



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:50 AM GMT

PDB ID : 4HT2
Title : Crystal structure of human carbonic anhydrase isozyme XII with the inhibitor.
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2012-10-31
Resolution : 1.45 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>

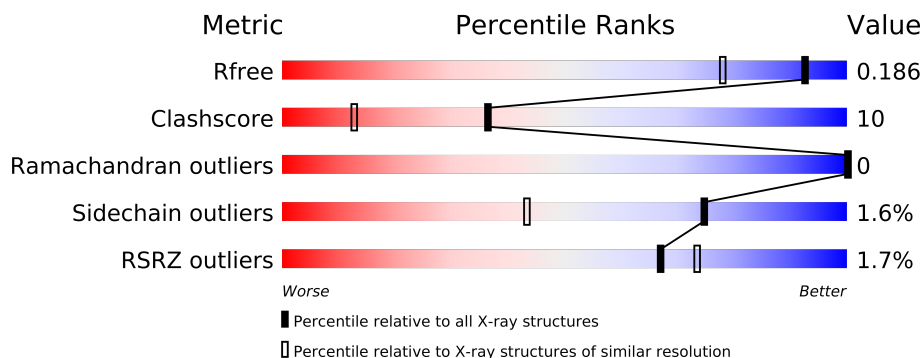
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.45 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	2476 (1.50-1.42)
Clashscore	79885	2834 (1.50-1.42)
Ramachandran outliers	78287	2769 (1.50-1.42)
Sidechain outliers	78261	2767 (1.50-1.42)
RSRZ outliers	66119	2477 (1.50-1.42)

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	263	
1	B	263	
1	C	263	
1	D	263	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	V50	A	302[B]	-	X
3	V50	A	302[C]	-	X
4	PEG	A	303	-	X
4	PEG	B	303	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	PEG	D	303	-	X
5	EDO	A	304[A]	-	X
5	EDO	A	304[B]	-	X
5	EDO	A	306	-	X
5	EDO	B	304	-	X
5	EDO	B	305	-	X
5	EDO	B	307	-	X
5	EDO	C	303	-	X
5	EDO	D	304	-	X
5	EDO	D	305[A]	-	X
5	EDO	D	305[B]	-	X
5	EDO	D	306	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10435 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	15	0
			2220	1405	382	426	7			
1	B	261	Total	C	N	O	S	0	7	0
			2154	1366	365	415	8			
1	C	261	Total	C	N	O	S	0	12	0
			2191	1387	376	421	7			
1	D	261	Total	C	N	O	S	0	9	0
			2170	1377	370	415	8			

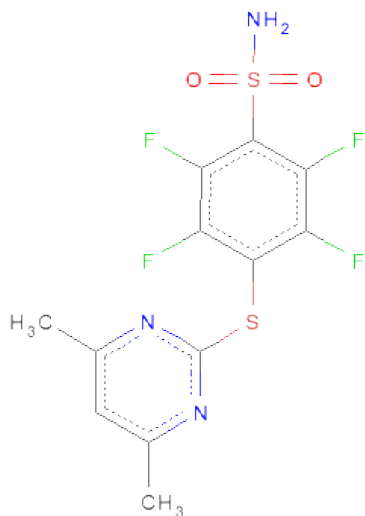
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP O43570
B	1	MET	-	EXPRESSION TAG	UNP O43570
C	1	MET	-	EXPRESSION TAG	UNP O43570
D	1	MET	-	EXPRESSION TAG	UNP O43570

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

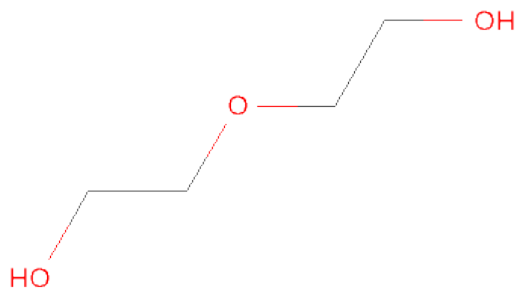
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-[(4,6-DIMETHYLPYRIMIDIN-2-YL)THIO]-2,3,5,6-TETRAFLUOROBENZENESULFONAMIDE (three-letter code: V50) (formula: C₁₂H₉F₄N₃O₂S₂).



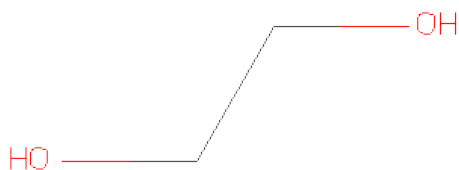
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	1
			46	24	8	6	4	4		
3	B	1	Total	C	F	N	O	S	0	0
			23	12	4	3	2	2		
3	C	1	Total	C	F	N	O	S	0	0
			23	12	4	3	2	2		
3	D	1	Total	C	F	N	O	S	0	0
			23	12	4	3	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 6 is water.

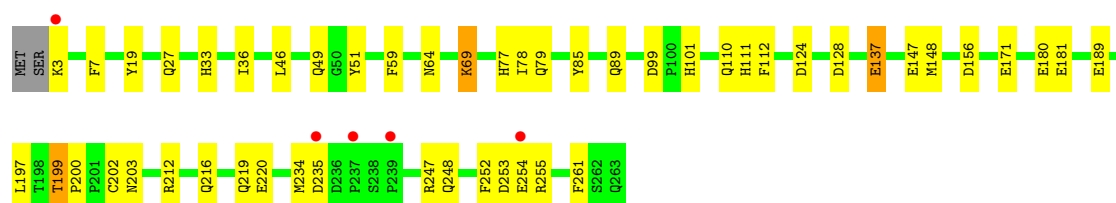
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	369	Total	O	0	0
			369	369		
6	B	375	Total	O	0	0
			375	375		
6	C	350	Total	O	0	0
			350	350		
6	D	410	Total	O	0	0
			410	410		

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.

