



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5G1W / pdb_00005g1w
Title : Apo Structure of Linalool Dehydratase-Isomerase
Authors : Chambers, S.; Hau, A.; Man, H.; Omar, M.; Turkenburg, J.P.; Grogan, G.
Deposited on : 2016-03-30
Resolution : 1.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

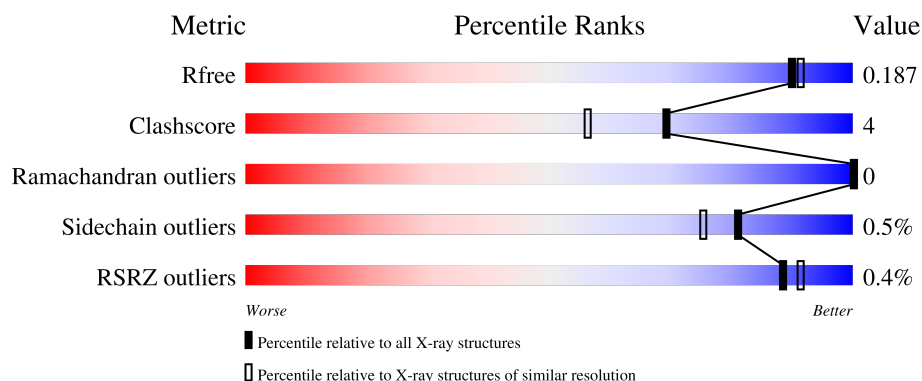
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	372	% 90% 8% .
1	B	372	91% 6% .
1	C	372	% 91% 7% ..
1	D	372	91% 6% ..
1	E	372	% 90% 7% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DXX	A	1370	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16596 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 LINALOOL DEHYDRATASE/ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	1	0
			2887	1868	478	528	13			
1	B	364	Total	C	N	O	S	0	1	0
			2885	1866	478	528	13			
1	C	365	Total	C	N	O	S	0	0	0
			2888	1868	479	528	13			
1	D	364	Total	C	N	O	S	0	2	0
			2899	1873	482	531	13			
1	E	365	Total	C	N	O	S	0	1	0
			2885	1867	478	527	13			

There are 5 discrepancies between the modelled and reference sequences:

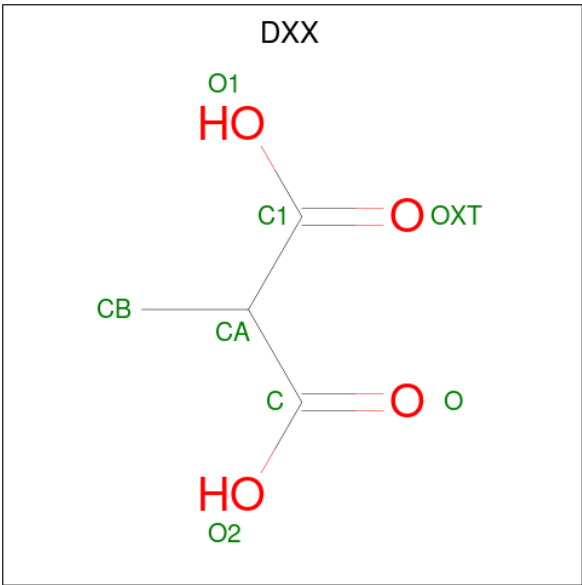
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP E1XUJ2
B	1	MET	-	expression tag	UNP E1XUJ2
C	1	MET	-	expression tag	UNP E1XUJ2
D	1	MET	-	expression tag	UNP E1XUJ2
E	1	MET	-	expression tag	UNP E1XUJ2

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



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

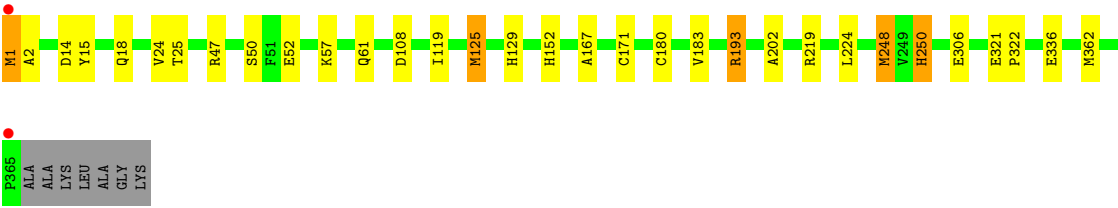
- Molecule 3 is METHYLMALONIC ACID (CCD ID: DXX) (formula: $C_4H_6O_4$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	466	Total	O	0	0
			466	466		
4	B	407	Total	O	0	0
			407	407		
4	C	416	Total	O	0	0
			416	416		
4	D	425	Total	O	0	0
			425	425		
4	E	380	Total	O	0	0
			380	380		



