



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2022 – 03:16 pm GMT

PDB ID : 7Q84
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

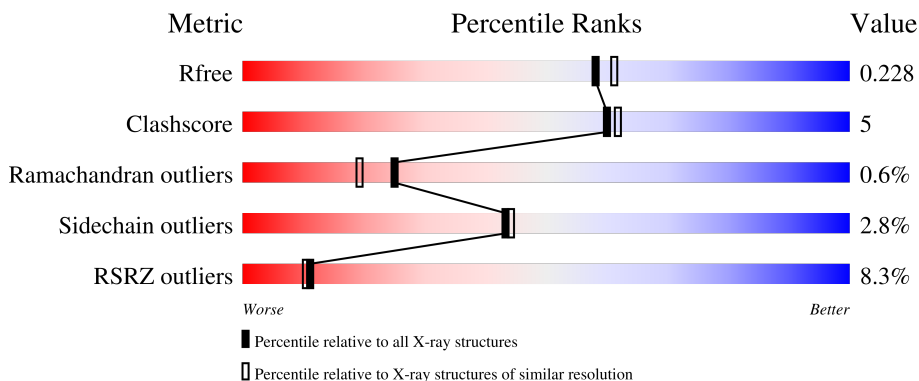
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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	 7% 82% 11% • 6%
1	B	667	 9% 83% 10% • 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	-
3	EDO	A	708	-	-	-	X

2 Entry composition [i](#)

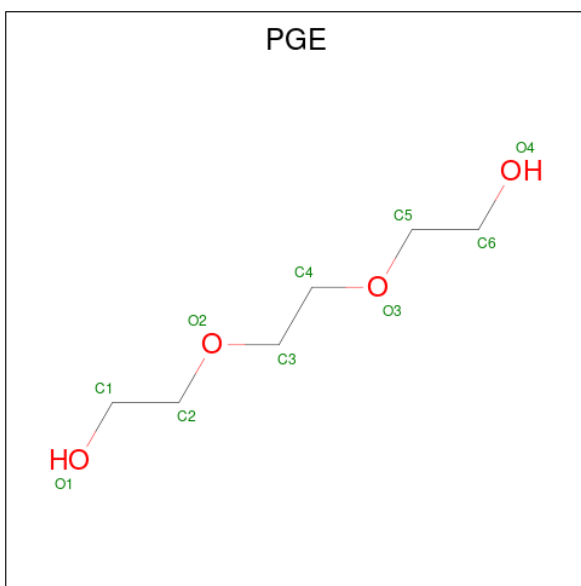
There are 6 unique types of molecules in this entry. The entry contains 10556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	628	5002	3185	868	920	29	0	0	0
1	B	625	4977	3169	863	916	29	0	0	0

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- 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		

- Molecule 5 is GLYCEROL (three-letter code: 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		

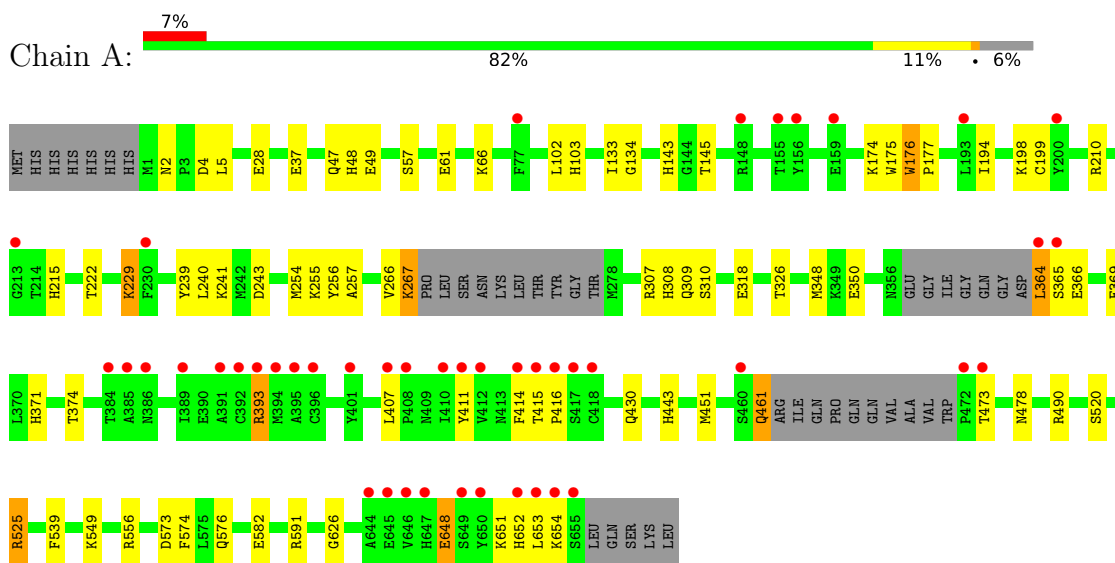
- Molecule 6 is water.

