



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:55 PM UTC

PDB ID : 7Q84 / pdb_00007q84
Title : Crystal structure of human peroxisomal acyl-Co-A oxidase 1a, apo-form
Authors : Sonani, R.R.; Blat, A.; Dubin, G.
Deposited on : 2021-11-10
Resolution : 2.00 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

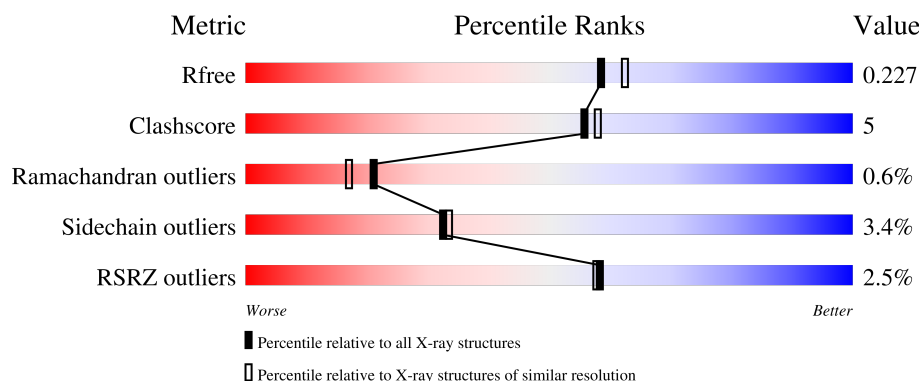
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	667	 2% 78% 15% • 6%
1	B	667	 2% 77% 16% • 6%

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
2	PGE	A	701	-	-	X	-

2 Entry composition [i](#)

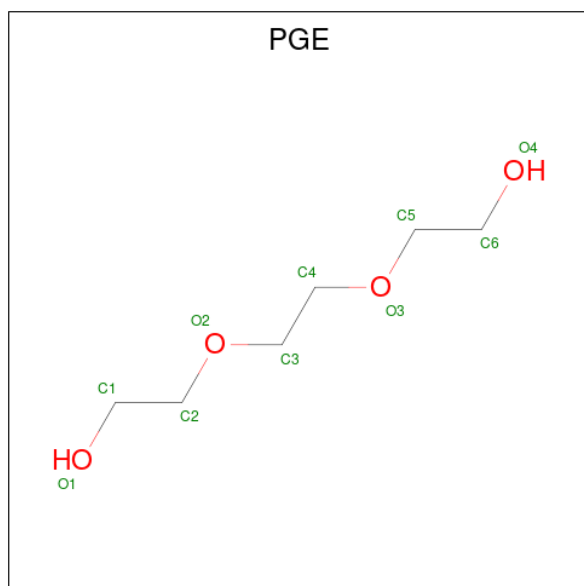
There are 6 unique types of molecules in this entry. The entry contains 10556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isoform 2 of Peroxisomal acyl-coenzyme A oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			5002	3185	868	920	29			
1	B	625	Total	C	N	O	S	0	0	0
			4977	3169	863	916	29			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



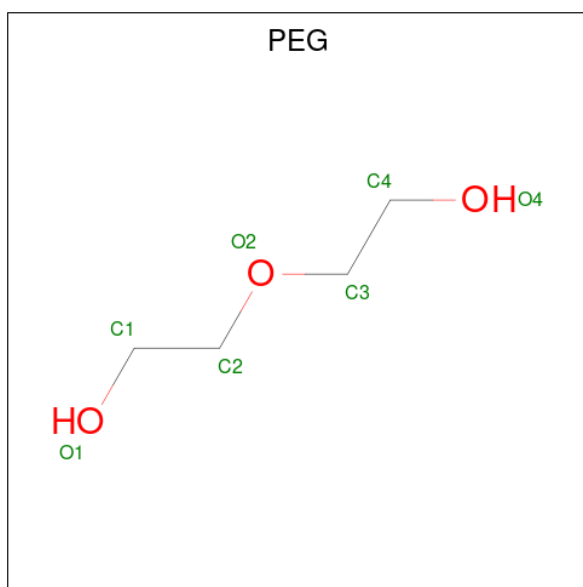
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



