



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:24 PM EDT

PDB ID : 5W3Z / pdb_00005w3z
Title : Crystal structure of SsoPox AsC6 mutant (L72I-Y99F-I122L-L228M-F229S-W263L)
Authors : Hiblot, J.; Gotthard, G.; Jacquet, P.; Daude, D.; Bergonzi, C.; Chabriere, E.; Elias, M.
Deposited on : 2017-06-08
Resolution : 2.55 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

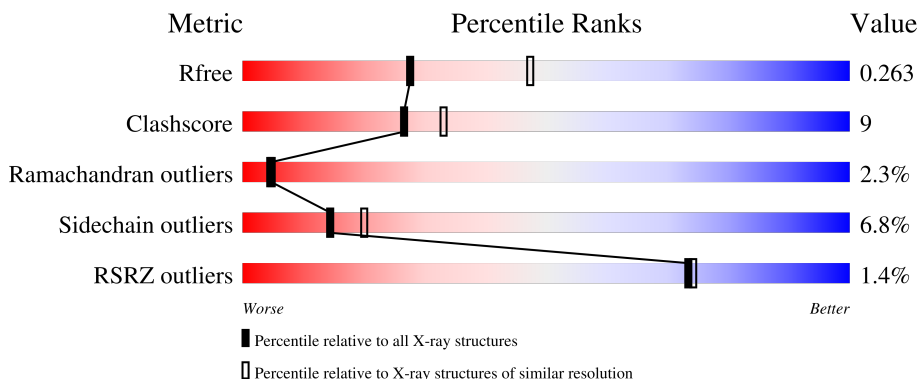
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	314	
1	B	314	
1	C	314	
1	D	314	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9811 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 Aryldialkylphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2333	1490	397	440	6			
1	B	302	Total	C	N	O	S	0	0	0
			2403	1535	407	453	8			
1	C	296	Total	C	N	O	S	0	0	0
			2364	1510	404	443	7			
1	D	314	Total	C	N	O	S	0	0	0
			2501	1600	425	468	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	ILE	LEU	engineered mutation	UNP Q97VT7
A	99	PHE	TYR	engineered mutation	UNP Q97VT7
A	122	LEU	ILE	engineered mutation	UNP Q97VT7
A	228	MET	LEU	engineered mutation	UNP Q97VT7
A	229	SER	PHE	engineered mutation	UNP Q97VT7
A	263	LEU	TRP	engineered mutation	UNP Q97VT7
B	72	ILE	LEU	engineered mutation	UNP Q97VT7
B	99	PHE	TYR	engineered mutation	UNP Q97VT7
B	122	LEU	ILE	engineered mutation	UNP Q97VT7
B	228	MET	LEU	engineered mutation	UNP Q97VT7
B	229	SER	PHE	engineered mutation	UNP Q97VT7
B	263	LEU	TRP	engineered mutation	UNP Q97VT7
C	72	ILE	LEU	engineered mutation	UNP Q97VT7
C	99	PHE	TYR	engineered mutation	UNP Q97VT7
C	122	LEU	ILE	engineered mutation	UNP Q97VT7
C	228	MET	LEU	engineered mutation	UNP Q97VT7
C	229	SER	PHE	engineered mutation	UNP Q97VT7
C	263	LEU	TRP	engineered mutation	UNP Q97VT7
D	72	ILE	LEU	engineered mutation	UNP Q97VT7
D	99	PHE	TYR	engineered mutation	UNP Q97VT7
D	122	LEU	ILE	engineered mutation	UNP Q97VT7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	228	MET	LEU	engineered mutation	UNP Q97VT7
D	229	SER	PHE	engineered mutation	UNP Q97VT7
D	263	LEU	TRP	engineered mutation	UNP Q97VT7

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co 1 1	0	0
3	B	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0
3	D	1	Total Co 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- 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	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

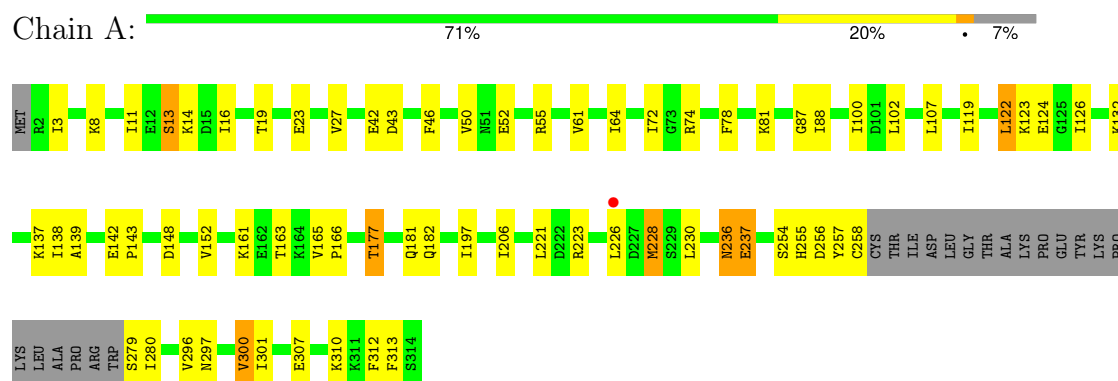
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total	O	0	0
			52	52		
6	B	33	Total	O	0	0
			33	33		
6	C	39	Total	O	0	0
			39	39		
6	D	30	Total	O	0	0
			30	30		