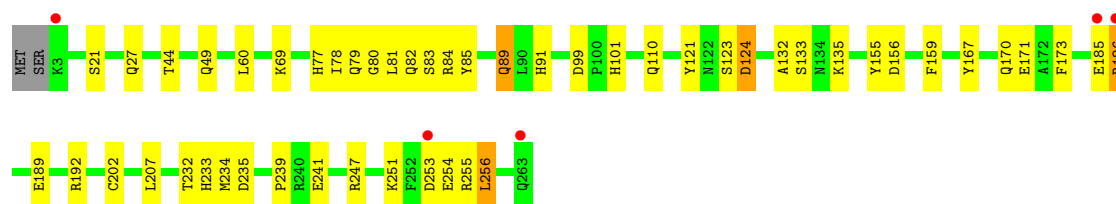
• Molecule 1: Carbonic anhydrase 12

Chain A: 



• Molecule 1: Carbonic anhydrase 12

Chain B: 



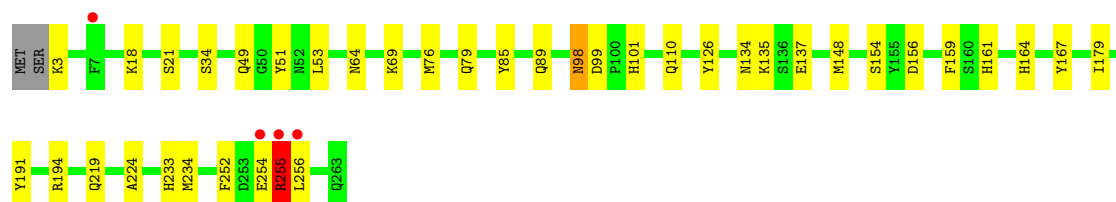
• Molecule 1: Carbonic anhydrase 12

Chain C: 



• Molecule 1: Carbonic anhydrase 12

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.71Å 67.26Å 80.69Å 81.78° 84.01° 86.48°	Depositor
Resolution (Å)	26.50 – 1.45 20.66 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (26.50-1.45) 97.1 (20.66-1.45)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.150 , 0.188 0.149 , 0.186	Depositor DCC
R_{free} test set	16448 reflections (10.99%)	DCC
Wilson B-factor (Å ²)	9.8	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 166178 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10435	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6825e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: ZN, PEG, EDO, V50

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	1.41	5/2285 (0.2%)	1.25	9/3113 (0.3%)
1	B	1.52	10/2217 (0.5%)	1.26	7/3016 (0.2%)
1	C	1.43	6/2254 (0.3%)	1.24	10/3067 (0.3%)
1	D	1.45	8/2234 (0.4%)	1.24	5/3039 (0.2%)
All	All	1.45	29/8990 (0.3%)	1.25	31/12235 (0.3%)

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	D	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	ALA	N-CA	5.97	1.58	1.46
1	B	133	SER	CB-OG	-5.92	1.34	1.42
1	B	173	PHE	CE2-CZ	5.86	1.48	1.37
1	D	137	GLU	CD-OE2	5.86	1.32	1.25
1	D	154	SER	CB-OG	5.83	1.49	1.42
1	B	85	TYR	CB-CG	-5.73	1.43	1.51
1	B	21	SER	CB-OG	5.51	1.49	1.42
1	A	69	LYS	CB-CG	-5.50	1.37	1.52
1	C	109	GLY	C-O	5.48	1.32	1.23
1	D	85	TYR	CE2-CZ	5.47	1.45	1.38
1	B	44	THR	C-O	5.44	1.33	1.23
1	B	135	LYS	CE-NZ	5.44	1.62	1.49
1	C	94	TRP	CG-CD1	5.42	1.44	1.36
1	B	155	TYR	CD1-CE1	5.42	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	GLU	CG-CD	5.40	1.60	1.51
1	A	189	GLU	CD-OE2	5.37	1.31	1.25
1	D	126	TYR	CE2-CZ	5.33	1.45	1.38
1	C	188	ALA	CA-CB	5.30	1.63	1.52
1	C	123	SER	CA-CB	5.27	1.60	1.52
1	C	123	SER	CB-OG	-5.23	1.35	1.42
1	B	123	SER	CB-OG	-5.19	1.35	1.42
1	A	112	PHE	CD2-CE2	5.19	1.49	1.39
1	D	167	TYR	CE1-CZ	-5.14	1.31	1.38
1	A	181	GLU	CD-OE1	5.12	1.31	1.25
1	D	191	TYR	CD2-CE2	5.12	1.47	1.39
1	D	98	ASN	CG-OD1	5.07	1.35	1.24
1	D	21	SER	CB-OG	5.05	1.48	1.42
1	B	186	ARG	C-O	5.02	1.32	1.23
1	C	177	PHE	CE2-CZ	5.01	1.46	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	76	MET	CG-SD-CE	-5.85	90.85	100.20
1	B	241	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	A	59	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	B	84	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	C	40	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	199[A]	THR	OG1-CB-CG2	-5.56	97.21	110.00
1	A	199[B]	THR	OG1-CB-CG2	-5.56	97.21	110.00
1	D	255	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	C	212	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	124	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	255[A]	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	255[B]	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	252	PHE	CB-CG-CD2	-5.52	116.93	120.80
1	B	121	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	C	85	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	D	159	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	B	232	THR	CA-CB-CG2	-5.41	104.83	112.40
1	C	51	TYR	CB-CG-CD1	5.39	124.23	121.00
1	A	85	TYR	CZ-CE2-CD2	-5.37	114.97	119.80
1	A	212	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	261	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	C	205	THR	CA-CB-CG2	-5.25	105.05	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	HIS	CB-CA-C	-5.23	99.94	110.40
1	D	255	ARG	CG-CD-NE	-5.22	100.83	111.80
1	D	191	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	128	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	167	TYR	CD1-CE1-CZ	-5.12	115.19	119.80
1	B	159	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	C	177	PHE	CZ-CE2-CD2	-5.06	114.03	120.10
1	A	128	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	255	ARG	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	2220	0	2095	43	0
1	B	2154	0	2033	46	0
1	C	2191	0	2073	19	0
1	D	2170	0	2051	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	46	0	18	2	0
3	B	23	0	9	0	0
3	C	23	0	9	0	0
3	D	23	0	9	0	0
4	A	7	0	10	15	0
4	B	7	0	10	7	0
4	D	7	0	10	6	0
5	A	16	0	24	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	0	30	9	0
5	C	4	0	6	0	0
5	D	16	0	22	16	0
6	A	369	0	0	10	0
6	B	375	0	0	17	0
6	C	350	0	0	2	0
6	D	410	0	0	19	0
All	All	10435	0	8409	178	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 10.