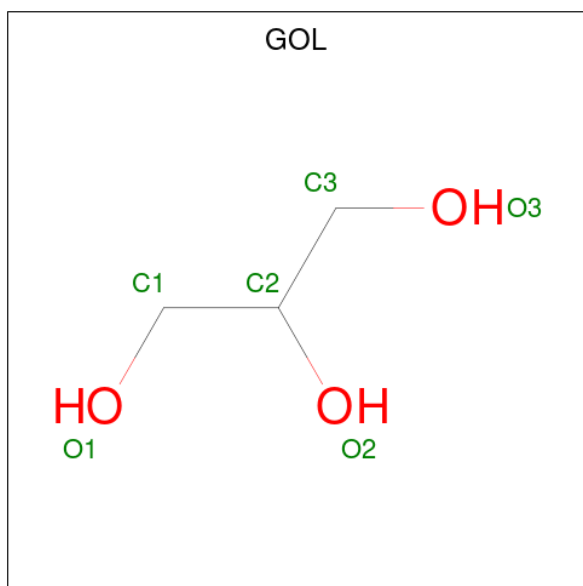
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total 221	O 221	0	0
6	B	271	Total 271	O 271	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.87Å 133.22Å 139.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.00 48.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.23-2.00) 99.1 (48.23-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.220 0.192 , 0.227	Depositor DCC
R_{free} test set	5573 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10556	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: CSO, PGE, GOL, PEG, EDO