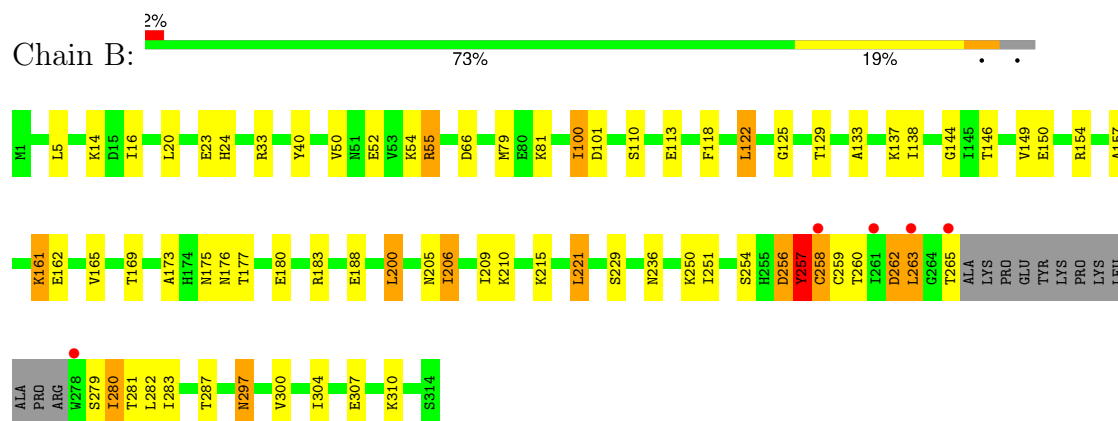
3 Residue-property plots [i](#)

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.

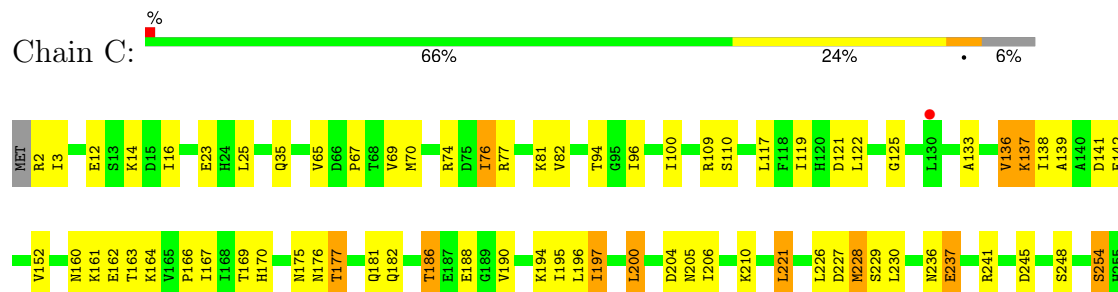
• Molecule 1: Aryldialkylphosphatase

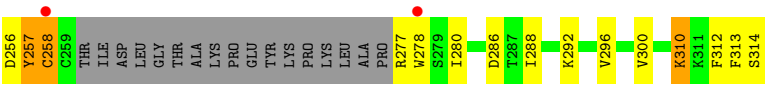


• Molecule 1: Aryldialkylphosphatase

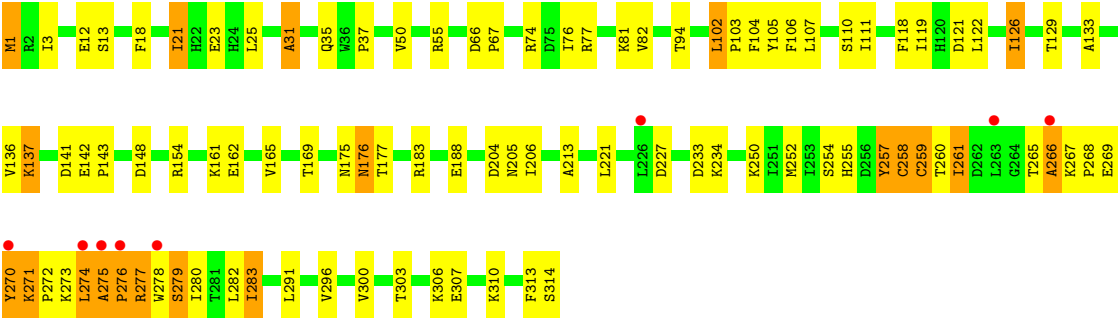


• Molecule 1: Aryldialkylphosphatase





● Molecule 1: Aryldialkylphosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.65Å 105.80Å 154.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.55 46.31 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.31-2.55) 97.3 (46.31-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.189 , 0.252 0.204 , 0.263	Depositor DCC
R_{free} test set	2161 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9811	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.01% 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: GOL, FE2, EDO, CO, KCX