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

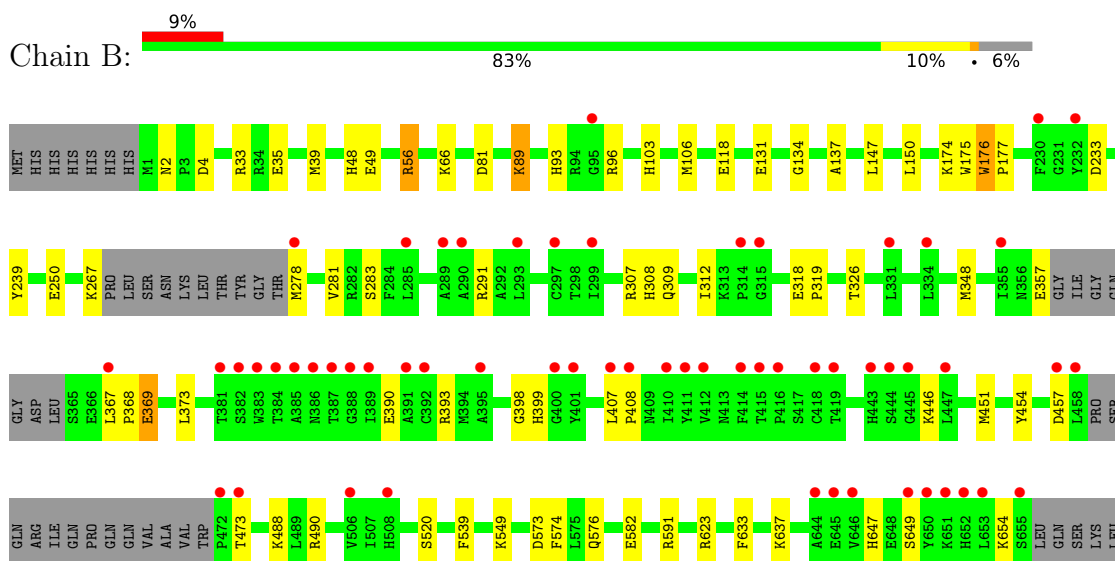
3 Residue-property plots [i](#)

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: Isoform 2 of Peroxisomal acyl-coenzyme A oxidase 1



