



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 04:25 pm BST

PDB ID : 6O4D
Title : Structure of ALDH7A1 mutant W175A complexed with L-pipecolic acid
Authors : Tanner, J.J.; Korasick, D.A.; Laciak, A.R.
Deposited on : 2019-02-28
Resolution : 1.88 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

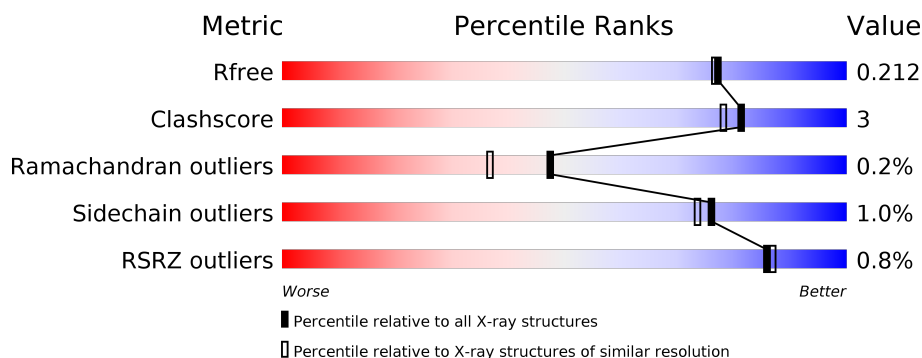
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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.



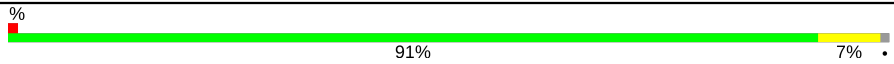
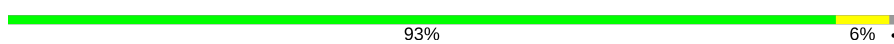
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 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	513	<div> <div></div> <div>93% 6% .</div> </div>
2	B	513	<div> <div>2%</div> <div>90% 9% .</div> </div>
2	G	513	<div> <div></div> <div>92% 7% .</div> </div>
3	C	513	<div> <div>2%</div> <div>92% 7% .</div> </div>
3	D	513	<div> <div>2%</div> <div>92% 8% .</div> </div>
3	E	513	<div> <div></div> <div>94% 6% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	513	 91% 7%
3	H	513	 93% 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
4	6PC	A	601	-	X	-	-
4	6PC	B	601	-	X	-	-
4	6PC	C	601	-	X	-	-
4	6PC	D	601	-	X	-	-
4	6PC	E	601	-	X	-	-
4	6PC	F	601	-	X	-	-
4	6PC	G	601	-	X	-	-
4	6PC	H	601	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 33068 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	3	0
			3841	2439	666	718	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	175	ALA	TRP	engineered mutation	UNP P49419

- Molecule 2 is a protein called Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	510	Total	C	N	O	S	0	1	0
			3850	2441	667	724	18			
2	G	508	Total	C	N	O	S	0	2	0
			3855	2445	668	724	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	175	ALA	TRP	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	175	ALA	TRP	engineered mutation	UNP P49419

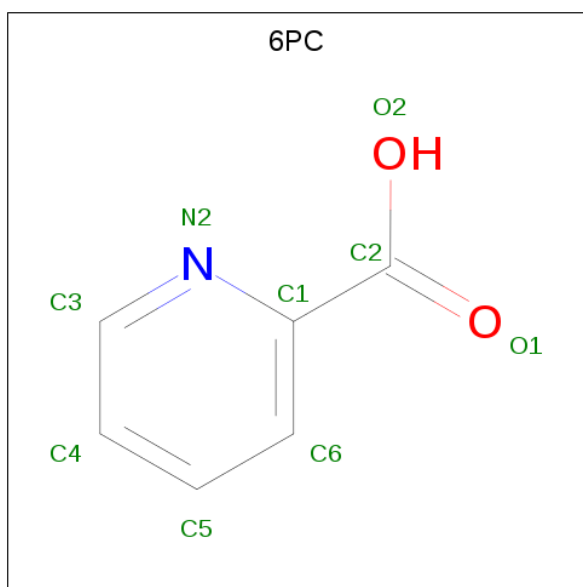
- Molecule 3 is a protein called Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	508	Total	C	N	O	S	0	1	0
			3823	2430	662	713	18			
3	D	509	Total	C	N	O	S	0	2	0
			3854	2445	669	722	18			
3	E	509	Total	C	N	O	S	0	1	0
			3843	2441	667	717	18			
3	F	509	Total	C	N	O	S	0	1	0
			3855	2447	669	721	18			
3	H	509	Total	C	N	O	S	0	3	0
			3859	2451	669	721	18			