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	1.32	19/5099 (0.4%)	1.51	19/6896 (0.3%)
1	B	1.30	19/5073 (0.4%)	1.50	28/6861 (0.4%)
All	All	1.31	38/10172 (0.4%)	1.50	47/13757 (0.3%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	HIS	CE1-NE2	8.27	1.40	1.32
1	B	298	THR	C-O	7.50	1.32	1.24
1	A	48	HIS	CE1-NE2	7.12	1.39	1.32
1	A	387	THR	C-O	-6.98	1.16	1.24
1	A	594	GLU	C-O	-6.77	1.15	1.24
1	A	530	HIS	CE1-NE2	6.72	1.39	1.32
1	B	609	ALA	C-O	6.70	1.32	1.24
1	A	143	HIS	CE1-NE2	6.61	1.39	1.32
1	A	505	GLU	C-O	6.21	1.31	1.24
1	A	48	HIS	C-O	6.15	1.30	1.23
1	A	537	LYS	C-O	6.12	1.31	1.24
1	A	512	LYS	C-O	6.10	1.31	1.24
1	A	85	ILE	C-O	6.08	1.31	1.24
1	A	21	HIS	CA-C	5.90	1.60	1.52
1	B	427	MET	C-O	5.88	1.30	1.24
1	B	323	ASP	C-O	-5.80	1.16	1.24
1	A	48	HIS	CG-ND1	5.76	1.44	1.38
1	A	31	ARG	C-O	5.76	1.30	1.24
1	B	264	THR	C-O	5.72	1.30	1.23
1	B	16	PRO	C-O	5.69	1.30	1.24
1	B	597	THR	CA-C	5.55	1.59	1.52
1	B	165	LEU	C-O	5.54	1.30	1.24
1	A	536	VAL	C-O	5.48	1.30	1.24
1	B	132	ILE	C-O	5.38	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	ILE	C-O	5.36	1.29	1.24
1	B	119	GLN	C-O	5.33	1.30	1.24
1	B	475	VAL	C-O	-5.30	1.18	1.24
1	B	166	ASN	C-O	5.27	1.30	1.23
1	B	524	VAL	C-O	5.25	1.30	1.24
1	B	196	LYS	C-O	5.20	1.29	1.24
1	B	175	TRP	C-O	5.15	1.30	1.23
1	B	93	HIS	CE1-NE2	5.15	1.37	1.32
1	B	601	SER	C-O	-5.13	1.17	1.24
1	A	292	ALA	C-O	-5.09	1.18	1.24
1	A	132	ILE	C-O	5.07	1.29	1.24
1	B	95	GLY	C-O	5.06	1.30	1.23
1	B	86	MET	C-O	5.03	1.29	1.24
1	A	598	LEU	C-O	-5.01	1.18	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	HIS	CA-CB-CG	-9.52	104.28	113.80
1	B	155	THR	CB-CA-C	7.58	122.23	109.80
1	B	94	ARG	CA-C-O	-7.25	113.17	121.65
1	B	283	SER	CA-C-N	6.86	129.77	120.38
1	B	283	SER	C-N-CA	6.86	129.77	120.38
1	B	623	ARG	CB-CA-C	-6.82	98.41	109.72
1	A	346	ALA	N-CA-C	-6.76	103.99	111.36
1	B	597	THR	N-CA-C	-6.73	103.87	111.07
1	A	43	ASP	CB-CA-C	6.69	116.80	110.17
1	B	84	GLU	N-CA-C	-6.43	104.35	111.36
1	B	339	TYR	CA-C-O	-6.33	114.17	120.82
1	B	79	ILE	CB-CA-C	6.22	118.48	110.96
1	A	350	GLU	CA-C-N	6.13	128.75	120.65
1	A	350	GLU	C-N-CA	6.13	128.75	120.65
1	B	90	ASN	CB-CA-C	-6.06	100.73	110.79
1	B	99	PRO	N-CA-C	5.78	121.14	114.03
1	B	170	VAL	N-CA-C	-5.76	103.88	111.09
1	B	8	GLU	N-CA-C	-5.74	104.93	111.07
1	A	369	GLU	N-CA-CB	5.73	118.64	110.16
1	B	414	PHE	CA-CB-CG	-5.73	108.07	113.80
1	B	131	GLU	N-CA-CB	-5.62	101.65	110.30
1	B	160	THR	O-C-N	5.60	128.81	122.20
1	A	623	ARG	CB-CA-C	-5.54	100.53	109.72
1	B	370	LEU	CA-C-O	-5.50	115.23	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	631	ASN	N-CA-C	-5.45	105.42	111.36
1	A	478	ASN	CB-CA-C	-5.45	100.99	110.09
1	A	208	PRO	N-CA-C	-5.44	102.66	111.14
1	A	75	ARG	CB-CG-CD	5.44	123.80	111.30
1	A	510	LYS	CB-CA-C	-5.40	104.06	111.73
1	B	145	THR	CA-C-O	-5.37	115.17	120.70
1	A	650	TYR	CA-C-O	-5.37	115.18	120.82
1	B	195	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	118	GLU	CA-C-O	-5.28	115.27	120.70
1	A	279	VAL	CA-C-O	-5.26	115.08	120.71
1	A	437	LYS	N-CA-C	-5.26	105.55	111.28
1	A	427	MET	N-CA-C	-5.25	105.45	111.07
1	B	38	ASN	N-CA-C	-5.24	105.57	111.28
1	A	350	GLU	CB-CG-CD	5.21	121.45	112.60
1	A	212	ILE	CA-C-O	-5.21	115.63	121.36
1	B	38	ASN	CB-CA-C	5.17	119.36	110.79
1	B	386	ASN	CA-C-N	5.16	127.15	120.44
1	B	386	ASN	C-N-CA	5.16	127.15	120.44
1	A	160	THR	CA-CB-OG1	-5.13	101.90	109.60
1	B	230	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	266	VAL	CA-C-O	-5.10	115.07	120.53
1	A	21	HIS	CB-CA-C	5.07	118.92	110.81
1	B	55	THR	CA-CB-OG1	-5.04	102.05	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5002	0	4973	51	0
1	B	4977	0	4945	45	0
2	A	10	0	14	6	0
2	B	10	0	14	4	0
3	A	24	0	36	3	0
3	B	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	7	0	10	0	0
5	A	6	0	8	2	0
5	B	12	0	16	1	0
6	A	221	0	0	5	0
6	B	271	0	0	4	0
All	All	10556	0	10040	94	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 5.