- Molecule 1: Isoform 2 of Peroxisomal acyl-coenzyme A oxidase 1



4 Data and refinement statistics i

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 48.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.23-2.00) 99.1 (48.18-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.220 0.192 , 0.228	Depositor DCC
R_{free} test set	5573 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtrriage
Anisotropy	0.822	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for -h,l,k	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, EDO, PEG, CSO, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	3/5099 (0.1%)	1.00	4/6896 (0.1%)
1	B	0.92	1/5073 (0.0%)	0.99	6/6861 (0.1%)
All	All	0.92	4/10172 (0.0%)	0.99	10/13757 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	GLU	CD-OE2	5.83	1.32	1.25
1	A	37	GLU	CD-OE1	-5.63	1.19	1.25
1	B	131	GLU	CD-OE1	5.40	1.31	1.25
1	A	28	GLU	CG-CD	5.10	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	623	ARG	CB-CA-C	-6.00	98.41	110.40
1	A	525	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	525	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	B	291	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	210	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	393	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	93	HIS	CA-CB-CG	-5.48	104.28	113.60
1	B	291	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	33	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	56	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4972	50	0
1	B	4977	0	4944	44	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
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	10038	92	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 (92) 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	1.60	0.81
1:A:307:ARG:HE	2:A:701:PGE:H12	1.45	0.79
1:A:348:MET:CE	1:A:374:THR:HG22	2.17	0.74
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:364:LEU:C	1:A:366:GLU:H	2.08	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
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: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: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:A:243:ASP:OD1	1:A:243:ASP:C	2.50	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:A:414:PHE:C	1:A:416:PRO:HD2	2.34	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:283:SER:HA	1:B:348:MET:HE1	1.95	0.48
1:B:369:GLU:OE1	1:B:451:MET:HG2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ASP:CG	6:B:825:HOH:O	2.52	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:B:35:GLU:HG2	1:B:39:MET:CE	2.45	0.46
1:B:35:GLU:HG2	1:B:39:MET:HE3	1.97	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:B:48:HIS:HE1	1:B:66:LYS:HZ3	1.61	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
1:A:326:THR:HG23	1:B:520:SER:HB3	1.98	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:176:TRP:O	1:A:177:PRO:C	2.55	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:48:HIS:HE1	1:A:66:LYS:HZ2	1.68	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: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: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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	618/667 (93%)	593 (96%)	21 (3%)	4 (1%)	25	19
1	B	615/667 (92%)	597 (97%)	15 (2%)	3 (0%)	29	23
All	All	1233/1334 (92%)	1190 (96%)	36 (3%)	7 (1%)	25	19

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	539/576 (94%)	522 (97%)	17 (3%)	39	38
1	B	536/576 (93%)	523 (98%)	13 (2%)	49	51
All	All	1075/1152 (93%)	1045 (97%)	30 (3%)	43	44

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	61	GLU
1	A	102	LEU
1	A	133	ILE
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	539	PHE
1	A	648	GLU
1	A	651	LYS
1	A	653	LEU
1	A	654	LYS
1	B	56	ARG
1	B	81	ASP
1	B	89	LYS
1	B	106	MET
1	B	278	MET
1	B	281	VAL
1	B	357	GLU
1	B	369	GLU
1	B	446	LYS
1	B	457	ASP
1	B	539	PHE
1	B	591	ARG
1	B	654	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	38	ASN
1	A	48	HIS
1	A	90	ASN
1	A	103	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	430	GLN
1	A	461	GLN
1	A	478	ASN
1	A	576	GLN
1	A	613	GLN
1	A	627	ASN
1	B	47	GLN
1	B	48	HIS
1	B	90	ASN
1	B	103	HIS
1	B	203	HIS
1	B	308	HIS
1	B	399	HIS
1	B	430	GLN
1	B	443	HIS
1	B	503	GLN
1	B	576	GLN
1	B	647	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	A	449	1	3,6,7	1.25	0	0,6,8	-	-
1	CSO	A	199	1	3,6,7	1.35	1 (33%)	0,6,8	-	-
1	CSO	B	449	1	3,6,7	1.17	0	0,6,8	-	-
1	CSO	B	199	1	3,6,7	1.16	0	0,6,8	-	-

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	A	449	1	-	0/1/5/7	-
1	CSO	A	199	1	-	0/1/5/7	-
1	CSO	B	449	1	-	0/1/5/7	-
1	CSO	B	199	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	CSO	O-C	2.21	1.28	1.19

