	0	5,5,5	1.64	2 (40%)
6	MPD	B	504	-	7,7,7	1.57	1 (14%)	9,10,10	1.78	3 (33%)
2	PO4	A	501	-	4,4,4	0.42	0	6,6,6	1.30	0
8	ACT	C	513	-	3,3,3	0.99	0	3,3,3	0.54	0
4	EDO	A	504	-	3,3,3	0.69	0	2,2,2	0.58	0
4	EDO	A	506	-	3,3,3	0.65	0	2,2,2	0.66	0
4	EDO	D	503	-	3,3,3	0.54	0	2,2,2	0.50	0
4	EDO	B	503	-	3,3,3	0.57	0	2,2,2	0.50	0
4	EDO	A	505	-	3,3,3	0.27	0	2,2,2	0.54	0
4	EDO	A	517	-	3,3,3	0.53	0	2,2,2	1.22	0
4	EDO	C	505	-	3,3,3	0.44	0	2,2,2	0.63	0
3	GOL	A	502	-	5,5,5	0.71	0	5,5,5	0.63	0
3	GOL	C	502	-	5,5,5	0.47	0	5,5,5	0.72	0
3	GOL	C	501	-	5,5,5	0.47	0	5,5,5	0.62	0
3	GOL	A	503	-	5,5,5	0.80	0	5,5,5	1.57	1 (20%)
3	GOL	D	501	-	5,5,5	0.56	0	5,5,5	1.31	0
4	EDO	A	508	-	3,3,3	0.53	0	2,2,2	0.23	0
4	EDO	B	502	-	3,3,3	0.72	0	2,2,2	0.69	0
4	EDO	A	510	-	3,3,3	0.39	0	2,2,2	0.44	0
4	EDO	C	504	-	3,3,3	0.43	0	2,2,2	0.60	0
4	EDO	A	509	-	3,3,3	0.63	0	2,2,2	1.30	0
4	EDO	D	502	-	3,3,3	0.89	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	504	-	5,5,5	0.54	0	5,5,5	0.68	0
7	PEG	C	507	-	6,6,6	1.23	0	5,5,5	1.85	1 (20%)
7	PEG	C	506	-	6,6,6	0.64	0	5,5,5	0.81	0
4	EDO	B	507	-	3,3,3	0.58	0	2,2,2	0.85	0
4	EDO	A	507	-	3,3,3	1.41	1 (33%)	2,2,2	1.20	0
4	EDO	A	511	-	3,3,3	0.37	0	2,2,2	1.31	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
4	EDO	C	503	-	-	0/1/1/1	-
3	GOL	B	501	-	-	0/4/4/4	-
4	EDO	A	512	-	-	1/1/1/1	-
7	PEG	D	505	-	-	2/4/4/4	-
6	MPD	B	504	-	-	4/5/5/5	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	A	517	-	-	1/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-
3	GOL	C	501	-	-	3/4/4/4	-
3	GOL	A	503	-	-	3/4/4/4	-
3	GOL	D	501	-	-	2/4/4/4	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	B	502	-	-	1/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	D	502	-	-	0/1/1/1	-
3	GOL	D	504	-	-	1/4/4/4	-
7	PEG	C	507	-	-	3/4/4/4	-
7	PEG	C	506	-	-	3/4/4/4	-
4	EDO	B	507	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	A	511	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	MPD	O2-C2	3.50	1.53	1.44
4	A	507	EDO	O2-C2	2.42	1.54	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	507	PEG	O2-C2-C1	3.43	125.21	110.11
6	B	504	MPD	CM-C2-C1	-3.42	102.98	110.63
6	B	504	MPD	O4-C4-C3	2.89	122.83	111.35
3	A	503	GOL	O1-C1-C2	2.51	121.69	110.38
6	B	504	MPD	O2-C2-CM	2.35	115.32	107.99
7	D	505	PEG	O2-C3-C4	2.35	120.45	110.11
4	A	512	EDO	O1-C1-C2	-2.07	96.62	112.39
7	D	505	PEG	O4-C4-C3	2.05	123.88	111.82

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
3	C	501	GOL	O1-C1-C2-O2
3	C	501	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
3	D	501	GOL	O1-C1-C2-C3
3	A	502	GOL	O2-C2-C3-O3
3	D	501	GOL	O1-C1-C2-O2
7	C	506	PEG	O2-C3-C4-O4
7	D	505	PEG	O2-C3-C4-O4
7	C	507	PEG	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
7	C	506	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	C	507	PEG	O2-C3-C4-O4
4	A	504	EDO	O1-C1-C2-O2
4	A	505	EDO	O1-C1-C2-O2
4	A	517	EDO	O1-C1-C2-O2
4	B	502	EDO	O1-C1-C2-O2
4	C	504	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
4	C	505	EDO	O1-C1-C2-O2
7	C	506	PEG	C4-C3-O2-C2
7	D	505	PEG	C1-C2-O2-C3
3	C	501	GOL	C1-C2-C3-O3
4	A	507	EDO	O1-C1-C2-O2
7	C	507	PEG	C1-C2-O2-C3
4	A	506	EDO	O1-C1-C2-O2
4	A	512	EDO	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-O2
4	A	508	EDO	O1-C1-C2-O2
4	A	510	EDO	O1-C1-C2-O2
3	A	503	GOL	C1-C2-C3-O3
6	B	504	MPD	O2-C2-C3-C4
6	B	504	MPD	C2-C3-C4-O4
4	A	509	EDO	O1-C1-C2-O2
6	B	504	MPD	C1-C2-C3-C4
6	B	504	MPD	CM-C2-C3-C4

There are no ring outliers.