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	1.34	10/2361 (0.4%)	1.26	4/3182 (0.1%)
1	B	1.27	3/2433 (0.1%)	1.25	9/3281 (0.3%)
1	C	1.31	11/2394 (0.5%)	1.23	5/3227 (0.2%)
1	D	1.20	2/2536 (0.1%)	1.20	3/3422 (0.1%)
All	All	1.28	26/9724 (0.3%)	1.23	21/13112 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	ASP	CA-C	8.04	1.61	1.53
1	A	139	ALA	N-CA	-7.45	1.36	1.45
1	C	117	LEU	C-O	7.45	1.33	1.24
1	D	126	ILE	C-O	7.18	1.31	1.24
1	A	74	ARG	C-O	-6.79	1.15	1.23
1	C	200	LEU	CA-C	6.15	1.61	1.52
1	A	142	GLU	C-O	-5.95	1.18	1.24
1	C	100	ILE	N-CA	5.89	1.53	1.46
1	A	61	VAL	C-O	-5.88	1.18	1.24
1	A	88	ILE	N-CA	5.86	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ILE	N-CA	5.75	1.53	1.46
1	C	258	CYS	CA-C	5.67	1.60	1.52
1	C	196	LEU	N-CA	5.65	1.53	1.46
1	A	43	ASP	C-O	-5.51	1.17	1.24
1	C	67	PRO	CA-C	5.43	1.60	1.52
1	D	121	ASP	CA-C	5.35	1.59	1.52
1	C	35	GLN	C-O	-5.34	1.17	1.24
1	C	74	ARG	C-O	-5.32	1.17	1.24
1	B	100	ILE	N-CA	5.31	1.52	1.46
1	A	142	GLU	N-CA	5.25	1.51	1.46
1	C	23	GLU	C-O	-5.18	1.18	1.23
1	B	55	ARG	C-O	-5.18	1.18	1.24
1	C	254	SER	C-O	5.15	1.29	1.23
1	B	304	ILE	CA-C	5.07	1.59	1.52
1	C	65	VAL	CA-C	5.06	1.59	1.52
1	A	143	PRO	C-O	-5.05	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ASP	N-CA-C	6.70	119.59	109.41
1	A	78	PHE	N-CA-C	-6.58	104.18	111.36
1	D	31	ALA	N-CA-C	6.02	117.52	111.07
1	B	256	ASP	CA-C-N	6.02	133.04	121.54
1	B	256	ASP	C-N-CA	6.02	133.04	121.54
1	C	248	SER	N-CA-C	5.89	118.45	111.33
1	B	16	ILE	CB-CA-C	-5.88	102.57	112.16
1	A	122	LEU	CB-CA-C	5.67	119.52	109.65
1	C	69	VAL	N-CA-CB	-5.65	106.12	112.45
1	B	250	LYS	N-CA-C	5.39	121.06	113.02
1	B	257	TYR	CA-CB-CG	5.29	123.43	113.90
1	B	209	ILE	N-CA-C	-5.24	105.61	110.53
1	B	257	TYR	N-CA-CB	5.22	119.32	110.49
1	B	215	LYS	N-CA-C	5.22	119.36	113.15
1	A	165	VAL	N-CA-CB	5.16	115.30	109.99
1	C	221	LEU	N-CA-C	-5.15	101.79	109.11
1	D	129	THR	N-CA-C	-5.12	101.51	109.14
1	C	139	ALA	N-CA-C	5.08	116.97	108.99
1	A	126	ILE	N-CA-C	5.08	115.17	107.80
1	C	117	LEU	O-C-N	5.07	128.51	122.27
1	D	21	ILE	N-CA-C	5.00	119.11	112.76

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	LEU	Peptide
1	B	221	LEU	Peptide
1	C	221	LEU	Peptide
1	D	221	LEU	Peptide

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	2333	0	2356	39	0
1	B	2403	0	2426	39	0
1	C	2364	0	2385	49	0
1	D	2501	0	2536	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	6	1	0
4	B	4	0	6	0	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	52	0	0	1	0
6	B	33	0	0	4	0
6	C	39	0	0	2	0
6	D	30	0	0	6	0
All	All	9811	0	9771	181	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 9.