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 monosaccharides 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	703	-	3,3,3	0.77	0	2,2,2	1.00	0
3	EDO	B	702	-	3,3,3	1.37	0	2,2,2	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	703	-	3,3,3	1.12	0	2,2,2	0.61	0
3	EDO	B	704	-	3,3,3	0.81	0	2,2,2	0.59	0
3	EDO	A	708	-	3,3,3	0.61	0	2,2,2	0.35	0
3	EDO	B	706	-	3,3,3	0.16	0	2,2,2	0.31	0
2	PGE	B	701	-	9,9,9	0.85	0	8,8,8	0.94	0
4	PEG	A	704	-	6,6,6	0.76	0	5,5,5	0.42	0
2	PGE	A	701	-	9,9,9	0.61	0	8,8,8	1.09	2 (25%)
3	EDO	A	706	-	3,3,3	0.26	0	2,2,2	0.37	0
3	EDO	A	709	-	3,3,3	0.20	0	2,2,2	0.32	0
5	GOL	B	705	-	5,5,5	0.16	0	5,5,5	0.42	0
5	GOL	A	707	-	5,5,5	0.27	0	5,5,5	0.58	0
5	GOL	B	707	-	5,5,5	0.20	0	5,5,5	0.50	0
3	EDO	A	705	-	3,3,3	0.73	0	2,2,2	0.25	0
3	EDO	A	702	-	3,3,3	1.31	0	2,2,2	1.10	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	703	-	-	0/1/1/1	-
3	EDO	B	702	-	-	1/1/1/1	-
3	EDO	B	703	-	-	1/1/1/1	-
3	EDO	B	704	-	-	1/1/1/1	-
3	EDO	A	708	-	-	1/1/1/1	-
3	EDO	B	706	-	-	1/1/1/1	-
2	PGE	B	701	-	-	4/7/7/7	-
4	PEG	A	704	-	-	3/4/4/4	-
2	PGE	A	701	-	-	3/7/7/7	-
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	A	709	-	-	1/1/1/1	-
5	GOL	B	705	-	-	4/4/4/4	-
5	GOL	A	707	-	-	0/4/4/4	-
5	GOL	B	707	-	-	0/4/4/4	-
3	EDO	A	705	-	-	1/1/1/1	-
3	EDO	A	702	-	-	1/1/1/1	-

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	-2.12	104.10	113.29
2	A	701	PGE	O2-C2-C1	-2.03	101.14	110.07