There are 15 discrepancies between the modelled and reference sequences:

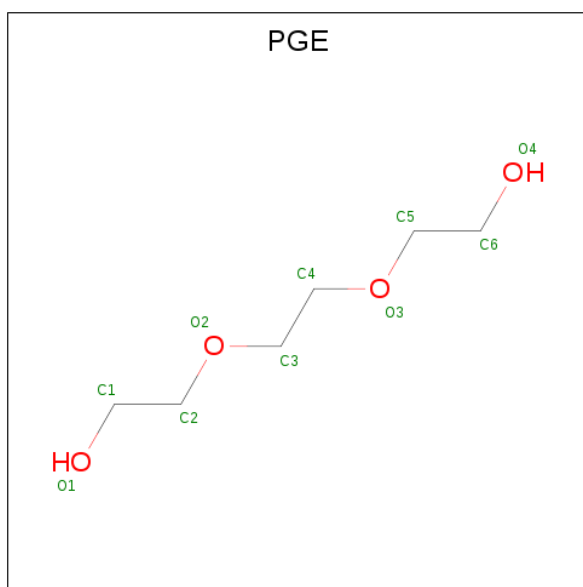
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	175	ALA	TRP	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	175	ALA	TRP	engineered mutation	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419
E	0	HIS	-	expression tag	UNP P49419
E	175	ALA	TRP	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	175	ALA	TRP	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	175	ALA	TRP	engineered mutation	UNP P49419

- Molecule 4 is PYRIDINE-2-CARBOXYLIC ACID (three-letter code: 6PC) (formula: $C_6H_5NO_2$).



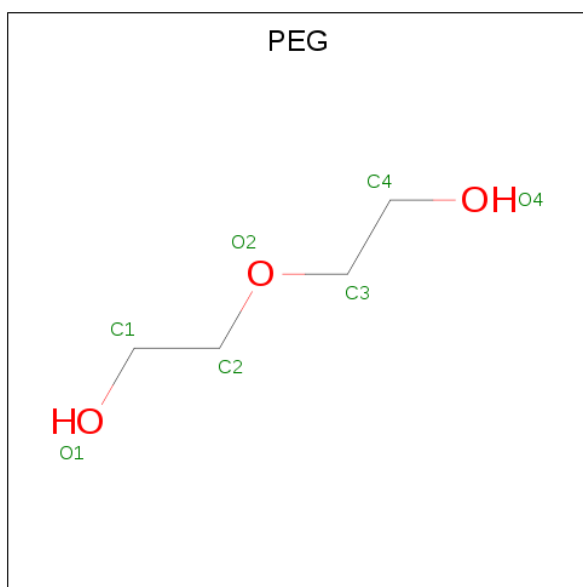
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	1	2		
4	B	1	Total	C	N	O	0	0
			9	6	1	2		
4	C	1	Total	C	N	O	0	0
			9	6	1	2		
4	D	1	Total	C	N	O	0	0
			9	6	1	2		
4	E	1	Total	C	N	O	0	0
			9	6	1	2		
4	F	1	Total	C	N	O	0	0
			9	6	1	2		
4	G	1	Total	C	N	O	0	0
			9	6	1	2		
4	H	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



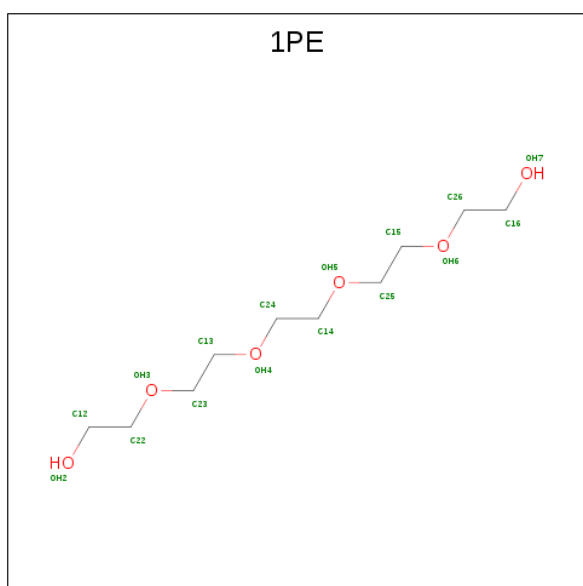
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



