



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 1, 2018 – 06:07 PM EST

PDB ID : 5W3W
Title : Crystal structure of SsoPox AsD6 mutant (V27A-Y97W-L228M-W263M) - open form
Authors : Hiblot, J.; Gotthard, G.; Jacquet, P.; Daude, D.; Bergonzi, C.; Chabriere, E.; Elias, M.
Deposited on : 2017-06-08
Resolution : 2.95 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

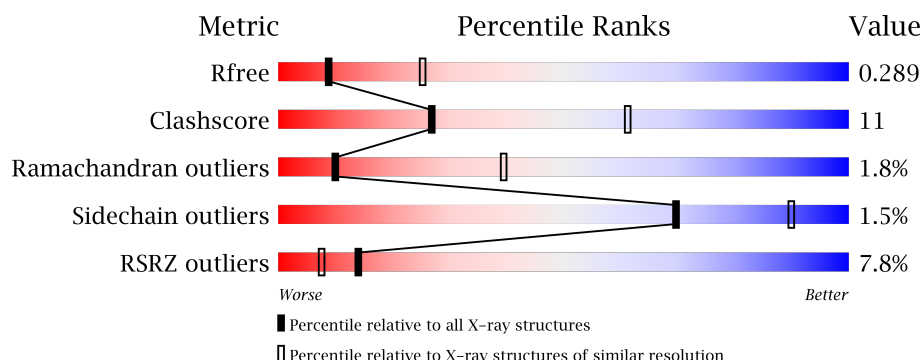
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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. 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	<div> <div>2%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	314	<div> <div>8%</div> <div>66%</div> <div>28%</div> <div>• 5%</div> </div>
1	C	314	<div> <div>19%</div> <div>71%</div> <div>23%</div> <div>• 5%</div> </div>
1	D	314	<div> <div>2%</div> <div>66%</div> <div>28%</div> <div>• •</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	404	-	-	-	X
4	EDO	B	403	-	-	-	X
4	EDO	B	405	-	-	-	X
4	EDO	C	405	-	-	-	X
4	EDO	D	403	-	-	-	X
4	EDO	D	406	-	-	-	X
5	GOL	C	404	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9703 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	300	Total	C	N	O	S	0	1	0
			2404	1539	409	448	8			
1	B	299	Total	C	N	O	S	0	1	0
			2398	1536	408	447	7			
1	C	298	Total	C	N	O	S	0	0	0
			2384	1526	407	444	7			
1	D	302	Total	C	N	O	S	0	1	0
			2420	1550	412	450	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	27	ALA	VAL	engineered mutation	UNP Q97VT7
D	97	TRP	TYR	engineered mutation	UNP Q97VT7
D	228	MET	LEU	engineered mutation	UNP Q97VT7
A	27	ALA	VAL	engineered mutation	UNP Q97VT7
A	97	TRP	TYR	engineered mutation	UNP Q97VT7
A	228	MET	LEU	engineered mutation	UNP Q97VT7
B	27	ALA	VAL	engineered mutation	UNP Q97VT7
B	97	TRP	TYR	engineered mutation	UNP Q97VT7
B	228	MET	LEU	engineered mutation	UNP Q97VT7
C	27	ALA	VAL	engineered mutation	UNP Q97VT7
C	97	TRP	TYR	engineered mutation	UNP Q97VT7
C	228	MET	LEU	engineered mutation	UNP Q97VT7

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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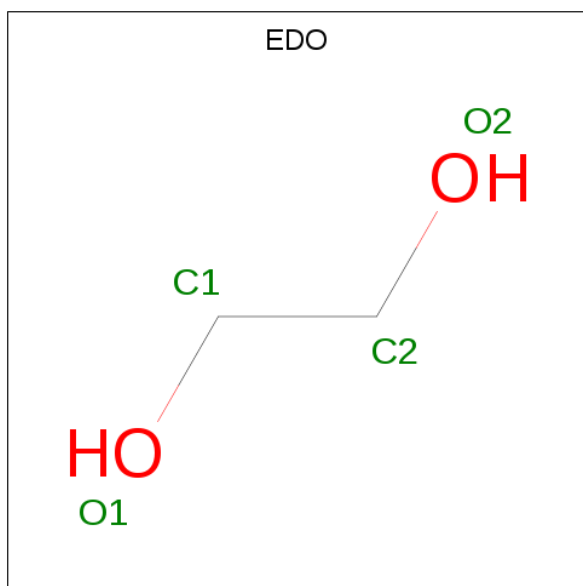
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