All (178) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:255:ARG:HB2	1:D:256[B]:LEU:CD2	1.67	1.23
1:D:255:ARG:HB2	1:D:256[B]:LEU:HD22	1.12	1.11
1:A:64:ASN:HD22	4:A:303:PEG:H11	1.05	1.11
1:A:64:ASN:ND2	4:A:303:PEG:H11	1.69	1.07
1:A:255[B]:ARG:NH2	6:A:468:HOH:O	1.88	1.04
1:D:134[A]:ASN:OD1	6:D:779:HOH:O	1.78	0.99
1:D:64:ASN:HD22	5:D:305[A]:EDO:H22	1.23	0.99
1:D:255:ARG:CB	1:D:256[B]:LEU:HD22	1.91	0.98
1:D:18:LYS:HD2	6:D:795:HOH:O	1.61	0.98
1:B:253[B]:ASP:O	6:B:653:HOH:O	1.82	0.97
1:B:253[B]:ASP:OD1	6:B:704:HOH:O	1.84	0.95
1:A:137:GLU:HG3	6:A:737:HOH:O	1.67	0.95
4:A:303:PEG:H32	5:A:304[B]:EDO:O1	1.67	0.95
1:B:234[B]:MET:HE1	6:B:721:HOH:O	1.67	0.93
1:B:89:GLN:HE22	1:B:91:HIS:HD1	1.07	0.93
1:A:69:LYS:NZ	4:A:303:PEG:H12	1.84	0.92
1:D:3[B]:LYS:N	6:D:600:HOH:O	2.03	0.91
1:A:64:ASN:HD22	4:A:303:PEG:C1	1.84	0.89
1:A:69:LYS:CE	4:A:303:PEG:H12	2.04	0.88
1:D:164:HIS:CD2	5:D:306:EDO:H21	2.13	0.83
1:C:164:HIS:HD2	6:C:590:HOH:O	1.60	0.83
4:B:303:PEG:H22	6:B:499:HOH:O	1.80	0.81
1:A:180:GLU:HG2	6:A:648:HOH:O	1.82	0.80
1:D:161[B]:HIS:CD2	5:D:306:EDO:O2	2.36	0.79
1:D:252:PHE:CZ	1:D:255:ARG:HG3	2.18	0.79
1:A:254[B]:GLU:C	1:A:255[B]:ARG:HG3	2.03	0.79
1:D:255:ARG:HB2	1:D:256[B]:LEU:HD23	1.63	0.78
1:A:254[B]:GLU:O	1:A:255[B]:ARG:HG3	1.84	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:46:LEU:HD22	1:A:78[B]:ILE:CG2	2.15	0.77
1:C:46[A]:LEU:HD22	1:C:78[A]:ILE:HG21	1.66	0.76
1:D:64:ASN:ND2	5:D:305[A]:EDO:H22	2.01	0.76
1:C:110[A]:GLN:NE2	1:D:110:GLN:NE2	2.33	0.76
1:B:78[B]:ILE:HD11	1:B:81:LEU:HD12	1.67	0.75
1:B:69:LYS:HZ3	5:B:305:EDO:C1	1.99	0.75
1:D:64:ASN:HD22	5:D:305[A]:EDO:C2	2.00	0.75
1:B:89:GLN:NE2	1:B:91:HIS:HD1	1.85	0.74
1:D:255:ARG:NH2	6:D:608:HOH:O	2.21	0.74
1:B:255:ARG:O	1:B:256:LEU:HD22	1.89	0.72
1:A:46:LEU:HD22	1:A:78[B]:ILE:HG21	1.72	0.72
4:D:303:PEG:H32	6:D:786:HOH:O	1.87	0.72
1:A:234:MET:O	1:A:235:ASP:HB2	1.88	0.71
1:A:27:GLN:HE22	1:A:202:CYS:HB3	1.56	0.71
1:A:111[B]:HIS:CE1	6:A:634:HOH:O	2.43	0.70
3:A:302[C]:V50:N16	6:A:592:HOH:O	2.24	0.70
1:D:164:HIS:NE2	5:D:306:EDO:H21	2.07	0.70
4:B:303:PEG:H32	6:B:499:HOH:O	1.90	0.70
1:B:69:LYS:HZ3	5:B:305:EDO:H12	1.56	0.70
1:B:255:ARG:C	1:B:256:LEU:HD23	2.11	0.70
1:A:69:LYS:HZ3	4:A:303:PEG:H12	1.57	0.69
1:B:234[A]:MET:O	1:B:235[A]:ASP:OD1	2.11	0.69
1:D:64:ASN:HD22	5:D:305[B]:EDO:H12	1.58	0.68
1:B:69:LYS:NZ	5:B:305:EDO:H12	2.07	0.68
4:A:303:PEG:C3	5:A:304[B]:EDO:O1	2.40	0.68
1:B:233:HIS:HE1	6:B:714:HOH:O	1.75	0.67
1:C:47:GLU:HG3	1:C:79:GLN:OE1	1.94	0.67
1:A:147:GLU:HG3	1:A:216:GLN:HG2	1.76	0.67
1:A:110[A]:GLN:NE2	1:B:110:GLN:OE1	2.28	0.65
1:B:255:ARG:C	1:B:256:LEU:CD2	2.65	0.65
1:A:7:PHE:CE1	1:B:253[B]:ASP:OD2	2.49	0.65
1:D:161[A]:HIS:HA	5:D:306:EDO:H22	1.77	0.65
1:B:186:ARG:NH2	1:B:189[B]:GLU:OE2	2.30	0.64
1:C:110[A]:GLN:HE21	1:D:110:GLN:HE22	1.46	0.64
1:C:46[A]:LEU:HD22	1:C:78[A]:ILE:CG2	2.28	0.64
1:A:99:ASP:OD1	1:A:101:HIS:HD2	1.81	0.63
1:A:7:PHE:HE1	1:B:253[B]:ASP:OD2	1.83	0.62