All (181) 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:B:122:LEU:HD12	1:B:133:ALA:HB3	1.61	0.82
1:D:94:THR:O	1:D:136:VAL:HA	1.80	0.81
1:B:257:TYR:O	1:B:259:CYS:N	2.16	0.79
1:C:14:LYS:HA	1:C:310:LYS:HD2	1.64	0.79
1:C:256:ASP:O	1:C:257:TYR:HB2	1.87	0.74
1:D:1:MET:SD	1:D:1:MET:N	2.57	0.73
1:D:291:LEU:O	1:D:296:VAL:HB	1.88	0.72
1:B:256:ASP:O	1:B:257:TYR:HD1	1.74	0.70
1:B:256:ASP:O	1:B:257:TYR:CD1	2.44	0.70
1:A:3:ILE:HG13	1:A:16:ILE:HD11	1.76	0.68
1:A:257:TYR:HD2	6:A:545:HOH:O	1.76	0.67
1:C:3:ILE:HD11	1:C:313:PHE:HB3	1.77	0.66
1:B:14:LYS:HA	1:B:310:LYS:CD	2.25	0.66
1:B:14:LYS:O	6:B:501:HOH:O	2.14	0.66
1:D:204:ASP:O	1:D:206:ILE:N	2.29	0.65
1:A:122:LEU:HD11	1:A:163:THR:HG21	1.78	0.65
1:C:236:ASN:O	1:C:237:GLU:HB2	1.97	0.64
1:D:67:PRO:HB2	1:D:137:KCX:HG2	1.80	0.64
1:A:177:THR:O	1:A:181:GLN:HG3	1.99	0.63
1:A:14:LYS:HA	1:A:310:LYS:CD	2.29	0.62
2:C:401:FE2:FE	6:C:503:HOH:O	1.51	0.62
1:A:52:GLU:OE1	1:A:55:ARG:NH2	2.32	0.62
1:C:137:KCX:OQ1	1:C:170:HIS:HB2	2.00	0.62
1:D:296:VAL:HG13	1:D:300:VAL:CG1	2.30	0.60
1:D:269:GLU:O	1:D:271:LYS:N	2.35	0.60
1:B:297:ASN:OD1	1:B:297:ASN:N	2.33	0.60
1:A:46:PHE:O	1:A:50:VAL:HG23	2.02	0.60
1:A:182:GLN:HB2	1:A:197:ILE:HD11	1.82	0.59
1:C:236:ASN:O	1:C:237:GLU:CB	2.49	0.59
1:D:213:ALA:O	1:D:250:LYS:NZ	2.33	0.59
1:B:150:GLU:OE1	1:B:154:ARG:NH1	2.33	0.59
1:C:296:VAL:HG13	1:C:300:VAL:CG1	2.32	0.58
1:C:122:LEU:HD13	1:C:163:THR:HG21	1.84	0.58
1:C:122:LEU:HD13	1:C:163:THR:CG2	2.34	0.58
1:C:296:VAL:HG13	1:C:300:VAL:HG11	1.85	0.58
1:D:122:LEU:HD22	1:D:165:VAL:HG11	1.86	0.58
1:A:3:ILE:HD11	1:A:313:PHE:HB3	1.85	0.57
1:C:182:GLN:O	1:C:186:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.40	0.57
1:B:14:LYS:HA	1:B:310:LYS:HD3	1.87	0.56
1:D:255:HIS:NE2	1:D:283:ILE:HB	2.20	0.56
1:D:25:LEU:HD13	1:D:82:VAL:HG11	1.87	0.56
1:A:27:VAL:HG23	1:A:72:ILE:HB	1.87	0.56
1:D:50:VAL:HG22	1:D:82:VAL:HG23	1.86	0.56
1:D:12:GLU:OE1	6:D:501:HOH:O	2.18	0.56
1:D:111:ILE:HD11	1:D:154:ARG:CB	2.35	0.55
1:C:195:ILE:HG22	1:C:197:ILE:HG22	1.88	0.55
1:A:13:SER:O	1:A:16:ILE:HG12	2.07	0.55
1:B:118:PHE:O	1:B:122:LEU:HD13	2.07	0.54
1:B:14:LYS:HA	1:B:310:LYS:HD2	1.90	0.54
1:B:79:MET:HE3	6:B:524:HOH:O	2.07	0.54
1:A:122:LEU:HD11	1:A:163:THR:CB	2.38	0.53
1:D:3:ILE:HD11	1:D:313:PHE:HB3	1.90	0.53
1:B:52:GLU:OE2	1:B:280:ILE:HG22	2.09	0.53
1:C:3:ILE:CD1	1:C:313:PHE:HB3	2.38	0.53
1:C:257:TYR:HB3	1:C:278:TRP:CZ2	2.42	0.53
1:B:100:ILE:HA	1:B:146:THR:HG21	1.90	0.53
1:A:119:ILE:HG23	1:A:123:LYS:HD3	1.91	0.53
1:B:257:TYR:CE1	1:B:262:ASP:HA	2.43	0.53
1:A:296:VAL:HG13	1:A:300:VAL:CG2	2.38	0.53
1:C:197:ILE:HD11	1:C:200:LEU:HD11	1.90	0.52
1:B:110:SER:HB3	1:B:113:GLU:HG3	1.91	0.52
1:C:256:ASP:O	1:C:257:TYR:CB	2.56	0.52