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.06Å 110.15Å 195.34Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	47.97 – 1.76 47.97 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.97-1.76) 96.9 (47.97-1.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.150 , 0.176 0.163 , 0.187	Depositor DCC
R_{free} test set	10822 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l 0.012 for -k,-h,-l 0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16596	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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: EDO, DXX

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	1.26	3/2976 (0.1%)	1.07	5/4051 (0.1%)
1	B	1.23	0/2974	1.06	4/4049 (0.1%)
1	C	1.30	5/2974 (0.2%)	1.09	8/4049 (0.2%)
1	D	1.29	2/2991 (0.1%)	1.07	9/4070 (0.2%)
1	E	1.30	9/2974 (0.3%)	1.08	10/4050 (0.2%)
All	All	1.28	19/14889 (0.1%)	1.07	36/20269 (0.2%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	SER	CA-C	8.86	1.63	1.52
1	C	2	ALA	N-CA	7.24	1.55	1.46
1	E	2	ALA	N-CA	6.58	1.54	1.46
1	E	248	MET	CG-SD	-6.05	1.65	1.80
1	C	2	ALA	CA-C	5.82	1.60	1.52
1	A	51	PHE	CA-C	-5.73	1.45	1.52
1	D	62	ARG	CA-C	5.68	1.60	1.52
1	E	2	ALA	CA-C	5.65	1.60	1.52
1	E	248	MET	SD-CE	-5.62	1.65	1.79
1	E	15	TYR	N-CA	5.58	1.53	1.46
1	E	250	HIS	N-CA	-5.34	1.39	1.46
1	A	3	GLU	C-O	-5.33	1.17	1.23
1	C	119	ILE	CA-CB	5.20	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	ALA	N-CA	5.19	1.52	1.46
1	E	193	ARG	CZ-NH2	-5.13	1.26	1.33
1	E	202	ALA	CA-C	5.09	1.59	1.52
1	E	119	ILE	CA-CB	5.09	1.61	1.54
1	C	193	ARG	C-O	-5.07	1.18	1.24
1	A	334	ARG	CA-C	5.02	1.58	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	ALA	N-CA-C	9.21	124.71	113.38
1	D	193	ARG	NE-CZ-NH2	-8.40	111.64	119.20
1	E	2	ALA	N-CA-C	8.18	123.44	113.38
1	C	1	MET	CA-C-N	8.03	136.16	122.26
1	C	1	MET	C-N-CA	8.03	136.16	122.26
1	D	193	ARG	CG-CD-NE	-7.98	94.45	112.00
1	E	1	MET	CA-C-N	7.93	135.97	122.26
1	E	1	MET	C-N-CA	7.93	135.97	122.26
1	A	193	ARG	NE-CZ-NH1	7.64	129.14	121.50
1	A	48	GLY	N-CA-C	6.13	119.07	112.33
1	A	193	ARG	CD-NE-CZ	5.92	132.69	124.40
1	C	50	SER	N-CA-CB	-5.92	101.17	110.69
1	C	193	ARG	CG-CD-NE	-5.88	99.08	112.00
1	A	119	ILE	CA-CB-CG2	5.86	120.45	110.50
1	B	363	PRO	O-C-N	5.73	123.84	121.15
1	D	193	ARG	NE-CZ-NH1	5.67	127.17	121.50
1	B	193	ARG	CG-CD-NE	-5.66	99.54	112.00
1	B	224	LEU	N-CA-C	5.62	117.85	111.11
1	D	193	ARG	CD-NE-CZ	5.52	132.12	124.40
1	E	119	ILE	CA-CB-CG2	5.48	119.82	110.50
1	E	119	ILE	N-CA-CB	-5.42	102.29	111.23
1	E	193	ARG	CG-CD-NE	-5.39	100.13	112.00
1	D	119	ILE	CA-CB-CG2	5.39	119.66	110.50
1	A	363	PRO	O-C-N	5.38	123.68	121.15
1	C	119	ILE	CA-CB-CG2	5.28	119.48	110.50
1	D	259	ARG	CB-CG-CD	5.26	123.41	111.30
1	E	47	ARG	CB-CA-C	-5.26	99.44	110.17
1	E	193	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	D	166	PHE	N-CA-C	-5.20	102.36	110.42
1	C	320	LEU	N-CA-C	5.19	117.73	111.40
1	B	47	ARG	CB-CA-C	-5.12	99.73	110.17
1	E	224	LEU	N-CA-C	5.09	116.52	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	224	LEU	N-CA-C	5.08	116.50	111.07
1	C	119	ILE	N-CA-CB	-5.06	102.88	111.23
1	E	125	MET	N-CA-CB	5.05	117.33	110.01
1	D	119	ILE	N-CA-CB	-5.02	102.94	111.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	193	ARG	Sidechain