1:D:51:TYR:O	1:D:179[B]:ILE:HD12	1.98	0.62
1:D:34:SER:HB3	6:D:756:HOH:O	1.98	0.62
1:D:161[A]:HIS:ND1	5:D:306:EDO:O2	2.29	0.61
1:D:179[B]:ILE:HD12	1:D:179[B]:ILE:H	1.66	0.61
1:B:27:GLN:NE2	1:B:247:ARG:HH12	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:161[A]:HIS:HD1	5:D:306:EDO:C2	2.13	0.60
1:B:27:GLN:HE22	1:B:202:CYS:HB3	1.68	0.59
1:D:3[A]:LYS:HG3	1:D:18:LYS:HZ3	1.67	0.59
1:D:255:ARG:NH1	6:D:517:HOH:O	2.24	0.59
1:D:255:ARG:CA	1:D:256[B]:LEU:HD22	2.33	0.58
1:D:161[B]:HIS:HA	5:D:306:EDO:H22	1.83	0.58
5:D:305[A]:EDO:H12	6:D:665:HOH:O	2.03	0.58
1:A:27:GLN:NE2	1:A:247:ARG:HH12	2.01	0.58
1:B:185:GLU:HG2	6:B:634:HOH:O	2.03	0.58
4:A:303:PEG:H32	5:A:304[A]:EDO:H21	1.86	0.57
1:D:53:LEU:CD1	1:D:179[B]:ILE:HD11	2.34	0.57
1:B:99:ASP:OD1	1:B:101:HIS:HD2	1.87	0.57
1:B:69:LYS:NZ	5:B:305:EDO:C1	2.65	0.57
1:A:79:GLN:NE2	6:A:525:HOH:O	2.36	0.57
1:D:255:ARG:HD2	6:D:444:HOH:O	2.04	0.57
1:A:78[B]:ILE:N	1:A:78[B]:ILE:HD13	2.20	0.57
3:A:302[C]:V50:S14	4:A:303:PEG:H41	2.44	0.56
1:B:255:ARG:O	1:B:256:LEU:CD2	2.54	0.56
1:A:51:TYR:OH	1:A:78[B]:ILE:HD11	2.06	0.56
1:B:83:SER:HA	5:B:307:EDO:H11	1.87	0.55
1:D:53:LEU:HG	1:D:179[B]:ILE:CD1	2.36	0.55
1:D:99:ASP:OD1	1:D:101:HIS:HD2	1.88	0.55
1:C:82[A]:GLN:HB2	6:C:584:HOH:O	2.06	0.55
1:A:197[A]:LEU:HD12	1:A:203[A]:ASN:OD1	2.07	0.54
4:B:303:PEG:C4	6:B:769:HOH:O	2.56	0.54
1:D:98:ASN:HB3	6:D:757:HOH:O	2.08	0.54
1:A:253:ASP:O	1:A:254[B]:GLU:HG2	2.07	0.54
1:D:255:ARG:HA	1:D:256[B]:LEU:HD22	1.90	0.53
1:A:234:MET:O	1:A:235:ASP:CB	2.54	0.53
1:A:199[B]:THR:HG21	4:A:303:PEG:O4	2.08	0.53
1:C:110[A]:GLN:NE2	1:D:110:GLN:HE21	2.04	0.53
1:D:233:HIS:HE1	6:D:676:HOH:O	1.91	0.53
1:A:254[B]:GLU:HG2	6:A:558:HOH:O	2.09	0.53
1:B:69:LYS:HD3	5:B:305:EDO:H11	1.90	0.52
1:D:53:LEU:HG	1:D:179[B]:ILE:HD11	1.92	0.52
4:B:303:PEG:C1	6:B:573:HOH:O	2.58	0.52
1:B:27:GLN:HE21	1:B:247:ARG:HH12	1.57	0.52
1:C:110[A]:GLN:HE22	1:D:110:GLN:HE21	1.57	0.52
1:A:36[B]:ILE:HD12	1:A:252:PHE:CD2	2.45	0.52
1:D:69:LYS:NZ	5:D:305[A]:EDO:H21	2.25	0.52
1:A:248:GLN:HE21	1:B:251:LYS:NZ	2.08	0.51
1:C:201:PRO:HG2	1:C:203[A]:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:234:MET:HE3	6:D:508:HOH:O	2.11	0.51
1:D:53:LEU:HD11	1:D:179[B]:ILE:HD11	1.92	0.51
1:A:69:LYS:HE2	4:A:303:PEG:H12	1.89	0.50
1:C:47:GLU:HB2	1:C:79:GLN:HB3	1.93	0.50
1:D:148[A]:MET:SD	1:D:219:GLN:HB2	2.52	0.50
1:A:220:GLU:OE1	6:A:716:HOH:O	2.20	0.50
1:C:19:TYR:CD1	1:C:200:PRO:HB3	2.48	0.48
4:D:303:PEG:H41	6:D:551:HOH:O	2.13	0.48
4:A:303:PEG:H32	5:A:304[B]:EDO:C1	2.42	0.48
1:A:254[B]:GLU:O	1:A:255[B]:ARG:CG	2.59	0.48
1:D:161[B]:HIS:HD2	5:D:306:EDO:O2	1.94	0.48
1:B:234[A]:MET:O	1:B:235[A]:ASP:CG	2.53	0.47
1:D:69:LYS:HZ2	5:D:305[A]:EDO:H21	1.79	0.47
1:B:254:GLU:HG3	6:B:702:HOH:O	2.14	0.47
1:D:3[B]:LYS:HG2	1:D:18:LYS:HZ3	1.80	0.47
4:B:303:PEG:H42	6:B:769:HOH:O	2.15	0.47
4:D:303:PEG:H41	6:D:582:HOH:O	2.14	0.47
1:A:27:GLN:HE21	1:A:247:ARG:HH12	1.62	0.47
1:A:111[A]:HIS:HE1	6:A:406:HOH:O	1.97	0.47