1:A:122:LEU:HD11	1:A:163:THR:CG2	2.39	0.52
1:D:142:GLU:HB2	1:D:143:PRO:HD3	1.91	0.52
1:A:236:ASN:O	1:A:237:GLU:HB2	2.11	0.51
1:A:296:VAL:CG1	1:A:300:VAL:HG22	2.40	0.51
1:C:136:VAL:HG13	1:C:167:ILE:HG12	1.90	0.51
6:B:531:HOH:O	1:D:37:PRO:HD2	2.11	0.51
1:C:204:ASP:O	1:C:206:ILE:N	2.43	0.51
1:D:111:ILE:HD11	1:D:154:ARG:HB3	1.93	0.51
1:A:100:ILE:H	4:A:403:EDO:H12	1.75	0.50
1:C:96:ILE:O	6:C:501:HOH:O	2.19	0.50
1:D:306:LYS:O	1:D:310:LYS:HB2	2.11	0.50
1:D:266:ALA:C	1:D:268:PRO:HD3	2.36	0.50
1:D:275:ALA:HB1	1:D:276:PRO:HD3	1.93	0.50
1:A:123:LYS:O	1:A:132:LYS:HE3	2.11	0.50
1:D:118:PHE:O	1:D:122:LEU:HG	2.12	0.50
1:C:160:ASN:O	1:C:164:LYS:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HD11	1:C:200:LEU:HD21	1.94	0.49
1:D:122:LEU:HD23	1:D:133:ALA:HB3	1.94	0.49
1:D:259:CYS:SG	1:D:260:THR:N	2.85	0.49
1:B:236:ASN:OD1	1:B:287:THR:HG23	2.12	0.49
1:D:272:PRO:HB2	1:D:274:LEU:HD13	1.95	0.49
1:A:102:LEU:HG	1:A:148:ASP:HB3	1.95	0.49
1:C:206:ILE:HD13	1:C:241:ARG:HG2	1.93	0.49
1:D:258:CYS:SG	1:D:259:CYS:N	2.85	0.49
1:B:101:ASP:N	6:B:503:HOH:O	2.45	0.49
1:C:76:ILE:HD12	1:C:77:ARG:N	2.28	0.48
1:C:210:LYS:NZ	1:C:245:ASP:OD2	2.44	0.48
1:C:227:ASP:O	1:C:229:SER:N	2.46	0.48
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.47	0.48
1:A:14:LYS:HA	1:A:310:LYS:HD2	1.95	0.48
1:B:55:ARG:HG2	1:B:281:THR:HG21	1.95	0.48
1:D:303:THR:HA	1:D:307:GLU:HB3	1.95	0.48
1:A:23:GLU:OE2	1:A:255:HIS:HB2	2.13	0.48
1:A:228:MET:N	1:A:228:MET:SD	2.87	0.48
1:A:296:VAL:HG13	1:A:300:VAL:HG21	1.96	0.48
1:B:154:ARG:NH2	1:B:188:GLU:OE1	2.38	0.48
1:D:161:LYS:CE	1:D:188:GLU:O	2.62	0.48
1:A:119:ILE:CG2	1:A:123:LYS:HD3	2.44	0.47
1:D:102:LEU:HB2	1:D:103:PRO:CD	2.45	0.47
1:D:1:MET:HB3	6:D:501:HOH:O	2.15	0.47
1:D:233:ASP:OD1	1:D:234:LYS:N	2.48	0.47
1:D:278:TRP:HB2	6:D:514:HOH:O	2.14	0.47
1:A:257:TYR:O	1:A:258:CYS:SG	2.70	0.47
1:C:94:THR:O	1:C:136:VAL:HA	2.15	0.47
1:B:307:GLU:O	1:B:310:LYS:HB3	2.15	0.46
1:D:31:ALA:O	1:D:35:GLN:HG2	2.15	0.46
1:D:1:MET:CB	6:D:501:HOH:O	2.63	0.46
1:D:13:SER:OG	1:D:314:SER:HB3	2.16	0.46
1:A:14:LYS:HA	1:A:310:LYS:HD3	1.98	0.46
1:C:226:LEU:HD13	1:C:228:MET:HE2	1.97	0.46
1:B:122:LEU:N	1:B:122:LEU:CD1	2.79	0.45
1:C:122:LEU:HD23	1:C:133:ALA:HB3	1.98	0.45
1:D:21:ILE:O	1:D:21:ILE:HG13	2.16	0.45
1:D:303:THR:HA	1:D:307:GLU:CB	2.46	0.45
1:B:206:ILE:HD11	1:B:210:LYS:HE3	1.99	0.45
1:C:194:LYS:HE2	1:C:314:SER:O	2.16	0.45
1:C:70:MET:HE2	1:C:96:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:C	1:A:122:LEU:HD12	2.42	0.44
1:D:278:TRP:O	1:D:279:SER:HB2	2.17	0.44
1:A:223:ARG:HA	1:A:255:HIS:O	2.17	0.44
1:B:122:LEU:HD13	1:B:122:LEU:N	2.33	0.44
1:A:297:ASN:OD1	1:A:297:ASN:N	2.48	0.44