All (94) 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:A:348:MET:HE1	1:A:374:THR:HG22	1.20	1.12
1:A:307:ARG:HE	2:A:701:PGE:H12	1.45	0.79
1:A:309:GLN:HG2	2:A:701:PGE:H2	1.73	0.71
1:A:103:HIS:HD2	1:A:134:GLY:H	1.39	0.70
1:A:143:HIS:ND1	6:A:801:HOH:O	2.29	0.66
1:B:549:LYS:HE2	6:B:987:HOH:O	1.96	0.65
1:A:308:HIS:HD2	1:A:318:GLU:O	1.80	0.65
1:B:103:HIS:HD2	1:B:134:GLY:H	1.45	0.65
1:B:4:ASP:OD2	1:B:308:HIS:HE1	1.79	0.65
1:B:103:HIS:CD2	1:B:134:GLY:H	2.16	0.64
1:B:267:LYS:HB2	6:B:1035:HOH:O	1.96	0.64
1:B:35:GLU:HG2	1:B:39:MET:HE3	1.81	0.63
1:B:283:SER:HA	1:B:348:MET:HE3	1.82	0.61
1:B:48:HIS:HE1	1:B:66:LYS:NZ	1.97	0.61
1:B:398:GLY:H	2:B:701:PGE:H4	1.65	0.61
1:A:364:LEU:C	1:A:366:GLU:H	2.08	0.61
1:A:4:ASP:OD2	1:A:308:HIS:HE1	1.82	0.61
1:B:367:LEU:N	1:B:368:PRO:HD2	2.16	0.60
1:A:103:HIS:CD2	1:A:134:GLY:H	2.17	0.60
1:A:525:ARG:HD2	5:A:707:GOL:O1	2.02	0.60
2:A:701:PGE:H4	3:A:702:EDO:C1	2.32	0.58
1:B:48:HIS:HD2	1:B:49:GLU:O	1.87	0.58
6:A:964:HOH:O	1:B:399:HIS:HD2	1.86	0.58
1:A:5:LEU:HD22	1:A:626:GLY:HA3	1.87	0.57
2:A:701:PGE:H4	3:A:702:EDO:H11	1.85	0.56
1:A:307:ARG:HE	2:A:701:PGE:C1	2.16	0.56
1:A:478:ASN:O	1:A:556:ARG:NH2	2.39	0.56
1:A:48:HIS:HD2	1:A:49:GLU:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TRP:O	1:B:176:TRP:HB2	2.07	0.55
5:B:705:GOL:H32	6:B:894:HOH:O	2.06	0.55
1:A:2:ASN:OD1	1:A:4:ASP:HB2	2.08	0.54
1:A:174:LYS:O	1:A:239:TYR:HA	2.07	0.54
1:A:243:ASP:OD1	1:A:243:ASP:C	2.50	0.54
1:A:414:PHE:C	1:A:416:PRO:HD2	2.34	0.53
1:B:147:LEU:O	1:B:150:LEU:HG	2.09	0.53
1:B:174:LYS:O	1:B:239:TYR:HA	2.09	0.53
1:A:255:LYS:HD3	1:A:256:TYR:CE1	2.44	0.53
1:B:307:ARG:HH21	2:B:701:PGE:H2	1.73	0.52
1:B:233:ASP:CG	6:B:825:HOH:O	2.52	0.52
1:B:48:HIS:HE1	1:B:66:LYS:HZ1	1.58	0.51
1:B:373:LEU:HD13	1:B:451:MET:SD	2.50	0.51
1:A:525:ARG:NH2	1:A:573:ASP:OD2	2.40	0.51
1:A:48:HIS:HE1	1:A:66:LYS:NZ	2.09	0.50
1:B:308:HIS:HD2	1:B:318:GLU:O	1.94	0.50
2:A:701:PGE:H4	3:A:702:EDO:O1	2.11	0.50
1:B:2:ASN:OD1	1:B:4:ASP:HB2	2.11	0.50
1:A:582:GLU:HG3	1:B:576:GLN:HE21	1.77	0.50
1:B:647:HIS:HD2	1:B:649:SER:H	1.60	0.50
1:A:254:MET:HA	1:A:257:ALA:O	2.12	0.49
1:B:283:SER:HA	1:B:348:MET:CE	2.42	0.49
1:B:309:GLN:HG2	2:B:701:PGE:H1	1.93	0.49
1:B:633:PHE:CE2	1:B:637:LYS:HE2	2.48	0.49
1:A:222:THR:HB	1:A:241:LYS:HB3	1.95	0.48