1:D:53:LEU:CG	1:D:179[B]:ILE:HD11	2.44	0.47
1:C:52:ASN:HA	1:C:178:ASN:HA	1.97	0.47
1:C:99:ASP:OD1	1:C:101:HIS:HD2	1.98	0.47
1:A:148:MET:HG3	1:A:219[B]:GLN:HE21	1.80	0.46
1:B:83:SER:CB	5:B:307:EDO:H11	2.46	0.46
4:D:303:PEG:C3	6:D:786:HOH:O	2.55	0.45
1:A:49:GLN:OE1	1:A:77[A]:HIS:NE2	2.43	0.45
1:C:147:GLU:HG3	1:C:216:GLN:HG2	1.99	0.45
1:D:148[B]:MET:C	1:D:148[B]:MET:HE3	2.38	0.44
1:B:185:GLU:CD	6:B:748:HOH:O	2.56	0.44
1:B:124:ASP:HB3	5:B:307:EDO:H22	2.00	0.44
1:D:224:ALA:CA	4:D:303:PEG:H12	2.48	0.43
1:B:83:SER:HA	5:B:307:EDO:C1	2.48	0.43
1:D:254:GLU:OE2	6:D:597:HOH:O	2.21	0.43
4:D:303:PEG:C4	6:D:551:HOH:O	2.65	0.43
1:C:46[B]:LEU:HD12	1:C:46[B]:LEU:N	2.32	0.43
1:A:33:HIS:O	1:A:36[A]:ILE:HG13	2.18	0.43
1:A:69:LYS:NZ	4:A:303:PEG:C1	2.71	0.43
1:D:135:LYS:NZ	6:D:779:HOH:O	2.50	0.43
1:B:82:GLN:HG2	6:B:719:HOH:O	2.18	0.43
1:D:49:GLN:HE22	1:D:79:GLN:NE2	2.17	0.42
5:A:304[B]:EDO:H22	6:A:498:HOH:O	2.19	0.42
4:B:303:PEG:H12	6:B:573:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:78[B]:ILE:CD1	1:B:81:LEU:HD12	2.45	0.42
1:D:69:LYS:HD3	5:D:305[A]:EDO:H21	2.02	0.42
1:D:161[B]:HIS:HE1	6:D:530:HOH:O	2.02	0.42
1:D:148[B]:MET:HE2	1:D:148[B]:MET:HB3	1.78	0.41
1:A:19:TYR:CD1	1:A:200:PRO:HB3	2.55	0.41
1:D:255:ARG:HG3	1:D:256[B]:LEU:H	1.85	0.41
1:B:170:GLN:HE22	1:B:234[A]:MET:CE	2.33	0.41
1:B:79:GLN:HG3	1:B:80:GLY:N	2.36	0.41
1:B:185:GLU:O	1:B:186:ARG:C	2.59	0.41
1:B:49:GLN:OE1	1:B:77:HIS:CD2	2.73	0.41
1:B:192:ARG:HD2	1:B:207:LEU:HD11	2.02	0.41
1:C:253:ASP:O	1:C:255[A]:ARG:HG3	2.21	0.41
1:C:192:ARG:HD2	1:C:207:LEU:HD11	2.03	0.41
1:C:110[A]:GLN:HE22	1:D:110:GLN:NE2	2.13	0.40
1:B:256:LEU:N	1:B:256:LEU:CD2	2.83	0.40
1:B:185:GLU:CG	6:B:748:HOH:O	2.69	0.40
1:B:185:GLU:HG2	6:B:748:HOH:O	2.20	0.40
1:D:255:ARG:HD2	1:D:255:ARG:HH11	1.55	0.40
4:A:303:PEG:H21	5:A:304[A]:EDO:O1	2.21	0.40
4:B:303:PEG:H11	6:B:573:HOH:O	2.20	0.40
1:A:49:GLN:HB2	1:A:77[A]:HIS:CD2	2.56	0.40
1:D:3[B]:LYS:HG2	1:D:18:LYS:NZ	2.36	0.40
1:B:60:LEU:HD11	1:B:171:GLU:HB3	2.02	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	274/263 (104%)	269 (98%)	5 (2%)	0	100	100
1	B	266/263 (101%)	258 (97%)	8 (3%)	0	100	100
1	C	271/263 (103%)	265 (98%)	6 (2%)	0	100	100
1	D	267/263 (102%)	262 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1078/1052 (102%)	1054 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	248/235 (106%)	244 (98%)	4 (2%)	75	43
1	B	240/235 (102%)	236 (98%)	4 (2%)	73	40
1	C	245/235 (104%)	242 (99%)	3 (1%)	82	56
1	D	242/235 (103%)	238 (98%)	4 (2%)	73	40
All	All	975/940 (104%)	960 (98%)	15 (2%)	75	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	89	GLN
1	A	137	GLU
1	A	156	ASP
1	B	89	GLN
1	B	156	ASP
1	B	239	PRO
1	B	256	LEU
1	C	25	LEU
1	C	89	GLN
1	C	156	ASP
1	D	89	GLN
1	D	156	ASP
1	D	194	ARG
1	D	255	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	233	HIS
1	A	248	GLN
1	B	27	GLN
1	B	56	ASN
1	B	89	GLN
1	B	111	HIS
1	B	170	GLN
1	B	219	GLN
1	B	233	HIS
1	C	111	HIS