25 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	GOL	2	0
4	A	512	EDO	2	0
7	D	505	PEG	2	0
6	B	504	MPD	2	0
2	A	501	PO4	1	0
8	C	513	ACT	1	0
4	A	504	EDO	1	0
4	D	503	EDO	2	0
4	B	503	EDO	3	0
4	A	505	EDO	3	0
4	C	505	EDO	1	0
3	A	502	GOL	3	0
3	C	502	GOL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	GOL	5	0
3	A	503	GOL	1	0
3	D	501	GOL	3	0
4	B	502	EDO	6	0
4	A	510	EDO	5	0
4	C	504	EDO	2	0
4	A	509	EDO	2	0
7	C	507	PEG	4	0
7	C	506	PEG	7	0
4	B	507	EDO	10	0
4	A	507	EDO	22	0
4	A	511	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	322/322 (100%)	0.44	30 (9%)	14 12	17, 26, 47, 86	18 (5%)
1	B	322/322 (100%)	0.44	29 (9%)	15 13	16, 26, 48, 80	20 (6%)
1	C	322/322 (100%)	0.68	34 (10%)	11 9	17, 28, 54, 84	19 (5%)
1	D	322/322 (100%)	0.39	23 (7%)	22 20	16, 28, 57, 78	14 (4%)
All	All	1288/1288 (100%)	0.49	116 (9%)	15 13	16, 27, 53, 86	71 (5%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	216	ALA	14.6
1	A	209	ALA	12.9
1	B	216	ALA	12.5
1	C	209	ALA	11.7
1	C	215	GLY	11.3
1	B	211	GLY	11.1
1	C	211	GLY	10.0
1	C	214	GLY	9.8
1	C	259	ALA	9.5
1	B	209	ALA	9.5
1	B	215	GLY	9.2
1	C	210	GLY	9.2
1	D	257	ASN	9.1
1	B	210	GLY	8.8
1	B	212	SER	8.7
1	A	210	GLY	8.6
1	A	214	GLY	8.2
1	C	213	ASN	8.1
1	C	212	SER	7.7
1	B	206	ASP	7.6
1	C	260	ASN	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	259	ALA	7.4
1	A	216	ALA	7.1
1	B	207	CYS	6.9
1	A	215	GLY	6.7
1	D	209	ALA	6.6
1	B	214	GLY	6.6
1	A	259	ALA	6.3
1	A	207	CYS	6.3
1	C	207	CYS	6.3
1	B	258	ASN	6.1
1	B	208	ASN	6.0
1	C	208	ASN	5.9
1	D	258	ASN	5.8
1	D	256	ALA	5.8
1	C	204	THR	5.7
1	A	261	CYS	5.6
1	A	212	SER	5.5
1	D	426	GLY	5.5
1	A	211	GLY	5.4
1	D	210	GLY	5.3
1	A	213	ASN	5.2
1	C	264	VAL	4.9
1	C	203	PRO	4.9
1	D	213	ASN	4.7
1	C	257	ASN	4.7
1	A	208	ASN	4.5
1	D	128	THR	4.5
1	D	259	ALA	4.5
1	A	263	ASN	4.4
1	C	449	PHE	4.4
1	A	203	PRO	4.4
1	B	217	ASP	4.3
1	B	128	THR	4.3
1	A	258	ASN	4.3
1	A	206	ASP	4.3
1	C	205	ARG	4.2
1	D	214	GLY	4.2
1	B	261	CYS	4.1
1	A	204	THR	4.1
1	A	262	ARG	4.0
1	A	205	ARG	3.9
1	A	260	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	257	ASN	3.9
1	A	449	PHE	3.9
1	C	258	ASN	3.8
1	B	260	ASN	3.7
1	D	212	SER	3.7
1	B	203	PRO	3.7
1	A	257	ASN	3.7
1	B	213	ASN	3.5
1	C	128	THR	3.5
1	C	206	ASP	3.5
1	B	152	GLN	3.5
1	A	128	THR	3.4
1	B	264	VAL	3.4
1	D	260	ASN	3.4
1	C	261	CYS	3.3
1	D	211	GLY	3.2
1	A	158	LEU	3.1
1	C	265	HIS	3.1
1	C	217	ASP	3.0
1	C	156	GLY	3.0
1	C	248	ASP	3.0
1	B	265[A]	HIS	3.0
1	A	221	THR	2.9
1	B	449	PHE	2.9