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
4	A	704	PEG	O2-C3-C4-O4
2	B	701	PGE	O2-C3-C4-O3
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
2	B	701	PGE	C6-C5-O3-C4
3	A	708	EDO	O1-C1-C2-O2
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	A	709	EDO	O1-C1-C2-O2
3	B	703	EDO	O1-C1-C2-O2
4	A	704	PEG	C4-C3-O2-C2
3	A	702	EDO	O1-C1-C2-O2
3	B	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
2	B	701	PGE	4	0
2	A	701	PGE	6	0
5	B	705	GOL	1	0
5	A	707	GOL	2	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%)	0.28	45 (7%) 15 14	30, 48, 81, 145	0
1	B	623/667 (93%)	0.34	59 (9%) 8 7	29, 45, 79, 125	0
All	All	1249/1334 (93%)	0.31	104 (8%) 11 10	29, 47, 80, 145	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	655	SER	8.7
1	A	472	PRO	6.8
1	B	472	PRO	5.8
1	B	355	ILE	5.6
1	B	653	LEU	5.6
1	A	365	SER	5.5
1	A	653	LEU	5.5
1	A	652	HIS	5.3
1	B	652	HIS	4.7
1	B	389	ILE	4.5
1	B	293	LEU	4.0
1	B	385	ALA	3.9
1	B	644	ALA	3.9
1	B	650	TYR	3.8
1	B	447	LEU	3.8
1	A	389	ILE	3.8
1	B	473	THR	3.8
1	B	411	TYR	3.6
1	B	334	LEU	3.6
1	B	412	VAL	3.5
1	A	649	SER	3.4
1	A	650	TYR	3.4
1	B	445	GLY	3.4
1	B	414	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	654	LYS	3.3
1	A	418	CYS	3.3
1	B	418	CYS	3.2
1	A	412	VAL	3.2
1	B	407	LEU	3.1
1	A	156	TYR	3.1
1	B	415	THR	3.1
1	B	392	CYS	3.0
1	A	77	PHE	3.0
1	B	649	SER	3.0
1	B	387	THR	2.9
1	B	367	LEU	2.9
1	B	410	ILE	2.9
1	B	289	ALA	2.9
1	B	391	ALA	2.9
1	B	646	VAL	2.8
1	B	443	HIS	2.8
1	A	385	ALA	2.8
1	A	644	ALA	2.8
1	A	230	PHE	2.8
1	A	411	TYR	2.8
1	B	331	LEU	2.8
1	A	646	VAL	2.7
1	A	460	SER	2.7
1	B	386	ASN	2.7
1	B	297	CYS	2.7
1	A	200	TYR	2.6
1	B	651	LYS	2.6
1	B	278	MET	2.6
1	B	383	TRP	2.6
1	B	444	SER	2.6
1	B	384	THR	2.6
1	B	655	SER	2.6
1	A	193	LEU	2.6
1	B	506	VAL	2.6
1	A	148	ARG	2.6
1	A	392	CYS	2.6
1	B	416	PRO	2.5
1	B	645	GLU	2.5
1	B	388	GLY	2.5
1	B	285	LEU	2.4
1	A	391	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	473	THR	2.4
1	B	400	GLY	2.4
1	A	386	ASN	2.4
1	B	419	THR	2.4
1	A	213	GLY	2.4
1	B	395	ALA	2.4
1	B	230	PHE	2.3
1	B	299	ILE	2.3
1	A	415	THR	2.3
1	A	395	ALA	2.3
1	A	414	PHE	2.3
1	A	410	ILE	2.3
1	B	457	ASP	2.2
1	B	315	GLY	2.2
1	A	407	LEU	2.2
1	B	314	PRO	2.2
1	A	647	HIS	2.2
1	B	95	GLY	2.2
1	B	401	TYR	2.2
1	A	393	ARG	2.2
1	B	408	PRO	2.2
1	B	458	LEU	2.1
1	A	401	TYR	2.1
1	B	382	SER	2.1
1	A	416	PRO	2.1
1	A	394	MET	2.1
1	A	155	THR	2.1
1	A	645	GLU	2.1
1	A	364	LEU	2.1
1	B	290	ALA	2.1
1	B	508	HIS	2.1
1	A	417	SER	2.1
1	A	384	THR	2.1
1	A	408	PRO	2.0
1	B	232	TYR	2.0
1	B	381	THR	2.0
1	A	159	GLU	2.0
1	A	396	CYS	2.0

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	A	199	7/8	0.83	0.31	20,20,20,20	0
1	CSO	A	449	7/8	0.85	0.27	20,20,20,20	0
1	CSO	B	449	7/8	0.86	0.39	20,20,20,20	0
1	CSO	B	199	7/8	0.91	0.28	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	A	708	4/4	0.72	0.49	63,68,70,73	0
5	GOL	A	707	6/6	0.82	0.16	63,65,72,73	0
2	PGE	A	701	10/10	0.85	0.39	43,54,64,70	0
3	EDO	A	709	4/4	0.86	0.25	59,64,67,72	0
2	PGE	B	701	10/10	0.87	0.37	41,64,72,77	0
3	EDO	B	703	4/4	0.89	0.16	52,57,57,61	0
3	EDO	B	704	4/4	0.91	0.17	42,58,62,63	0
3	EDO	A	702	4/4	0.92	0.19	44,52,52,54	0
3	EDO	A	705	4/4	0.92	0.15	53,60,67,69	0
4	PEG	A	704	7/7	0.92	0.21	61,65,72,75	0
3	EDO	B	702	4/4	0.92	0.45	38,50,59,59	0
3	EDO	B	706	4/4	0.93	0.17	49,59,62,65	0
3	EDO	A	703	4/4	0.94	0.28	36,48,50,54	0
3	EDO	A	706	4/4	0.94	0.15	50,53,57,57	0
5	GOL	B	707	6/6	0.94	0.23	54,58,59,64	0
5	GOL	B	705	6/6	0.95	0.14	63,70,75,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.