1:B:125:GLY:HA3	1:B:129:THR:O	2.18	0.44
1:C:277:ARG:HH12	1:C:286:ASP:HB2	1.81	0.44
1:A:307:GLU:O	1:A:310:LYS:HB3	2.18	0.43
1:B:146:THR:OG1	1:B:149:VAL:HG23	2.18	0.43
1:A:11:ILE:HD11	1:A:16:ILE:HD13	2.00	0.43
1:D:104:PHE:O	1:D:106:PHE:N	2.51	0.43
1:D:252:MET:HG2	6:D:515:HOH:O	2.17	0.43
1:C:2:ARG:HH22	1:C:314:SER:HA	1.83	0.43
1:C:197:ILE:HD12	1:C:197:ILE:C	2.43	0.43
1:C:288:ILE:HG22	1:C:292:LYS:HE2	1.99	0.43
1:C:161:LYS:NZ	1:C:188:GLU:O	2.48	0.43
1:D:275:ALA:CB	1:D:276:PRO:CD	2.95	0.43
1:B:175:ASN:O	1:B:176:ASN:HB3	2.19	0.43
1:B:157:ALA:O	1:B:161:LYS:HD3	2.19	0.43
1:C:175:ASN:O	1:C:176:ASN:HB3	2.19	0.42
1:B:122:LEU:CD1	1:B:133:ALA:HB3	2.43	0.42
1:C:176:ASN:O	1:C:176:ASN:ND2	2.52	0.42
1:C:197:ILE:CD1	1:C:200:LEU:HD11	2.49	0.42
1:A:3:ILE:CD1	1:A:313:PHE:HB3	2.49	0.42
1:B:23:GLU:O	1:B:66:ASP:HA	2.19	0.42
1:C:119:ILE:HA	1:C:122:LEU:HD12	2.02	0.42
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.92	0.42
1:A:296:VAL:CG1	1:A:300:VAL:CG2	2.98	0.42
1:B:50:VAL:O	1:B:54:LYS:HG2	2.19	0.42
1:B:221:LEU:HD12	1:B:251:ILE:HG23	2.02	0.42
1:C:197:ILE:CG1	1:C:200:LEU:HD11	2.50	0.42
1:D:102:LEU:CD2	1:D:148:ASP:HB3	2.49	0.42
1:B:24:HIS:H	1:B:257:TYR:HB3	1.84	0.42
1:B:33:ARG:HG3	1:B:40:TYR:CD2	2.54	0.42
1:B:180:GLU:OE2	1:B:183:ARG:NH1	2.53	0.42
1:C:25:LEU:HD13	1:C:82:VAL:HG11	2.00	0.42
1:C:160:ASN:OD1	1:C:190:VAL:HG13	2.20	0.42
1:D:18:PHE:C	1:D:18:PHE:CD1	2.97	0.42
1:D:23:GLU:O	1:D:66:ASP:HA	2.20	0.42
1:A:16:ILE:HG22	1:A:19:THR:OG1	2.20	0.41
1:C:226:LEU:HD21	1:C:278:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ALA:HB2	1:B:200:LEU:HA	2.01	0.41
1:C:177:THR:O	1:C:181:GLN:HG3	2.21	0.41
1:D:175:ASN:O	1:D:176:ASN:HB3	2.20	0.41
1:D:257:TYR:CG	1:D:258:CYS:N	2.88	0.41
1:A:8:LYS:NZ	1:A:87:GLY:O	2.38	0.41
1:A:138:ILE:HG22	1:A:152:VAL:HG12	2.01	0.41
1:C:138:ILE:HG22	1:C:152:VAL:HG12	2.01	0.41
1:D:3:ILE:CD1	1:D:313:PHE:HB3	2.50	0.41
1:D:119:ILE:HD13	6:D:519:HOH:O	2.20	0.41
1:A:257:TYR:CE1	1:A:279:SER:HA	2.55	0.41
1:B:20:LEU:HD21	1:B:283:ILE:HD11	2.02	0.41
1:C:121:ASP:HA	1:C:125:GLY:O	2.21	0.41
1:D:74:ARG:CZ	1:D:126:ILE:HG23	2.51	0.41
1:D:175:ASN:OD1	1:D:177:THR:HG23	2.21	0.41
1:D:277:ARG:HH21	1:D:278:TRP:HB3	1.86	0.41
1:D:275:ALA:CB	1:D:276:PRO:HD3	2.51	0.41
1:D:296:VAL:HG13	1:D:300:VAL:HG11	2.03	0.40
1:B:138:ILE:HD11	1:B:169:THR:HG22	2.04	0.40
1:B:258:CYS:O	1:B:279:SER:HA	2.22	0.40
1:C:141:ASP:OD1	1:C:142:GLU:N	2.51	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	288/314 (92%)	275 (96%)	11 (4%)	2 (1%)	18	25
1	B	297/314 (95%)	267 (90%)	24 (8%)	6 (2%)	6	6
1	C	291/314 (93%)	263 (90%)	23 (8%)	5 (2%)	7	8
1	D	311/314 (99%)	268 (86%)	29 (9%)	14 (4%)	2	1
All	All	1187/1256 (94%)	1073 (90%)	87 (7%)	27 (2%)	5	4