1	C	164	HIS
1	D	79	GLN
1	D	111	HIS
1	D	233	HIS
1	D	263	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	V50	A	302[B]	2	24,24,24	1.37	3 (12%)	37,37,37	2.17	12 (32%)
3	V50	A	302[C]	2	24,24,24	1.16	3 (12%)	37,37,37	2.38	15 (40%)
4	PEG	A	303	-	6,6,6	0.89	0	5,5,5	1.27	1 (20%)
5	EDO	A	304[A]	-	3,3,3	0.82	0	2,2,2	0.83	0
5	EDO	A	304[B]	-	3,3,3	0.50	0	2,2,2	0.69	0
5	EDO	A	305	-	3,3,3	0.51	0	2,2,2	0.21	0
5	EDO	A	306	-	3,3,3	0.62	0	2,2,2	0.48	0
3	V50	B	302	2	24,24,24	1.97	7 (29%)	37,37,37	2.28	14 (37%)
4	PEG	B	303	-	6,6,6	0.98	0	5,5,5	1.43	1 (20%)
5	EDO	B	304	-	3,3,3	0.52	0	2,2,2	0.97	0
5	EDO	B	305	-	3,3,3	0.18	0	2,2,2	0.93	0
5	EDO	B	306	-	3,3,3	0.97	0	2,2,2	0.16	0
5	EDO	B	307	-	3,3,3	0.31	0	2,2,2	0.83	0
5	EDO	B	308	-	3,3,3	0.51	0	2,2,2	0.53	0
3	V50	C	302	2	24,24,24	1.64	6 (25%)	37,37,37	2.45	16 (43%)
5	EDO	C	303	-	3,3,3	0.57	0	2,2,2	0.56	0
3	V50	D	302	2	24,24,24	1.12	1 (4%)	37,37,37	1.72	9 (24%)
4	PEG	D	303	-	6,6,6	1.06	0	5,5,5	1.37	1 (20%)
5	EDO	D	304	-	3,3,3	0.67	0	2,2,2	0.72	0
5	EDO	D	305[A]	-	3,3,3	1.06	0	2,2,2	0.93	0
5	EDO	D	305[B]	-	3,3,3	0.57	0	2,2,2	0.31	0
5	EDO	D	306	-	3,3,3	1.12	0	2,2,2	1.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	V50	A	302[B]	2	-	0/10/10/10	0/2/2/2
3	V50	A	302[C]	2	-	0/10/10/10	0/2/2/2
4	PEG	A	303	-	-	0/4/4/4	0/0/0/0
5	EDO	A	304[A]	-	-	0/1/1/1	0/0/0/0
5	EDO	A	304[B]	-	-	0/1/1/1	0/0/0/0
5	EDO	A	305	-	-	0/1/1/1	0/0/0/0
5	EDO	A	306	-	-	0/1/1/1	0/0/0/0
3	V50	B	302	2	-	0/10/10/10	0/2/2/2
4	PEG	B	303	-	-	0/4/4/4	0/0/0/0
5	EDO	B	304	-	-	0/1/1/1	0/0/0/0
5	EDO	B	305	-	-	0/1/1/1	0/0/0/0
5	EDO	B	306	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	307	-	-	0/1/1/1	0/0/0/0
5	EDO	B	308	-	-	0/1/1/1	0/0/0/0
3	V50	C	302	2	-	0/10/10/10	0/2/2/2
5	EDO	C	303	-	-	0/1/1/1	0/0/0/0
3	V50	D	302	2	-	0/10/10/10	0/2/2/2
4	PEG	D	303	-	-	0/4/4/4	0/0/0/0
5	EDO	D	304	-	-	0/1/1/1	0/0/0/0
5	EDO	D	305[A]	-	-	0/1/1/1	0/0/0/0
5	EDO	D	305[B]	-	-	0/1/1/1	0/0/0/0
5	EDO	D	306	-	-	0/1/1/1	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	V50	C5-S7	4.51	1.87	1.78
3	B	302	V50	F11-C6	-3.37	1.29	1.35
3	C	302	V50	C5-S7	3.34	1.85	1.78
3	A	302[C]	V50	C4-C5	3.11	1.43	1.39
3	A	302[B]	V50	C6-C5	2.93	1.43	1.39
3	A	302[B]	V50	C4-C5	2.91	1.43	1.39
3	B	302	V50	C4-C5	2.90	1.43	1.39
3	B	302	V50	C15-S14	2.87	1.80	1.76
3	C	302	V50	C4-C5	2.83	1.43	1.39
3	B	302	V50	C15-N20	-2.81	1.29	1.34
3	C	302	V50	O9-S7	2.59	1.48	1.43
3	B	302	V50	C15-N16	2.48	1.37	1.34
3	C	302	V50	F11-C6	-2.37	1.31	1.35
3	C	302	V50	C22-C17	2.22	1.56	1.50
3	A	302[C]	V50	O9-S7	-2.22	1.40	1.43
3	C	302	V50	C6-C5	2.19	1.42	1.39
3	D	302	V50	C2-C3	2.19	1.42	1.38
3	A	302[C]	V50	O8-S7	2.16	1.47	1.43
3	A	302[B]	V50	C6-C1	2.12	1.42	1.37
3	B	302	V50	C2-C1	-2.08	1.35	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	V50	C6-C5-S7	6.36	131.82	121.83
3	A	302[C]	V50	C1-C6-C5	5.86	126.90	121.85
3	C	302	V50	C1-C6-C5	5.58	126.66	121.85