1:A:369:GLU:OE1	1:A:451:MET:N	2.35	0.48
1:B:89:LYS:HB2	1:B:89:LYS:HE2	1.58	0.48
1:A:145:THR:H	2:B:701:PGE:H22	1.79	0.48
1:B:369:GLU:OE1	1:B:451:MET:HG2	2.14	0.48
1:A:176:TRP:O	1:A:177:PRO:C	2.55	0.48
1:A:174:LYS:HB2	1:A:240:LEU:HB3	1.96	0.47
1:B:393:ARG:HA	1:B:407:LEU:HD13	1.97	0.47
1:A:348:MET:HB3	1:A:348:MET:HE3	1.55	0.47
1:A:478:ASN:HD22	1:A:591:ARG:NH1	2.13	0.46
1:A:549:LYS:HG2	6:A:926:HOH:O	2.15	0.46
1:A:371:HIS:NE2	1:A:430:GLN:NE2	2.64	0.46
1:A:415:THR:N	1:A:416:PRO:HD2	2.31	0.46
1:A:57:SER:OG	1:B:647:HIS:HE1	1.98	0.46
1:A:411:TYR:OH	1:B:390:GLU:OE1	2.29	0.45
1:B:312:ILE:HG13	1:B:319:PRO:HG3	2.00	0.44
1:A:443:HIS:HA	1:A:461:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:HG2	1:B:39:MET:CE	2.45	0.44
1:A:326:THR:HG23	1:B:520:SER:HB3	1.98	0.44
1:B:624:TYR:CD2	1:B:624:TYR:C	2.95	0.44
1:B:137:ALA:HA	1:B:177:PRO:HG2	1.99	0.44
1:A:229:LYS:HE2	6:A:862:HOH:O	2.17	0.43
1:A:520:SER:HB3	1:B:326:THR:HG23	1.99	0.43
1:A:175:TRP:O	1:A:176:TRP:HB2	2.19	0.42
1:A:310:SER:O	1:A:318:GLU:HG2	2.20	0.42
1:A:490:ARG:HG3	1:A:573:ASP:HB3	2.02	0.42
1:B:407:LEU:N	1:B:408:PRO:CD	2.82	0.42
1:B:490:ARG:HG3	1:B:573:ASP:HB3	2.02	0.42
1:B:118:GLU:OE1	1:B:250:GLU:HB3	2.20	0.42
1:A:364:LEU:C	1:A:366:GLU:N	2.76	0.41
1:A:393:ARG:HA	1:A:407:LEU:HD13	2.02	0.41
1:A:267:LYS:HD2	1:A:267:LYS:HA	1.53	0.41
1:A:648:GLU:H	1:A:648:GLU:HG3	1.59	0.41
1:A:490:ARG:HD2	1:A:574:PHE:CZ	2.56	0.41
1:A:66:LYS:NZ	6:A:822:HOH:O	2.54	0.41
1:A:157:ASP:C	1:A:157:ASP:OD1	2.64	0.41
1:A:576:GLN:HE21	1:B:582:GLU:HG3	1.84	0.41
1:B:633:PHE:CZ	1:B:637:LYS:HE2	2.55	0.41
1:B:647:HIS:CD2	1:B:649:SER:H	2.39	0.41
1:B:454:TYR:HB2	1:B:488:LYS:HG3	2.03	0.41
1:A:525:ARG:HD2	5:A:707:GOL:C1	2.51	0.40
1:B:490:ARG:HD2	1:B:574:PHE:CZ	2.56	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	618/667 (93%)	593 (96%)	21 (3%)	4 (1%)	21 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	615/667 (92%)	597 (97%)	15 (2%)	3 (0%)	24	21
All	All	1233/1334 (92%)	1190 (96%)	36 (3%)	7 (1%)	21	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	A	473	THR
1	B	176	TRP
1	B	473	THR
1	A	365	SER
1	A	652	HIS
1	B	96	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	539/576 (94%)	516 (96%)	23 (4%)	26	25
1	B	536/576 (93%)	522 (97%)	14 (3%)	40	44
All	All	1075/1152 (93%)	1038 (97%)	37 (3%)	32	33