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	GLU
1	B	258	CYS
1	B	260	THR
1	C	205	ASN
1	C	237	GLU
1	C	257	TYR
1	C	258	CYS
1	D	105	TYR
1	D	205	ASN
1	D	257	TYR
1	D	267	LYS
1	D	270	TYR
1	D	271	LYS
1	D	275	ALA
1	D	279	SER
1	B	263	LEU
1	C	228	MET
1	D	259	CYS
1	D	261	ILE
1	B	205	ASN
1	B	257	TYR
1	D	176	ASN
1	D	266	ALA
1	D	277	ARG
1	A	236	ASN
1	B	144	GLY
1	D	276	PRO

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	254/272 (93%)	239 (94%)	15 (6%)	18	27
1	B	262/272 (96%)	244 (93%)	18 (7%)	14	20
1	C	257/272 (94%)	242 (94%)	15 (6%)	18	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	272/272 (100%)	249 (92%)	23 (8%)	10	13
All	All	1045/1088 (96%)	974 (93%)	71 (7%)	14	20

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	42	GLU
1	A	81	LYS
1	A	107	LEU
1	A	124	GLU
1	A	161	LYS
1	A	177	THR
1	A	206	ILE
1	A	226	LEU
1	A	228	MET
1	A	230	LEU
1	A	254	SER
1	A	280	ILE
1	A	300	VAL
1	A	301	ILE
1	B	5	LEU
1	B	81	LYS
1	B	122	LEU
1	B	161	LYS
1	B	162	GLU
1	B	165	VAL
1	B	177	THR
1	B	200	LEU
1	B	206	ILE
1	B	229	SER
1	B	254	SER
1	B	257	TYR
1	B	263	LEU
1	B	265	THR
1	B	280	ILE
1	B	282	LEU
1	B	297	ASN
1	B	300	VAL
1	C	12	GLU
1	C	16	ILE
1	C	76	ILE

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Mol	Chain	Res	Type
1	C	81	LYS
1	C	109	ARG
1	C	110	SER
1	C	136	VAL
1	C	162	GLU
1	C	169	THR
1	C	177	THR
1	C	186	THR
1	C	197	ILE
1	C	254	SER
1	C	280	ILE
1	C	310	LYS
1	D	1	MET
1	D	55	ARG
1	D	76	ILE
1	D	77	ARG
1	D	81	LYS
1	D	102	LEU
1	D	107	LEU
1	D	110	SER
1	D	141	ASP
1	D	162	GLU
1	D	169	THR
1	D	183	ARG
1	D	227	ASP
1	D	254	SER
1	D	258	CYS
1	D	261	ILE
1	D	265	THR
1	D	270	TYR
1	D	273	LYS
1	D	274	LEU
1	D	280	ILE
1	D	282	LEU
1	D	283	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	176	ASN
1	B	182	GLN
1	C	131	ASN

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Mol	Chain	Res	Type
1	D	294	ASN

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	KCX	B	137	3,2,1	10,11,12	1.07	1 (10%)	6,12,14	0.80	0
1	KCX	A	137	2,1	10,11,12	0.95	0	6,12,14	2.58	2 (33%)
1	KCX	D	137	3,2,1	10,11,12	0.54	0	6,12,14	1.55	2 (33%)
1	KCX	C	137	3,2,1	10,11,12	0.87	0	6,12,14	1.95	2 (33%)