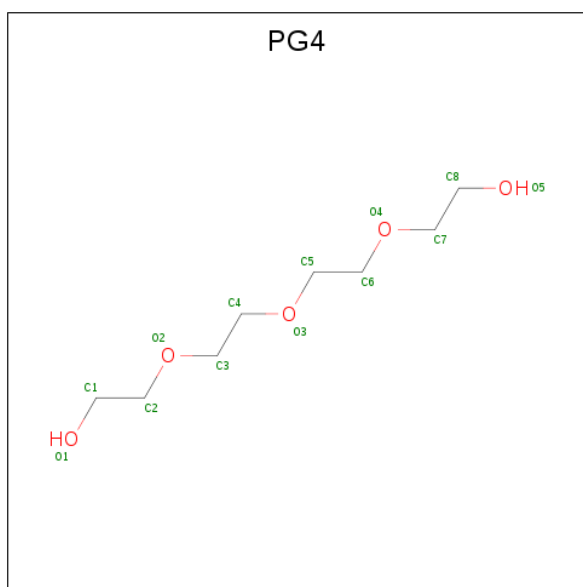
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



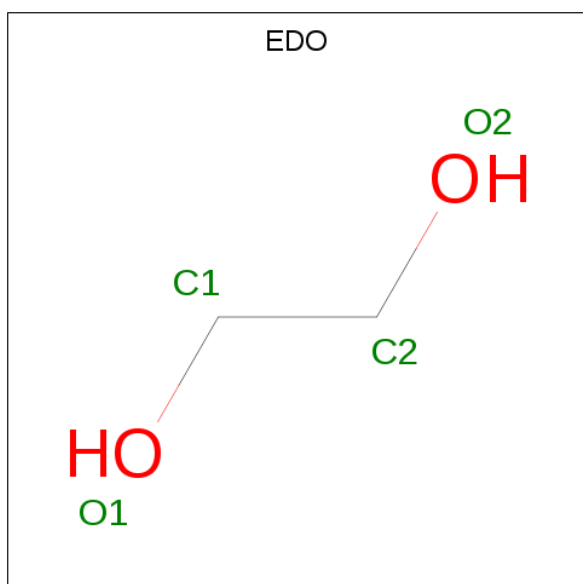
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	8	5		
8	D	1	Total	C	O	0	0
			13	8	5		
8	F	1	Total	C	O	0	0
			13	8	5		
8	G	1	Total	C	O	0	0
			13	8	5		
8	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

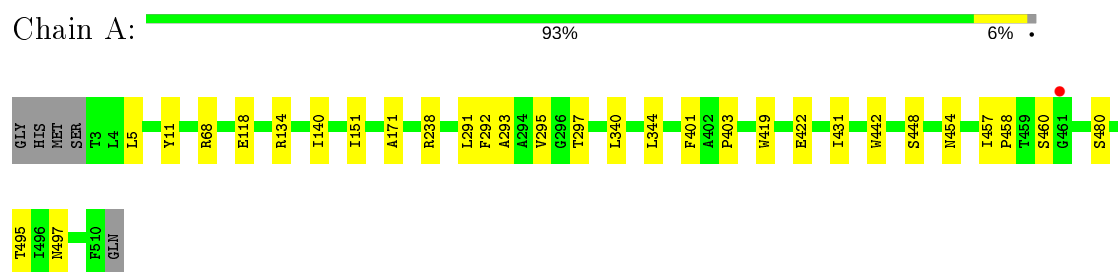
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	261	Total	O	0	0
			261	261		
10	B	263	Total	O	0	0
			263	263		
10	C	241	Total	O	0	1
			242	242		
10	D	223	Total	O	0	0
			223	223		
10	E	273	Total	O	0	0
			273	273		
10	F	254	Total	O	0	0
			254	254		
10	G	276	Total	O	0	1
			277	277		
10	H	264	Total	O	0	0
			264	264		