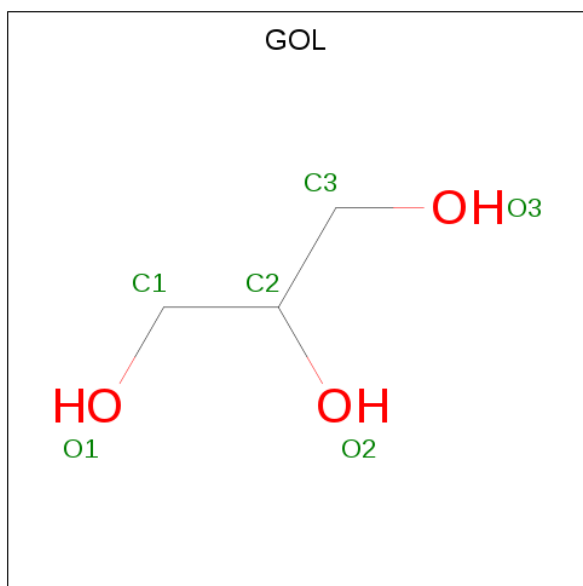
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

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

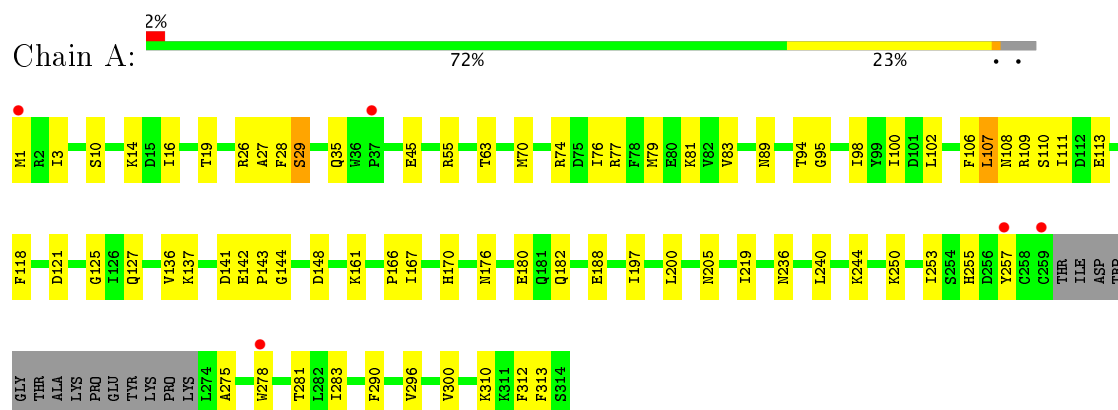
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total 10	O 10	0	0
6	B	3	Total 3	O 3	0	0
6	C	2	Total 2	O 2	0	0
6	D	8	Total 8	O 8	0	0

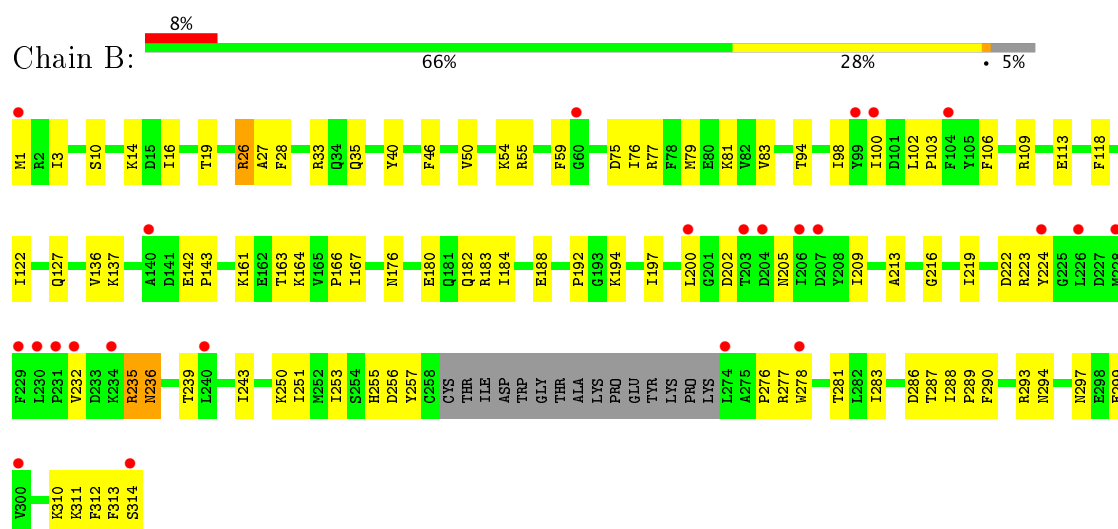
3 Residue-property plots [i](#)