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	KCX	B	137	3,2,1	-	3/9/10/12	-
1	KCX	A	137	2,1	-	2/9/10/12	-
1	KCX	D	137	3,2,1	-	3/9/10/12	-
1	KCX	C	137	3,2,1	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	KCX	CB-CA	2.57	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	KCX	OQ1-CX-NZ	-5.28	116.89	124.92
1	C	137	KCX	CD-CE-NZ	3.58	122.25	112.20
1	A	137	KCX	CD-CE-NZ	3.09	120.85	112.20
1	D	137	KCX	CE-NZ-CX	2.52	126.25	121.98
1	D	137	KCX	OQ1-CX-NZ	-2.34	121.37	124.92
1	C	137	KCX	OQ1-CX-NZ	-2.19	121.59	124.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	137	KCX	N-CA-CB-CG
1	A	137	KCX	C-CA-CB-CG
1	B	137	KCX	C-CA-CB-CG
1	C	137	KCX	N-CA-CB-CG
1	C	137	KCX	C-CA-CB-CG
1	D	137	KCX	N-CA-CB-CG
1	D	137	KCX	C-CA-CB-CG
1	C	137	KCX	CG-CD-CE-NZ
1	B	137	KCX	N-CA-CB-CG
1	D	137	KCX	CA-CB-CG-CD
1	B	137	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	137	KCX	1	0
1	C	137	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	A	404	-	5,5,5	0.40	0	5,5,5	0.78	0
5	GOL	B	404	-	5,5,5	0.35	0	5,5,5	0.57	0
4	EDO	D	405	-	3,3,3	0.81	0	2,2,2	0.04	0
4	EDO	C	403	-	3,3,3	0.69	0	2,2,2	0.65	0
4	EDO	B	403	-	3,3,3	0.95	0	2,2,2	0.34	0
4	EDO	C	404	-	3,3,3	0.70	0	2,2,2	0.30	0
5	GOL	C	405	-	5,5,5	0.34	0	5,5,5	0.51	0
5	GOL	D	404	-	5,5,5	0.28	0	5,5,5	0.27	0
4	EDO	D	403	-	3,3,3	0.50	0	2,2,2	0.51	0
4	EDO	A	403	-	3,3,3	1.24	0	2,2,2	0.12	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
5	GOL	A	404	-	-	2/4/4/4	-
5	GOL	B	404	-	-	2/4/4/4	-
4	EDO	D	405	-	-	1/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	C	404	-	-	0/1/1/1	-
5	GOL	C	405	-	-	2/4/4/4	-
5	GOL	D	404	-	-	2/4/4/4	-
4	EDO	D	403	-	-	1/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	GOL	C1-C2-C3-O3
5	B	404	GOL	C1-C2-C3-O3
5	D	404	GOL	O1-C1-C2-O2
5	D	404	GOL	O1-C1-C2-C3
5	A	404	GOL	O2-C2-C3-O3
5	B	404	GOL	O2-C2-C3-O3
4	A	403	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2
4	D	403	EDO	O1-C1-C2-O2
4	D	405	EDO	O1-C1-C2-O2
5	C	405	GOL	O2-C2-C3-O3
4	C	403	EDO	O1-C1-C2-O2
5	C	405	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	EDO	1	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	292/314 (92%)	-0.33	1 (0%) 90 92	34, 61, 98, 135	0
1	B	301/314 (95%)	-0.20	5 (1%) 69 69	34, 69, 119, 168	0
1	C	295/314 (93%)	-0.07	3 (1%) 79 80	39, 76, 108, 135	0
1	D	313/314 (99%)	0.09	8 (2%) 57 58	44, 94, 137, 187	0
All	All	1201/1256 (95%)	-0.12	17 (1%) 73 74	34, 75, 124, 187	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	ILE	4.1
1	B	263	LEU	3.5
1	B	265	THR	3.5
1	D	276	PRO	3.1
1	D	263	LEU	2.7
1	C	258	CYS	2.7
1	D	278	TRP	2.6
1	D	275	ALA	2.6
1	B	278	TRP	2.5
1	A	226	LEU	2.5
1	D	226	LEU	2.5
1	C	278	TRP	2.4
1	D	274	LEU	2.3
1	D	270	TYR	2.2
1	C	130	LEU	2.1
1	B	258	CYS	2.1
1	D	266	ALA	2.0

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

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	KCX	C	137	12/13	0.95	0.07	36,48,55,57	0
1	KCX	D	137	12/13	0.95	0.09	66,74,75,78	0
1	KCX	B	137	12/13	0.96	0.07	36,38,40,41	0
1	KCX	A	137	12/13	0.97	0.06	35,35,36,36	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	EDO	D	405	4/4	0.73	0.20	31,32,33,33	0
5	GOL	C	405	6/6	0.78	0.16	49,53,55,55	0
4	EDO	A	403	4/4	0.83	0.13	24,27,28,29	0
4	EDO	C	403	4/4	0.83	0.12	47,52,53,54	0
4	EDO	D	403	4/4	0.84	0.10	48,56,58,61	0
5	GOL	D	404	6/6	0.86	0.16	35,37,38,40	0
5	GOL	A	404	6/6	0.90	0.13	27,30,31,31	0
5	GOL	B	404	6/6	0.91	0.15	35,37,37,38	0
4	EDO	C	404	4/4	0.92	0.11	28,30,32,36	0
4	EDO	B	403	4/4	0.93	0.15	34,35,37,38	0
3	CO	D	402	1/1	0.97	0.09	39,39,39,39	0
2	FE2	D	401	1/1	0.99	0.10	30,30,30,30	0
2	FE2	C	401	1/1	0.99	0.09	20,20,20,20	0
2	FE2	B	401	1/1	1.00	0.10	16,16,16,16	0
3	CO	A	402	1/1	1.00	0.12	16,16,16,16	0
3	CO	B	402	1/1	1.00	0.13	22,22,22,22	0
3	CO	C	402	1/1	1.00	0.11	14,14,14,14	0
2	FE2	A	401	1/1	1.00	0.10	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.