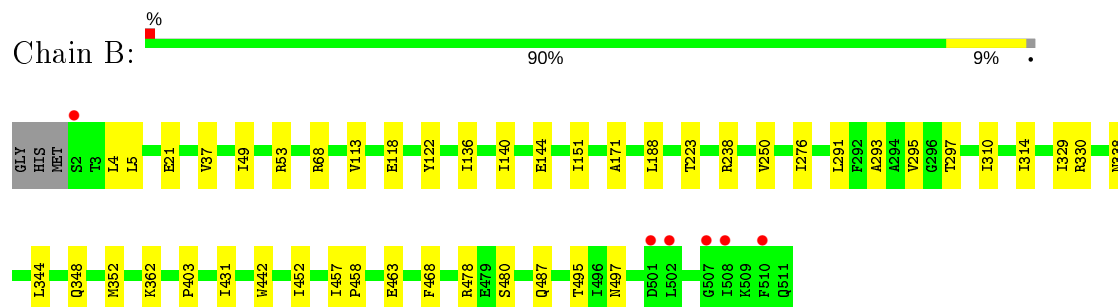
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

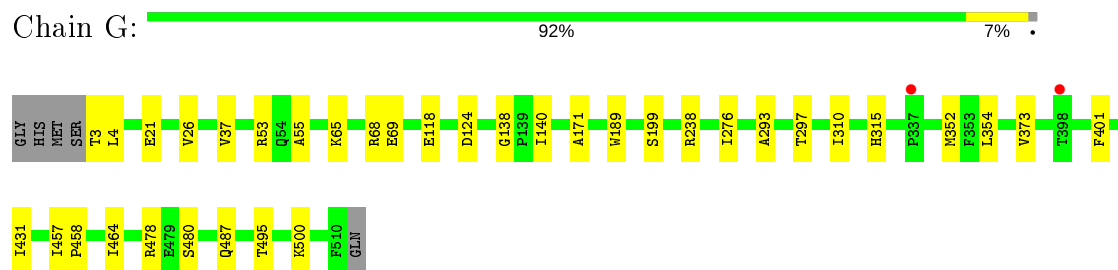
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



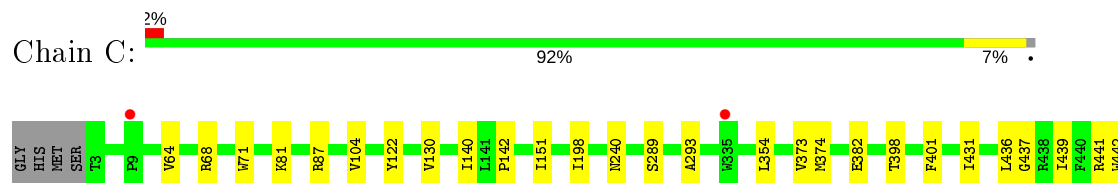
- Molecule 2: Alpha-aminoadipic semialdehyde dehydrogenase

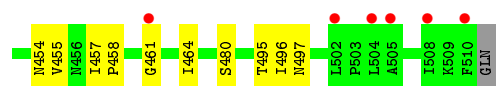


- Molecule 2: Alpha-aminoadipic semialdehyde dehydrogenase

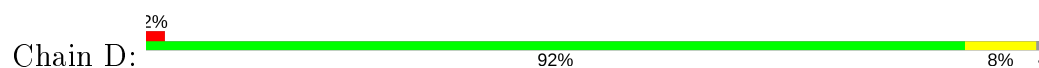


- Molecule 3: Alpha-aminoadipic semialdehyde dehydrogenase

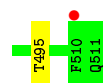




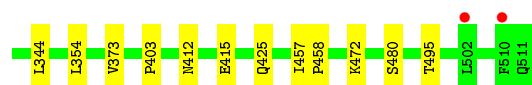
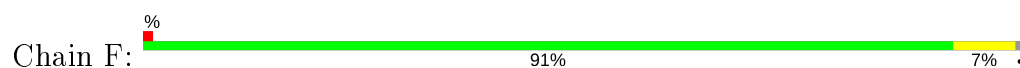
- Molecule 3: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 3: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 3: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 3: Alpha-aminoadipic semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.78Å 161.97Å 159.04Å 90.00° 94.88° 90.00°	Depositor
Resolution (Å)	57.96 – 1.88 57.96 – 1.88	Depositor EDS
% Data completeness (in resolution range)	94.7 (57.96-1.88) 99.5 (57.96-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, R_{free}	0.172 , 0.215 0.169 , 0.212	Depositor DCC
R_{free} test set	15255 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33068	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% 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: CSO, PGE, EDO, 1PE, PG4, 6PC, OCS, PEG

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	0.37	0/3919	0.53	0/5318
2	B	0.36	0/3921	0.53	0/5320
2	G	0.36	0/3929	0.52	0/5328
3	C	0.37	0/3904	0.51	0/5301
3	D	0.35	0/3938	0.51	0/5343
3	E	0.36	0/3924	0.53	0/5325
3	F	0.36	0/3936	0.52	0/5339
3	H	0.35	0/3946	0.52	0/5353
All	All	0.36	0/31417	0.52	0/42627

There are no bond length outliers.