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	2887	0	2771	20	0
1	B	2885	0	2767	17	0
1	C	2888	0	2769	21	0
1	D	2899	0	2792	18	0
1	E	2885	0	2763	24	0
2	A	16	0	24	0	0
2	B	12	0	18	0	0
2	C	4	0	6	0	0
2	D	8	0	12	0	0
2	E	4	0	6	0	0
3	A	7	0	0	0	11
3	B	7	0	0	0	0
4	A	466	0	0	9	0
4	B	407	0	0	7	0
4	C	416	0	0	9	0
4	D	425	0	0	9	0
4	E	380	0	0	11	0
All	All	16596	0	13928	100	11

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 4.

All (100) 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:C:125:MET:HE3	4:C:2200:HOH:O	1.62	1.00
1:A:171:CYS:SG	4:A:2285:HOH:O	2.27	0.91
1:C:180:CYS:SG	4:C:2243:HOH:O	2.33	0.86
1:A:180:CYS:SG	4:A:2285:HOH:O	2.41	0.79
1:E:171:CYS:SG	4:E:2213:HOH:O	2.43	0.76
1:E:14:ASP:OD2	4:E:2030:HOH:O	2.04	0.74
1:C:171:CYS:SG	4:C:2243:HOH:O	2.45	0.73
1:B:29:MET:CE	4:B:2026:HOH:O	2.35	0.73
1:E:250:HIS:HD2	1:E:306:GLU:OE2	1.72	0.73
1:C:250:HIS:HD2	1:C:306:GLU:OE2	1.72	0.73
1:B:250:HIS:HD2	1:B:306:GLU:OE2	1.72	0.72
1:C:125:MET:HE2	1:C:129:HIS:CD2	2.25	0.71
1:A:125:MET:HE2	1:A:129:HIS:CD2	2.25	0.71
1:D:125:MET:HE2	1:D:129:HIS:CD2	2.26	0.70
1:A:50:SER:OG	1:A:52:GLU:OE1	2.10	0.70
1:E:125:MET:HE2	1:E:129:HIS:CD2	2.27	0.70
1:D:250:HIS:HD2	1:D:306:GLU:OE2	1.75	0.69
1:E:50:SER:OG	1:E:52:GLU:OE1	2.11	0.69
1:E:180:CYS:SG	4:E:2213:HOH:O	2.52	0.68
1:B:50:SER:OG	1:B:52:GLU:OE1	2.11	0.68
1:A:250:HIS:HD2	1:A:306:GLU:OE2	1.76	0.68
1:D:50[B]:SER:OG	1:D:52:GLU:OE1	2.11	0.67
1:B:125:MET:HE2	1:B:129:HIS:CD2	2.29	0.67
1:C:50:SER:OG	1:C:52:GLU:OE1	2.12	0.67
4:A:2168:HOH:O	1:D:230:SER:HB2	1.93	0.67
1:B:29:MET:HE2	4:B:2026:HOH:O	1.94	0.65
1:B:144:ARG:CG	4:B:2212:HOH:O	2.47	0.62
1:A:152:HIS:HE1	4:A:2264:HOH:O	1.84	0.60
1:A:152:HIS:HD2	4:A:2261:HOH:O	1.84	0.59
1:D:250:HIS:HE1	4:D:2302:HOH:O	1.85	0.59
1:D:212:LYS:HE2	4:D:2280:HOH:O	2.03	0.58
1:E:1:MET:CB	4:E:2002:HOH:O	2.51	0.58
1:E:183:VAL:HG22	1:E:248:MET:HE2	1.86	0.58
1:E:1:MET:HA	4:E:2002:HOH:O	2.04	0.57
1:E:152:HIS:HE1	4:E:2197:HOH:O	1.86	0.57
1:B:152:HIS:HE1	4:B:2217:HOH:O	1.87	0.56
1:D:361:ARG:NH2	4:D:2421:HOH:O	2.36	0.56
1:A:159:ASP:OD2	4:A:2275:HOH:O	2.17	0.56
1:A:18:GLN:HE21	1:A:25:THR:H	1.55	0.55
1:D:152:HIS:HE1	4:D:2222:HOH:O	1.89	0.54
1:E:219:ARG:NH1	4:E:2246:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:HIS:HE1	4:C:2224:HOH:O	1.91	0.54
1:C:334:ARG:CB	4:C:2401:HOH:O	2.55	0.54
1:C:193:ARG:NH2	1:C:362:MET:O	2.37	0.54
1:E:125:MET:HA	1:E:125:MET:HE3	1.89	0.53
1:D:2:ALA:HB1	4:D:2003:HOH:O	2.07	0.52
1:D:125:MET:HE3	1:D:125:MET:HA	1.90	0.52
1:B:125:MET:HA	1:B:125:MET:HE3	1.92	0.52
1:B:18:GLN:HE21	1:B:25:THR:H	1.58	0.51
1:A:125:MET:HE3	1:A:125:MET:HA	1.91	0.51
1:E:18:GLN:HE21	1:E:25:THR:H	1.59	0.51