1	B	218	ASN	2.9
1	A	264	VAL	2.8
1	C	256	ALA	2.8
1	D	449	PHE	2.7
1	C	129	SER	2.7
1	B	263	ASN	2.7
1	D	261	CYS	2.7
1	B	205	ARG	2.7
1	C	313	ARG	2.6
1	A	156	GLY	2.6
1	B	256	ALA	2.6
1	B	204	THR	2.6
1	B	262	ARG	2.5
1	D	414	ALA	2.4
1	D	215	GLY	2.4
1	D	155	SER	2.3
1	D	152	GLN	2.3
1	D	427	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	265[A]	HIS	2.2
1	D	206	ASP	2.2
1	A	293	HIS	2.1
1	C	218	ASN	2.1
1	D	433	TRP	2.1
1	A	202	ILE	2.1
1	C	201[A]	MET	2.1
1	C	262	ARG	2.1
1	C	240	ARG	2.1
1	D	413	SER	2.0
1	C	263	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ACT	C	513	4/4	0.68	0.29	39,46,51,53	0
4	EDO	A	506	4/4	0.70	0.17	39,40,49,59	0
6	MPD	B	504	8/8	0.78	0.22	28,43,49,50	0
4	EDO	A	517	4/4	0.80	0.23	47,51,57,59	0
3	GOL	D	501	6/6	0.80	0.17	43,56,56,59	0
3	GOL	A	503	6/6	0.80	0.15	44,55,58,63	0
3	GOL	A	502	6/6	0.82	0.19	40,56,59,69	0
3	GOL	C	502	6/6	0.83	0.20	37,40,55,61	0
2	PO4	A	501	5/5	0.84	0.13	57,57,61,67	0
4	EDO	D	503	4/4	0.84	0.36	46,50,51,52	0
3	GOL	D	504	6/6	0.85	0.15	52,57,60,62	0
7	PEG	C	507	7/7	0.85	0.14	35,36,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PEG	D	505	7/7	0.85	0.14	33,40,49,51	0
4	EDO	A	510	4/4	0.85	0.17	40,41,46,48	0
3	GOL	C	501	6/6	0.86	0.16	37,45,48,50	0
4	EDO	A	504	4/4	0.87	0.22	31,33,44,53	0
5	NH4	C	510	1/1	0.87	0.16	31,31,31,31	0
4	EDO	B	502	4/4	0.87	0.22	32,34,36,49	0
4	EDO	C	505	4/4	0.88	0.18	46,47,52,58	0
5	NH4	D	507	1/1	0.88	0.16	32,32,32,32	0
4	EDO	C	503	4/4	0.88	0.16	48,55,56,57	0
7	PEG	C	506	7/7	0.89	0.14	35,47,53,54	0
4	EDO	A	509	4/4	0.89	0.23	38,39,40,51	0
4	EDO	C	504	4/4	0.89	0.25	38,38,40,41	0
5	NH4	A	513	1/1	0.89	0.17	39,39,39,39	0
4	EDO	A	512	4/4	0.90	0.21	28,38,41,48	0
4	EDO	A	505	4/4	0.90	0.26	28,38,39,47	0
3	GOL	B	501	6/6	0.90	0.13	35,43,53,57	0
4	EDO	B	503	4/4	0.90	0.14	32,40,43,57	0
5	NH4	A	515	1/1	0.91	0.12	31,31,31,31	0
5	NH4	C	512	1/1	0.92	0.11	15,15,15,15	0
4	EDO	A	508	4/4	0.93	0.11	34,48,51,62	0
5	NH4	C	511	1/1	0.93	0.14	34,34,34,34	0
4	EDO	A	511	4/4	0.93	0.15	29,29,43,43	0
4	EDO	A	507	4/4	0.94	0.22	28,28,29,33	0
4	EDO	B	507	4/4	0.94	0.12	29,31,35,47	0
5	NH4	B	505	1/1	0.94	0.10	23,23,23,23	0
4	EDO	D	502	4/4	0.95	0.17	22,22,24,29	0
5	NH4	C	509	1/1	0.96	0.12	22,22,22,22	0
5	NH4	B	506	1/1	0.96	0.10	32,32,32,32	0
5	NH4	A	514	1/1	0.98	0.05	15,15,15,15	0
5	NH4	D	506	1/1	0.98	0.17	32,32,32,32	0
5	NH4	A	516	1/1	0.98	0.05	14,14,14,14	0
5	NH4	C	508	1/1	0.98	0.13	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.