There are no bond angle outliers.

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	3841	0	3812	18	0
2	B	3850	0	3817	30	0
2	G	3855	0	3845	21	0
3	C	3823	0	3788	27	0
3	D	3854	0	3833	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3843	0	3823	17	0
3	F	3855	0	3845	27	0
3	H	3859	0	3849	22	0
4	A	9	0	4	0	0
4	B	9	0	4	0	0
4	C	9	0	4	0	0
4	D	9	0	4	0	0
4	E	9	0	4	1	0
4	F	9	0	4	0	0
4	G	9	0	4	0	0
4	H	9	0	4	0	0
5	A	10	0	14	0	0
5	D	10	0	14	2	0
5	E	20	0	28	2	0
5	H	20	0	28	4	0
6	B	7	0	10	1	0
6	F	7	0	10	0	0
7	B	16	0	22	0	0
8	C	13	0	18	6	0
8	D	13	0	18	2	0
8	F	13	0	18	1	0
8	G	13	0	18	1	0
8	H	13	0	18	2	0
9	H	4	0	6	0	0
10	A	261	0	0	1	0
10	B	263	0	0	2	0
10	C	242	0	0	0	0
10	D	223	0	0	3	0
10	E	273	0	0	0	0
10	F	254	0	0	1	0
10	G	277	0	0	0	0
10	H	264	0	0	0	0
All	All	33068	0	30866	163	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 3.

The worst 5 of 163 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)
3:C:68:ARG:HH22	8:C:602:PG4:H71	1.31	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:ASN:HD21	8:C:602:PG4:H72	1.36	0.89
3:F:293:ALA:HB2	3:F:458:PRO:HB3	1.56	0.87
3:E:293:ALA:HB2	3:E:458:PRO:HB3	1.55	0.86
2:B:140:ILE:HD11	3:C:151:ILE:HB	1.65	0.78

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	508/513 (99%)	493 (97%)	14 (3%)	1 (0%)	47	37
2	B	508/513 (99%)	491 (97%)	16 (3%)	1 (0%)	47	37
2	G	507/513 (99%)	492 (97%)	14 (3%)	1 (0%)	47	37
3	C	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	37
3	D	509/513 (99%)	492 (97%)	16 (3%)	1 (0%)	47	37
3	E	508/513 (99%)	492 (97%)	15 (3%)	1 (0%)	47	37
3	F	508/513 (99%)	493 (97%)	14 (3%)	1 (0%)	47	37
3	H	510/513 (99%)	493 (97%)	16 (3%)	1 (0%)	47	37
All	All	4065/4104 (99%)	3936 (97%)	121 (3%)	8 (0%)	47	37

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	480	SER
1	A	480	SER
3	E	480	SER
3	F	480	SER
2	G	480	SER

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	395/408 (97%)	391 (99%)	4 (1%)	76	73
2	B	397/408 (97%)	395 (100%)	2 (0%)	88	88
2	G	401/408 (98%)	397 (99%)	4 (1%)	76	73
3	C	392/409 (96%)	388 (99%)	4 (1%)	76	73
3	D	400/409 (98%)	393 (98%)	7 (2%)	59	52
3	E	397/409 (97%)	394 (99%)	3 (1%)	81	80
3	F	401/409 (98%)	396 (99%)	5 (1%)	71	67
3	H	401/409 (98%)	397 (99%)	4 (1%)	76	73
All	All	3184/3269 (97%)	3151 (99%)	33 (1%)	76	73