1:D:61:GLN:HE22	1:D:108:ASP:HB3	1.76	0.51
1:C:152:HIS:HD2	4:C:2222:HOH:O	1.93	0.51
1:C:125:MET:HE3	1:C:125:MET:HA	1.92	0.50
1:D:21:LYS:HE3	4:D:2038:HOH:O	2.10	0.50
1:C:61:GLN:HE22	1:C:108:ASP:HB3	1.76	0.50
1:C:19:GLN:OE1	4:C:2047:HOH:O	2.20	0.49
1:E:336:GLU:CB	4:E:2359:HOH:O	2.60	0.49
1:E:193:ARG:NH2	1:E:362:MET:O	2.29	0.48
1:C:18:GLN:HE21	1:C:25:THR:H	1.60	0.48
1:C:145:ARG:NH2	4:C:2144:HOH:O	2.47	0.47
1:D:18:GLN:HE21	1:D:25:THR:H	1.61	0.47
1:B:193:ARG:NE	4:B:2253:HOH:O	2.48	0.46
1:C:250:HIS:CD2	1:C:306:GLU:OE2	2.62	0.46
1:E:61:GLN:HE22	1:E:108:ASP:HB3	1.81	0.46
1:A:2:ALA:HB3	4:A:2035:HOH:O	2.16	0.46
1:B:152:HIS:HD2	4:B:2213:HOH:O	1.99	0.45
1:A:61:GLN:HE22	1:A:108:ASP:HB3	1.82	0.45
1:C:321:GLU:HB3	1:C:322:PRO:HD3	1.99	0.44
1:A:125:MET:HE2	1:A:129:HIS:NE2	2.33	0.44
1:C:18:GLN:HE21	1:C:24:VAL:HA	1.82	0.44
1:A:250:HIS:CD2	1:A:306:GLU:OE2	2.65	0.44
1:B:2:ALA:HB1	4:B:2002:HOH:O	2.18	0.44
1:E:57:LYS:NZ	4:E:2065:HOH:O	2.50	0.44
1:E:152:HIS:HD2	4:E:2193:HOH:O	2.00	0.44
1:A:321:GLU:HB3	1:A:322:PRO:HD3	2.00	0.43
1:D:21:LYS:CE	4:D:2038:HOH:O	2.66	0.43
1:A:250:HIS:HE1	1:A:258:GLU:OE2	2.02	0.43
1:E:250:HIS:CD2	1:E:306:GLU:OE2	2.61	0.43
1:E:321:GLU:HB3	1:E:322:PRO:HD3	2.00	0.43
1:D:211:GLN:HE22	1:D:259:ARG:HH21	1.67	0.43
1:E:248:MET:HE3	1:E:248:MET:HB3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:HIS:CE1	4:D:2302:HOH:O	2.67	0.42
1:B:61:GLN:HE22	1:B:108:ASP:HB3	1.84	0.42
1:E:125:MET:HE2	1:E:129:HIS:NE2	2.35	0.41
1:E:167:ALA:HA	4:E:2209:HOH:O	2.18	0.41
1:C:125:MET:CE	4:C:2200:HOH:O	2.41	0.41
1:B:321:GLU:HB3	1:B:322:PRO:HD3	2.02	0.41
1:A:121:LYS:NZ	4:A:2235:HOH:O	2.53	0.41
1:A:2:ALA:CB	4:A:2035:HOH:O	2.68	0.41
1:B:18:GLN:HE21	1:B:24:VAL:HA	1.86	0.41
1:C:125:MET:HE2	1:C:129:HIS:NE2	2.36	0.41
1:A:18:GLN:HE21	1:A:24:VAL:HA	1.86	0.41
1:D:125:MET:HE2	1:D:129:HIS:NE2	2.36	0.41
1:B:193:ARG:NH2	1:B:362:MET:O	2.48	0.41
1:C:48:GLY:C	1:C:50:SER:H	2.29	0.40
1:B:250:HIS:CD2	1:B:306:GLU:OE2	2.62	0.40
1:A:261:TYR:HB3	1:A:262:PRO:HD3	2.03	0.40
1:D:152:HIS:HD2	4:D:2221:HOH:O	2.03	0.40
1:E:18:GLN:HE21	1:E:24:VAL:HA	1.86	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1370:DXX:C1	3:A:1370:DXX:C[2_555]	0.00	2.20
3:A:1370:DXX:O1	3:A:1370:DXX:O[2_555]	0.00	2.20
3:A:1370:DXX:OXT	3:A:1370:DXX:O2[2_555]	0.00	2.20
3:A:1370:DXX:C1	3:A:1370:DXX:O2[2_555]	1.20	1.00
3:A:1370:DXX:OXT	3:A:1370:DXX:C[2_555]	1.20	1.00
3:A:1370:DXX:C1	3:A:1370:DXX:O[2_555]	1.20	1.00
3:A:1370:DXX:O1	3:A:1370:DXX:C[2_555]	1.20	1.00
3:A:1370:DXX:C1	3:A:1370:DXX:CA[2_555]	1.50	0.70
3:A:1370:DXX:CA	3:A:1370:DXX:C[2_555]	1.50	0.70
3:A:1370:DXX:O1	3:A:1370:DXX:O2[2_555]	2.11	0.09
3:A:1370:DXX:OXT	3:A:1370:DXX:O[2_555]	2.11	0.09