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.

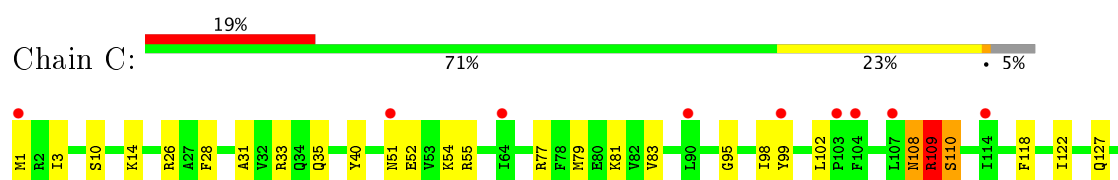
• Molecule 1: Aryldialkylphosphatase

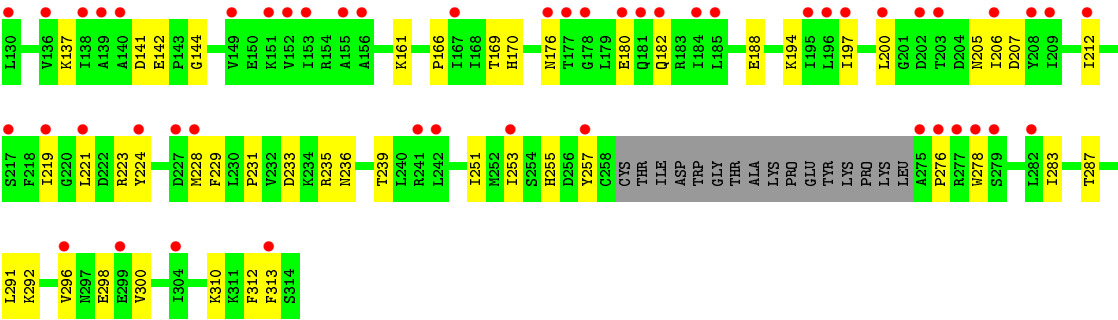


• Molecule 1: Aryldialkylphosphatase

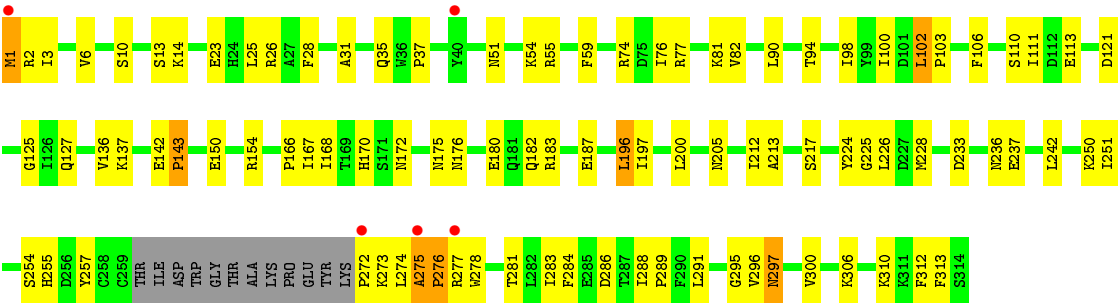


• Molecule 1: Aryldialkylphosphatase





● 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	82.34Å 105.01Å 153.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 2.95 49.67 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.67-2.95) 98.3 (49.67-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.229 , 0.288 0.232 , 0.289	Depositor DCC
R_{free} test set	1409 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.9	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	0.94	EDS
Total number of atoms	9703	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.38% 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: GOL, KCX, CO, EDO, FE