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	389	LEU
3	E	297	THR
3	H	297	THR
3	D	401	PHE
3	D	424	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
2	B	506	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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
2	OCS	G	302	2	7,8,9	0.91	0	6,11,13	1.63	1 (16%)
2	OCS	B	302	2	7,8,9	0.98	0	6,11,13	2.06	2 (33%)
1	CSO	A	302	1	3,6,7	0.67	0	0,6,8	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OCS	G	302	2	-	0/4/7/9	-
2	OCS	B	302	2	-	0/4/7/9	-
1	CSO	A	302	1	-	0/1/5/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	OCS	OD3-SG-CB	3.35	110.92	106.94
2	B	302	OCS	OD2-SG-CB	2.82	110.23	105.74
2	G	302	OCS	OD2-SG-CB	2.81	110.22	105.74

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

23 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
7	1PE	B	603	-	15,15,15	0.53	0	14,14,14	0.28	0
5	PGE	A	602	-	9,9,9	0.36	0	8,8,8	0.33	0
6	PEG	F	603	-	6,6,6	0.48	0	5,5,5	0.26	0
4	6PC	E	601	-	6,9,9	6.07	6 (100%)	7,11,11	5.14	7 (100%)
4	6PC	C	601	-	6,9,9	5.87	6 (100%)	7,11,11	5.11	6 (85%)
8	PG4	D	603	-	12,12,12	0.51	0	11,11,11	0.24	0
8	PG4	F	602	-	12,12,12	0.51	0	11,11,11	0.42	0
5	PGE	H	605	-	9,9,9	0.53	0	8,8,8	0.26	0
4	6PC	H	601	-	6,9,9	6.04	6 (100%)	7,11,11	5.03	7 (100%)
4	6PC	F	601	-	6,9,9	6.10	6 (100%)	7,11,11	5.16	6 (85%)
9	EDO	H	602	-	3,3,3	0.53	0	2,2,2	0.21	0
5	PGE	H	603	-	9,9,9	0.34	0	8,8,8	0.27	0
8	PG4	C	602	-	12,12,12	0.49	0	11,11,11	0.35	0
6	PEG	B	602	-	6,6,6	0.49	0	5,5,5	0.24	0
5	PGE	E	603	-	9,9,9	0.28	0	8,8,8	0.41	0
8	PG4	H	604	-	12,12,12	0.56	0	11,11,11	0.48	0
4	6PC	A	601	-	6,9,9	5.87	6 (100%)	7,11,11	4.83	5 (71%)
5	PGE	E	602	-	9,9,9	0.28	0	8,8,8	0.24	0
8	PG4	G	602	-	12,12,12	0.52	0	11,11,11	0.24	0
4	6PC	D	601	-	6,9,9	5.91	6 (100%)	7,11,11	5.70	7 (100%)
4	6PC	B	601	-	6,9,9	5.90	6 (100%)	7,11,11	5.40	6 (85%)
5	PGE	D	602	-	9,9,9	0.34	0	8,8,8	0.32	0
4	6PC	G	601	-	6,9,9	5.90	6 (100%)	7,11,11	5.53	6 (85%)

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
7	1PE	B	603	-	-	4/13/13/13	-
5	PGE	A	602	-	-	3/7/7/7	-
6	PEG	F	603	-	-	3/4/4/4	-
4	6PC	E	601	-	-	0/0/4/4	0/1/1/1
4	6PC	C	601	-	-	0/0/4/4	0/1/1/1
8	PG4	D	603	-	-	8/10/10/10	-
8	PG4	F	602	-	-	2/10/10/10	-
5	PGE	H	605	-	-	6/7/7/7	-
4	6PC	H	601	-	-	0/0/4/4	0/1/1/1
4	6PC	F	601	-	-	0/0/4/4	0/1/1/1
9	EDO	H	602	-	-	0/1/1/1	-
5	PGE	H	603	-	-	5/7/7/7	-
8	PG4	C	602	-	-	5/10/10/10	-
6	PEG	B	602	-	-	3/4/4/4	-
5	PGE	E	603	-	-	4/7/7/7	-
8	PG4	H	604	-	-	4/10/10/10	-
4	6PC	A	601	-	-	0/0/4/4	0/1/1/1
5	PGE	E	602	-	-	2/7/7/7	-
8	PG4	G	602	-	-	5/10/10/10	-
4	6PC	D	601	-	-	0/0/4/4	0/1/1/1
4	6PC	B	601	-	-	0/0/4/4	0/1/1/1
5	PGE	D	602	-	-	4/7/7/7	-
4	6PC	G	601	-	-	0/0/4/4	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	6PC	C3-N2	7.37	1.50	1.34
4	E	601	6PC	C3-N2	7.20	1.49	1.34
4	F	601	6PC	C1-N2	7.19	1.49	1.35
4	D	601	6PC	C3-N2	7.12	1.49	1.34
4	A	601	6PC	C3-N2	7.11	1.49	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	601	6PC	C6-C1-C2	-9.27	108.66	120.19
4	D	601	6PC	C6-C1-C2	-8.74	109.33	120.19
4	B	601	6PC	C6-C1-C2	-8.69	109.38	120.19
4	G	601	6PC	C6-C1-C2	-8.51	109.61	120.19
4	H	601	6PC	C6-C1-C2	-8.36	109.80	120.19