3	A	302[C]	V50	O9-S7-N23	5.28	115.45	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[B]	V50	C6-C5-S7	-5.01	113.96	121.83
3	A	302[B]	V50	C3-C4-C5	-5.00	117.55	121.85
3	B	302	V50	C22-C17-N16	-4.85	107.67	116.55
3	B	302	V50	C1-C6-C5	-4.70	117.81	121.85
3	A	302[C]	V50	C17-C18-C19	-4.66	111.58	118.88
3	A	302[B]	V50	C17-C18-C19	-4.42	111.96	118.88
3	B	302	V50	C15-N16-C17	-4.35	110.61	115.97
3	C	302	V50	C17-C18-C19	-4.31	112.14	118.88
3	C	302	V50	C3-C4-C5	4.23	125.49	121.85
3	B	302	V50	C18-C17-N16	4.22	128.66	121.50
3	D	302	V50	C4-C5-S7	4.16	128.37	121.83
3	A	302[C]	V50	C22-C17-C18	-4.01	115.03	121.83
3	A	302[C]	V50	C4-C5-S7	3.89	127.94	121.83
3	B	302	V50	C4-C5-S7	-3.89	115.72	121.83
3	A	302[B]	V50	O9-S7-C5	-3.85	101.69	107.34
3	D	302	V50	O8-S7-N23	3.76	113.10	107.28
3	C	302	V50	C4-C5-C6	-3.75	110.06	117.48
3	C	302	V50	O9-S7-N23	3.73	113.05	107.28
3	D	302	V50	C6-C5-S7	-3.71	116.01	121.83
3	A	302[C]	V50	C4-C5-C6	-3.63	110.30	117.48
3	C	302	V50	F11-C6-C5	-3.56	115.66	121.16
3	A	302[B]	V50	C15-S14-C2	3.53	108.24	102.26
3	B	302	V50	C6-C5-S7	3.42	127.21	121.83
3	B	302	V50	C17-C18-C19	-3.31	113.70	118.88
3	A	302[C]	V50	F11-C6-C1	-3.20	112.33	119.29
3	A	302[B]	V50	C4-C5-S7	3.00	126.54	121.83
3	C	302	V50	C5-S7-N23	-2.98	103.06	108.23
3	D	302	V50	C17-C18-C19	-2.91	114.32	118.88
3	A	302[C]	V50	C3-C4-C5	2.87	124.32	121.85
3	A	302[C]	V50	C18-C19-N20	2.86	126.36	121.50
3	B	302	V50	F10-C1-C6	-2.86	113.07	119.29
3	B	302	V50	O9-S7-N23	2.85	111.69	107.28
3	A	302[B]	V50	F12-C3-C4	-2.82	113.16	119.29
3	A	302[C]	V50	O8-S7-N23	-2.81	102.93	107.28
3	A	302[B]	V50	C18-C19-N20	2.76	126.18	121.50
3	A	302[C]	V50	F13-C4-C3	-2.72	113.38	119.29
3	C	302	V50	O8-S7-N23	2.70	111.47	107.28
4	A	303	PEG	O1-C1-C2	2.69	129.23	111.80
3	C	302	V50	C18-C17-N16	2.67	126.03	121.50
3	B	302	V50	C15-S14-C2	2.62	106.69	102.26
4	B	303	PEG	C3-O2-C2	2.59	124.78	113.38
3	A	302[C]	V50	C18-C17-N16	2.59	125.90	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	V50	C3-C2-S14	-2.57	118.01	121.47
3	A	302[C]	V50	O8-S7-C5	-2.52	103.64	107.34
4	D	303	PEG	C3-O2-C2	2.50	124.37	113.38
3	D	302	V50	C18-C17-N16	2.45	125.66	121.50
3	C	302	V50	C4-C5-S7	-2.40	118.05	121.83
3	A	302[C]	V50	C15-S14-C2	2.40	106.33	102.26
3	D	302	V50	F11-C6-C1	-2.29	114.31	119.29
3	D	302	V50	O9-S7-C5	-2.26	104.03	107.34
3	D	302	V50	C15-S14-C2	2.26	106.09	102.26
3	A	302[B]	V50	C21-C19-N20	-2.24	112.44	116.55
3	A	302[B]	V50	O9-S7-O8	2.23	122.64	118.78
3	A	302[B]	V50	C18-C17-N16	2.20	125.24	121.50
3	B	302	V50	O8-S7-C5	-2.16	104.17	107.34
3	B	302	V50	F10-C1-C2	2.15	122.86	119.83
3	A	302[B]	V50	C3-C2-S14	-2.15	118.58	121.47
3	D	302	V50	F10-C1-C2	-2.14	116.81	119.83
3	B	302	V50	C2-C3-C4	-2.09	118.81	122.01
3	B	302	V50	O8-S7-N23	2.09	110.52	107.28
3	C	302	V50	C1-C2-S14	2.09	124.28	121.47
3	A	302[C]	V50	F12-C3-C2	-2.07	116.91	119.83
3	C	302	V50	C21-C19-N20	-2.06	112.77	116.55
3	C	302	V50	F13-C4-C3	-2.06	114.80	119.29
3	C	302	V50	C22-C17-C18	-2.01	118.42	121.83