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	0.59	0/2440	0.72	0/3291
1	B	0.51	0/2434	0.64	0/3283
1	C	0.48	0/2417	0.66	0/3260
1	D	0.62	0/2457	0.69	0/3313
All	All	0.56	0/9748	0.68	0/13147

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	2404	0	2426	55	0
1	B	2398	0	2421	62	0
1	C	2384	0	2404	47	0
1	D	2420	0	2447	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	12	1	0
4	B	8	0	12	1	0
4	C	8	0	12	0	0
4	D	12	0	18	0	0
5	A	6	0	8	0	0
5	B	6	0	8	1	0
5	C	6	0	8	1	0
5	D	12	0	16	0	0
6	A	10	0	0	2	0
6	B	3	0	0	0	0
6	C	2	0	0	0	0
6	D	8	0	0	0	0
All	All	9703	0	9792	223	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 11.

All (223) 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:14:LYS:HA	1:A:310:LYS:HD2	1.43	1.01
1:C:223:ARG:O	1:C:235:ARG:NH2	2.06	0.87
1:B:219:ILE:HG22	1:B:251:ILE:HA	1.60	0.83
1:D:14:LYS:HA	1:D:310:LYS:HD2	1.61	0.79
1:A:182:GLN:HB2	1:A:197:ILE:HD11	1.64	0.79
1:C:182:GLN:HB2	1:C:197:ILE:HD11	1.62	0.79
1:B:14:LYS:HA	1:B:310:LYS:HD2	1.64	0.79
1:B:106:PHE:HA	1:B:109:ARG:HG2	1.66	0.78
1:D:1:MET:N	1:D:10:SER:OG	2.18	0.77
1:B:182:GLN:HB2	1:B:197:ILE:HD11	1.68	0.76
1:C:229:PHE:HB2	1:C:235:ARG:HH11	1.51	0.75
1:D:102:LEU:HD13	1:D:106:PHE:HB2	1.69	0.74
1:D:111:ILE:HD11	1:D:154:ARG:HB3	1.70	0.73
1:B:213:ALA:O	1:B:250:LYS:NZ	2.22	0.72
1:C:14:LYS:HA	1:C:310:LYS:HD2	1.70	0.72
1:B:35:GLN:HA	1:C:127:GLN:HE21	1.54	0.71
1:B:109:ARG:NH2	1:B:113:GLU:OE2	2.23	0.71
1:B:26:ARG:HD2	1:B:28:PHE:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ILE:HG13	1:B:127:GLN:HE21	1.57	0.70
1:B:26:ARG:HD2	1:B:28:PHE:HD2	1.59	0.68
1:D:233:ASP:O	1:D:237:GLU:HG2	1.95	0.67
1:D:182:GLN:HB2	1:D:197:ILE:HD11	1.76	0.67
1:C:31:ALA:O	1:C:35:GLN:HG2	1.94	0.66
1:D:98:ILE:HD13	1:D:102:LEU:HB3	1.77	0.66
1:C:33:ARG:HG2	1:C:40:TYR:CE2	2.31	0.66
1:A:106:PHE:HA	1:A:109:ARG:HG3	1.79	0.65
1:C:231:PRO:HB2	1:C:233:ASP:OD1	1.97	0.65
1:C:52:GLU:OE1	1:C:55:ARG:NH2	2.26	0.64
1:A:35:GLN:HE22	1:D:74:ARG:HB3	1.62	0.64
1:D:110:SER:HB3	1:D:113:GLU:HG3	1.80	0.64
1:C:229:PHE:HB2	1:C:235:ARG:NH1	2.12	0.64
1:A:176:ASN:O	1:A:180[B]:GLU:HG2	1.98	0.63
1:B:277:ARG:NH1	1:B:286:ASP:OD2	2.30	0.63
1:D:297:ASN:HD22	1:D:297:ASN:H	1.45	0.63
1:D:257:TYR:HA	1:D:278:TRP:CZ2	2.33	0.63
1:C:221:LEU:HD22	1:C:239:THR:HG22	1.82	0.62