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	602	PGE	C1-C2-O2-C3
8	C	602	PG4	C4-C3-O2-C2
8	H	604	PG4	O4-C7-C8-O5
5	H	603	PGE	O2-C3-C4-O3
5	E	603	PGE	O2-C3-C4-O3

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	601	6PC	1	0
8	D	603	PG4	2	0
8	F	602	PG4	1	0
5	H	605	PGE	2	0
5	H	603	PGE	2	0
8	C	602	PG4	6	0
6	B	602	PEG	1	0
5	E	603	PGE	1	0
8	H	604	PG4	2	0
5	E	602	PGE	1	0
8	G	602	PG4	1	0
5	D	602	PGE	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	507/513 (98%)	-0.19	1 (0%) 95 95	15, 26, 42, 62	0
2	B	509/513 (99%)	-0.21	6 (1%) 79 80	16, 26, 43, 75	0
2	G	507/513 (98%)	-0.30	2 (0%) 92 93	16, 25, 41, 64	0
3	C	508/513 (99%)	-0.20	8 (1%) 72 74	15, 25, 48, 69	0
3	D	509/513 (99%)	-0.05	10 (1%) 65 67	16, 30, 54, 77	0
3	E	509/513 (99%)	-0.25	1 (0%) 95 95	19, 26, 40, 61	0
3	F	509/513 (99%)	-0.17	4 (0%) 86 87	18, 27, 44, 64	0
3	H	509/513 (99%)	-0.23	0 100 100	16, 26, 43, 57	0
All	All	4067/4104 (99%)	-0.20	32 (0%) 86 87	15, 26, 45, 77	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	510	PHE	6.1
3	C	502	LEU	4.6
2	B	2	SER	4.2
3	C	510	PHE	3.9
3	D	508	ILE	3.8

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	302	7/8	0.93	0.10	23,26,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OCS	B	302	9/10	0.97	0.10	17,20,44,51	0
2	OCS	G	302	9/10	0.97	0.10	18,28,41,53	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
5	PGE	D	602	10/10	0.78	0.18	51,54,55,55	0
5	PGE	H	605	10/10	0.83	0.14	42,48,54,58	0
9	EDO	H	602	4/4	0.86	0.21	40,43,43,44	0
5	PGE	H	603	10/10	0.86	0.17	43,48,51,53	0
8	PG4	H	604	13/13	0.86	0.16	22,39,43,46	0
4	6PC	D	601	9/9	0.86	0.17	41,45,49,51	0
6	PEG	F	603	7/7	0.86	0.23	46,47,54,56	0
5	PGE	A	602	10/10	0.87	0.15	34,38,44,46	0
8	PG4	G	602	13/13	0.88	0.16	36,44,59,60	0
8	PG4	C	602	13/13	0.88	0.11	30,36,44,46	0
5	PGE	E	602	10/10	0.88	0.14	31,40,46,50	0
4	6PC	F	601	9/9	0.89	0.14	41,44,47,48	0
8	PG4	D	603	13/13	0.89	0.13	37,42,46,48	0
4	6PC	B	601	9/9	0.89	0.14	33,36,40,43	0
4	6PC	C	601	9/9	0.89	0.19	32,35,44,45	0
5	PGE	E	603	10/10	0.90	0.14	39,46,50,53	0
4	6PC	E	601	9/9	0.90	0.12	39,41,43,44	0
4	6PC	A	601	9/9	0.90	0.12	38,43,53,55	0
7	1PE	B	603	16/16	0.90	0.16	36,42,58,60	0
8	PG4	F	602	13/13	0.91	0.13	36,43,51,51	0
4	6PC	H	601	9/9	0.92	0.10	24,29,33,34	0
6	PEG	B	602	7/7	0.92	0.15	37,46,50,50	0
4	6PC	G	601	9/9	0.94	0.11	25,32,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.