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	SER
1	A	47	GLN
1	A	61	GLU
1	A	75	ARG
1	A	102	LEU
1	A	108	LEU
1	A	125	MET
1	A	133	ILE

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Mol	Chain	Res	Type
1	A	194	ILE
1	A	198	LYS
1	A	215	HIS
1	A	229	LYS
1	A	266	VAL
1	A	267	LYS
1	A	364	LEU
1	A	461	GLN
1	A	630	GLU
1	A	648	GLU
1	A	651	LYS
1	A	652	HIS
1	A	653	LEU
1	A	654	LYS
1	B	70	MET
1	B	81	ASP
1	B	89	LYS
1	B	278	MET
1	B	281	VAL
1	B	357	GLU
1	B	366	GLU
1	B	369	GLU
1	B	446	LYS
1	B	457	ASP
1	B	472	PRO
1	B	506	VAL
1	B	591	ARG
1	B	654	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	48	HIS
1	A	90	ASN
1	A	103	HIS
1	A	113	HIS
1	A	146	HIS
1	A	203	HIS
1	A	215	HIS
1	A	245	HIS
1	A	308	HIS

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Mol	Chain	Res	Type
1	A	356	ASN
1	A	430	GLN
1	A	441	GLN
1	A	478	ASN
1	A	576	GLN
1	A	587	GLN
1	A	613	GLN
1	A	627	ASN
1	B	47	GLN
1	B	48	HIS
1	B	90	ASN
1	B	93	HIS
1	B	103	HIS
1	B	114	GLN
1	B	203	HIS
1	B	244	ASN
1	B	308	HIS
1	B	399	HIS
1	B	430	GLN
1	B	576	GLN
1	B	587	GLN
1	B	613	GLN
1	B	627	ASN
1	B	647	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CSO	B	449	1	3,6,7	1.22	1 (33%)	1,6,8	0.40	0
1	CSO	A	449	1	3,6,7	1.29	1 (33%)	1,6,8	0.49	0
1	CSO	A	199	1	3,6,7	1.40	1 (33%)	1,6,8	0.30	0
1	CSO	B	199	1	3,6,7	1.20	0	1,6,8	0.53	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
1	CSO	B	449	1	-	0/1/5/7	-
1	CSO	A	449	1	-	0/1/5/7	-
1	CSO	A	199	1	-	0/1/5/7	-
1	CSO	B	199	1	-	0/1/5/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	CSO	O-C	2.30	1.28	1.20
1	A	449	CSO	O-C	2.08	1.27	1.20
1	B	449	CSO	O-C	2.04	1.27	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands 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	$\# Z > 2$
3	EDO	A	708	-	3,3,3	0.62	0	2,2,2	0.32	0
3	EDO	A	709	-	3,3,3	0.21	0	2,2,2	0.32	0
3	EDO	B	704	-	3,3,3	0.79	0	2,2,2	0.49	0
4	PEG	A	704	-	6,6,6	0.77	0	5,5,5	0.41	0
5	GOL	A	707	-	5,5,5	0.27	0	5,5,5	0.59	0
2	PGE	A	701	-	9,9,9	0.61	0	8,8,8	1.08	2 (25%)
3	EDO	B	703	-	3,3,3	1.11	0	2,2,2	0.52	0
3	EDO	B	706	-	3,3,3	0.14	0	2,2,2	0.35	0
3	EDO	B	702	-	3,3,3	1.34	0	2,2,2	0.86	0
3	EDO	A	705	-	3,3,3	0.73	0	2,2,2	0.30	0
2	PGE	B	701	-	9,9,9	0.86	0	8,8,8	0.94	0
5	GOL	B	705	-	5,5,5	0.16	0	5,5,5	0.44	0
3	EDO	A	702	-	3,3,3	1.31	0	2,2,2	0.98	0
3	EDO	A	706	-	3,3,3	0.26	0	2,2,2	0.38	0
3	EDO	A	703	-	3,3,3	0.77	0	2,2,2	0.92	0
5	GOL	B	707	-	5,5,5	0.20	0	5,5,5	0.51	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	EDO	A	708	-	-	1/1/1/1	-
3	EDO	A	709	-	-	1/1/1/1	-
3	EDO	B	704	-	-	1/1/1/1	-
4	PEG	A	704	-	-	3/4/4/4	-
5	GOL	A	707	-	-	0/4/4/4	-
2	PGE	A	701	-	-	3/7/7/7	-
3	EDO	B	703	-	-	1/1/1/1	-
3	EDO	B	706	-	-	1/1/1/1	-
3	EDO	B	702	-	-	1/1/1/1	-
3	EDO	A	705	-	-	1/1/1/1	-
2	PGE	B	701	-	-	4/7/7/7	-
5	GOL	B	705	-	-	4/4/4/4	-
3	EDO	A	702	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
5	GOL	B	707	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PGE	C3-O2-C2	-2.09	104.10	113.26
2	A	701	PGE	O2-C2-C1	-2.04	101.14	110.11