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	261/263 (99%)	-0.31	5 (1%) 64 70	4, 9, 21, 36	2 (0%)
1	B	261/263 (99%)	-0.28	5 (1%) 64 70	5, 11, 21, 38	1 (0%)
1	C	261/263 (99%)	-0.28	4 (1%) 70 76	5, 10, 22, 36	1 (0%)
1	D	261/263 (99%)	-0.38	4 (1%) 70 76	4, 9, 18, 41	0
All	All	1044/1052 (99%)	-0.31	18 (1%) 67 73	4, 10, 21, 41	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	4.3
1	D	254	GLU	3.9
1	A	235	ASP	3.8
1	A	3	LYS	3.8
1	C	235	ASP	3.4
1	D	256[A]	LEU	3.2
1	C	3	LYS	2.8
1	C	237	PRO	2.8
1	B	185	GLU	2.6
1	C	254	GLU	2.5
1	B	3	LYS	2.4
1	B	263	GLN	2.4
1	B	253[A]	ASP	2.4
1	A	254[A]	GLU	2.3
1	D	7	PHE	2.2
1	D	255	ARG	2.1
1	B	186	ARG	2.0
1	A	239	PRO	2.0

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

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

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
5	EDO	B	305	4/4	0.21	17.14	18,22,31,32	0
4	PEG	D	303	7/7	0.23	12.42	17,21,36,38	0
4	PEG	B	303	7/7	0.23	11.64	19,25,31,32	0
5	EDO	D	305[A]	4/4	0.17	9.49	8,13,17,17	4
5	EDO	D	305[B]	4/4	0.17	9.49	13,20,21,22	4
5	EDO	D	306	4/4	0.16	8.44	14,21,29,34	0
5	EDO	A	304[B]	4/4	0.18	8.40	11,17,19,22	4
5	EDO	A	304[A]	4/4	0.18	6.45	9,12,15,20	4
5	EDO	B	304	4/4	0.11	5.61	15,18,19,20	0
5	EDO	D	304	4/4	0.13	5.37	18,19,19,20	0
4	PEG	A	303	7/7	0.15	5.07	23,27,33,38	0
5	EDO	C	303	4/4	0.12	4.70	22,23,23,24	0
5	EDO	A	306	4/4	0.19	4.63	35,37,40,42	0
5	EDO	B	307	4/4	0.24	3.27	25,35,36,37	0
3	V50	A	302[B]	23/23	0.11	2.19	3,8,11,13	23
3	V50	A	302[C]	23/23	0.11	2.10	6,11,18,19	23
5	EDO	B	308	4/4	0.10	1.92	21,29,31,33	0
3	V50	C	302	23/23	0.10	1.28	6,12,21,23	0
3	V50	B	302	23/23	0.07	1.26	7,9,15,16	0
5	EDO	A	305	4/4	0.07	0.49	10,14,14,17	0
3	V50	D	302	23/23	0.06	0.37	5,9,13,17	0
5	EDO	B	306	4/4	0.06	-0.53	10,11,12,12	0
2	ZN	D	301	1/1	0.03	-3.23	4,4,4,4	0
2	ZN	B	301	1/1	0.03	-5.40	5,5,5,5	0
2	ZN	A	301	1/1	0.02	-5.88	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	C	301	1/1	0.02	-6.69	5,5,5,5	0

6.5 Other polymers ⓘ

There are no such residues in this entry.