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	363/372 (98%)	356 (98%)	7 (2%)	0	100	100
1	B	363/372 (98%)	357 (98%)	6 (2%)	0	100	100
1	C	363/372 (98%)	354 (98%)	9 (2%)	0	100	100
1	D	364/372 (98%)	357 (98%)	7 (2%)	0	100	100
1	E	364/372 (98%)	358 (98%)	6 (2%)	0	100	100
All	All	1817/1860 (98%)	1782 (98%)	35 (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	293/303 (97%)	291 (99%)	2 (1%)	76	67
1	B	293/303 (97%)	291 (99%)	2 (1%)	76	67
1	C	292/303 (96%)	290 (99%)	2 (1%)	76	67
1	D	297/303 (98%)	296 (100%)	1 (0%)	86	83
1	E	291/303 (96%)	291 (100%)	0	100	100
All	All	1466/1515 (97%)	1459 (100%)	7 (0%)	81	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	TYR
1	A	248	MET
1	B	57	LYS
1	B	248	MET
1	C	240	TYR
1	C	248	MET
1	D	248	MET

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	18	GLN
1	A	61	GLN
1	A	152	HIS
1	A	227	HIS
1	A	250	HIS
1	A	310	GLN
1	B	18	GLN
1	B	61	GLN
1	B	152	HIS
1	B	227	HIS
1	B	250	HIS
1	B	310	GLN
1	C	18	GLN
1	C	36	ASN
1	C	61	GLN
1	C	152	HIS
1	C	211	GLN
1	C	227	HIS
1	C	250	HIS
1	C	310	GLN
1	D	18	GLN
1	D	61	GLN
1	D	152	HIS
1	D	211	GLN
1	D	227	HIS
1	D	250	HIS
1	E	18	GLN
1	E	61	GLN
1	E	152	HIS
1	E	211	GLN
1	E	227	HIS
1	E	250	HIS