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	705	GOL	O1-C1-C2-O2
5	B	705	GOL	O1-C1-C2-C3
5	B	705	GOL	C1-C2-C3-O3
2	B	701	PGE	O2-C3-C4-O3
4	A	704	PEG	O2-C3-C4-O4
2	A	701	PGE	O2-C3-C4-O3
5	B	705	GOL	O2-C2-C3-O3
3	B	706	EDO	O1-C1-C2-O2
2	A	701	PGE	O1-C1-C2-O2
2	B	701	PGE	O3-C5-C6-O4
3	A	708	EDO	O1-C1-C2-O2
2	B	701	PGE	C6-C5-O3-C4
2	B	701	PGE	C4-C3-O2-C2
4	A	704	PEG	C1-C2-O2-C3
2	A	701	PGE	C3-C4-O3-C5
3	B	703	EDO	O1-C1-C2-O2
3	A	709	EDO	O1-C1-C2-O2
4	A	704	PEG	C4-C3-O2-C2
3	B	702	EDO	O1-C1-C2-O2
3	A	702	EDO	O1-C1-C2-O2
3	A	705	EDO	O1-C1-C2-O2
3	B	704	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	707	GOL	2	0
2	A	701	PGE	6	0
2	B	701	PGE	4	0
5	B	705	GOL	1	0
3	A	702	EDO	3	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	626/667 (93%)	0.14	16 (2%) 57 56	30, 48, 81, 145	0
1	B	623/667 (93%)	0.08	15 (2%) 59 59	29, 45, 79, 125	0
All	All	1249/1334 (93%)	0.11	31 (2%) 58 58	29, 47, 80, 145	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	LEU	4.8
1	B	458	LEU	4.6
1	A	472	PRO	4.2
1	A	653	LEU	3.8
1	B	278	MET	3.7
1	B	355	ILE	3.7
1	B	653	LEU	3.3
1	A	654	LYS	3.2
1	A	473	THR	3.0
1	A	365	SER	3.0
1	B	95	GLY	2.9
1	A	652	HIS	2.9
1	A	655	SER	2.7
1	B	447	LEU	2.7
1	B	472	PRO	2.7
1	A	650	TYR	2.6
1	B	473	THR	2.5
1	B	644	ALA	2.5
1	A	649	SER	2.4
1	B	279	VAL	2.4
1	B	652	HIS	2.4
1	A	280	PHE	2.4
1	B	649	SER	2.4
1	B	42	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	124	PHE	2.3
1	A	95	GLY	2.3
1	A	176	TRP	2.3
1	A	355	ILE	2.2
1	B	176	TRP	2.2
1	B	267	LYS	2.1
1	A	267	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	B	449	7/8	0.83	0.32	20,20,20,20	0
1	CSO	A	449	7/8	0.84	0.25	20,20,20,20	0
1	CSO	A	199	7/8	0.90	0.27	20,20,20,20	0
1	CSO	B	199	7/8	0.93	0.25	20,20,20,20	0

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
3	EDO	B	703	4/4	0.82	0.17	52,57,57,61	0
3	EDO	A	708	4/4	0.83	0.18	63,68,70,73	0
3	EDO	B	704	4/4	0.85	0.15	42,58,62,63	0
3	EDO	B	706	4/4	0.85	0.17	49,59,62,65	0
3	EDO	A	702	4/4	0.87	0.15	44,52,52,54	0
3	EDO	A	705	4/4	0.87	0.16	53,60,67,69	0
2	PGE	B	701	10/10	0.88	0.19	41,64,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	706	4/4	0.88	0.14	50,53,57,57	0
2	PGE	A	701	10/10	0.88	0.20	43,54,64,70	0
4	PEG	A	704	7/7	0.88	0.18	61,65,72,75	0
3	EDO	B	702	4/4	0.89	0.23	38,50,59,59	0
5	GOL	A	707	6/6	0.89	0.12	63,65,72,73	0
5	GOL	B	707	6/6	0.90	0.10	54,58,59,64	0
3	EDO	A	703	4/4	0.91	0.12	36,48,50,54	0
3	EDO	A	709	4/4	0.92	0.14	59,64,67,72	0
5	GOL	B	705	6/6	0.94	0.11	63,70,75,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.