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Mol	Chain	Res	Type
1	E	310	GLN
1	E	337	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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
2	EDO	B	1366	-	3,3,3	0.52	0	2,2,2	0.54	0
2	EDO	B	1368	-	3,3,3	0.48	0	2,2,2	0.39	0
2	EDO	C	1366	-	3,3,3	0.46	0	2,2,2	0.39	0
2	EDO	A	1368	-	3,3,3	0.54	0	2,2,2	0.20	0
2	EDO	B	1367	-	3,3,3	0.66	0	2,2,2	0.52	0
2	EDO	D	1366	-	3,3,3	0.71	0	2,2,2	0.01	0
3	DXX	B	1369	-	6,6,7	1.20	0	7,7,9	1.21	0
3	DXX	A	1370	-	6,6,7	1.82	2 (33%)	7,7,9	1.00	0
2	EDO	E	1366	-	3,3,3	0.65	0	2,2,2	0.17	0
2	EDO	A	1367	-	3,3,3	0.53	0	2,2,2	0.60	0
2	EDO	A	1369	-	3,3,3	0.30	0	2,2,2	0.67	0
2	EDO	A	1366	-	3,3,3	0.37	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	D	1367	-	3,3,3	0.61	0	2,2,2	0.54	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
2	EDO	B	1366	-	-	0/1/1/1	-
2	EDO	B	1368	-	-	0/1/1/1	-
2	EDO	C	1366	-	-	0/1/1/1	-
2	EDO	A	1368	-	-	0/1/1/1	-
2	EDO	B	1367	-	-	0/1/1/1	-
2	EDO	D	1366	-	-	0/1/1/1	-
3	DXX	B	1369	-	-	4/4/4/8	-
3	DXX	A	1370	-	-	4/4/4/8	-
2	EDO	E	1366	-	-	0/1/1/1	-
2	EDO	A	1367	-	-	0/1/1/1	-
2	EDO	A	1369	-	-	1/1/1/1	-
2	EDO	A	1366	-	-	0/1/1/1	-
2	EDO	D	1367	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1370	DXX	O2-C	-3.15	1.20	1.30
3	A	1370	DXX	O1-C1	-3.09	1.20	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1370	DXX	O1-C1-CA-C
3	B	1369	DXX	O1-C1-CA-C
3	A	1370	DXX	OXT-C1-CA-C
3	B	1369	DXX	OXT-C1-CA-C
3	A	1370	DXX	O-C-CA-C1
2	A	1369	EDO	O1-C1-C2-O2
3	A	1370	DXX	O2-C-CA-C1
3	B	1369	DXX	O2-C-CA-C1

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Mol	Chain	Res	Type	Atoms
3	B	1369	DXX	O-C-CA-C1

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1370	DXX	0	11

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	364/372 (97%)	-0.38	2 (0%) 87 90	12, 17, 30, 45	1 (0%)
1	B	364/372 (97%)	-0.33	0 100 100	11, 18, 30, 41	1 (0%)
1	C	365/372 (98%)	-0.30	3 (0%) 82 86	13, 18, 30, 52	0
1	D	364/372 (97%)	-0.37	0 100 100	12, 18, 30, 47	2 (0%)
1	E	365/372 (98%)	-0.31	2 (0%) 87 90	12, 18, 31, 44	1 (0%)
All	All	1822/1860 (97%)	-0.34	7 (0%) 88 91	11, 18, 31, 52	5 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	3.1
1	A	365	PRO	2.9
1	A	2	ALA	2.4
1	C	1	MET	2.4
1	E	1	MET	2.2
1	E	365	PRO	2.0
1	C	244	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	1369	4/4	0.93	0.10	25,31,37,43	0
2	EDO	B	1366	4/4	0.95	0.08	24,31,31,36	0
2	EDO	B	1368	4/4	0.95	0.08	23,28,29,31	0
2	EDO	D	1367	4/4	0.96	0.08	24,25,25,25	0
2	EDO	E	1366	4/4	0.96	0.14	20,20,20,20	0
3	DXX	A	1370	7/8	0.96	0.15	16,17,160,161	0
2	EDO	D	1366	4/4	0.97	0.07	18,21,23,23	0
2	EDO	A	1368	4/4	0.97	0.07	22,23,25,27	0
2	EDO	A	1366	4/4	0.97	0.09	25,27,28,30	0
2	EDO	C	1366	4/4	0.97	0.06	22,23,24,24	0
2	EDO	A	1367	4/4	0.98	0.05	23,24,24,27	0
2	EDO	B	1367	4/4	0.98	0.05	21,22,25,27	0
3	DXX	B	1369	7/8	0.98	0.05	16,18,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.