1:D:297:ASN:H	1:D:297:ASN:ND2	1.98	0.61
1:A:95:GLY:HA2	1:A:118:PHE:CE1	2.36	0.60
1:D:168:ILE:HG23	1:D:196:LEU:HD12	1.83	0.60
1:A:35:GLN:NE2	1:D:74:ARG:HE	1.99	0.59
1:B:16:ILE:HG22	1:B:19:THR:OG1	2.02	0.59
1:A:257:TYR:HA	1:A:278:TRP:CZ2	2.39	0.58
1:D:296:VAL:HG12	1:D:300:VAL:HB	1.86	0.58
1:B:232:VAL:O	1:B:236:ASN:HB2	2.05	0.57
1:B:59:PHE:CE1	1:D:59:PHE:CE2	2.93	0.57
1:A:28:PHE:O	6:A:501:HOH:O	2.18	0.56
1:A:77:ARG:O	1:A:81:LYS:HB2	2.05	0.56
1:C:224:TYR:HE2	1:C:236:ASN:OD1	1.88	0.56
1:D:2:ARG:HH11	1:D:13:SER:HB3	1.71	0.56
1:B:163:THR:O	1:B:164:LYS:HE3	2.06	0.55
1:A:161:LYS:HE3	1:A:188:GLU:O	2.06	0.55
1:C:99:TYR:CE1	1:C:141:ASP:HB2	2.41	0.55
1:D:3:ILE:HD11	1:D:313:PHE:HB3	1.88	0.55
1:A:26:ARG:HG2	1:A:27:ALA:N	2.21	0.55
1:B:142:GLU:HB2	1:B:143:PRO:HD3	1.89	0.55
1:A:35:GLN:HE22	1:D:74:ARG:HE	1.55	0.54
1:B:202:ASP:OD1	1:B:235:ARG:NH1	2.40	0.54
1:C:296:VAL:HG13	1:C:300:VAL:CG1	2.38	0.54
1:A:127:GLN:NE2	1:D:35:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:O	1:A:113:GLU:N	2.39	0.53
1:C:28:PHE:CD1	1:C:33:ARG:HD3	2.44	0.53
1:A:296:VAL:HA	6:A:503:HOH:O	2.08	0.53
1:D:166:PRO:HB2	1:D:312:PHE:CZ	2.43	0.53
1:D:213:ALA:O	1:D:250:LYS:NZ	2.40	0.53
1:B:136:VAL:HG13	1:B:167:ILE:HG12	1.90	0.52
1:C:77:ARG:O	1:C:81:LYS:HB2	2.09	0.52
1:A:26:ARG:HD3	1:A:28:PHE:CE1	2.43	0.52
1:A:121:ASP:HA	1:A:125:GLY:O	2.08	0.52
1:C:257:TYR:HA	1:C:278:TRP:CZ2	2.45	0.52
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.44	0.52
1:B:255:HIS:NE2	1:B:283:ILE:HB	2.24	0.52
1:C:141:ASP:O	1:C:144:GLY:N	2.41	0.52
1:A:55:ARG:HD2	1:A:281:THR:HG21	1.91	0.52
1:B:3:ILE:HD11	1:B:313:PHE:HB3	1.92	0.52
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.45	0.52
1:C:26:ARG:HD3	1:C:28:PHE:CD2	2.45	0.52
1:D:274:LEU:O	1:D:274:LEU:HG	2.10	0.52
1:B:209:ILE:HG23	1:B:219:ILE:HD11	1.91	0.52
1:D:176:ASN:O	1:D:180[B]:GLU:HG2	2.10	0.52
1:C:137:KCX:OQ1	1:C:170:HIS:HB2	2.10	0.52
1:D:3:ILE:CD1	1:D:313:PHE:HB3	2.39	0.52
1:C:161:LYS:HE3	1:C:188:GLU:O	2.10	0.51
1:D:255:HIS:NE2	1:D:283:ILE:HB	2.26	0.51
1:A:106:PHE:O	1:A:107:LEU:O	2.28	0.51
1:C:292:LYS:NZ	1:C:298:GLU:OE1	2.44	0.51
1:D:26:ARG:HD3	1:D:28:PHE:CD2	2.45	0.51
1:A:253:ILE:CG2	1:A:283:ILE:HD11	2.41	0.51
1:C:255:HIS:NE2	1:C:283:ILE:HB	2.26	0.51
1:C:287:THR:O	1:C:291:LEU:HG	2.11	0.51
1:A:74:ARG:HB3	1:D:35:GLN:OE1	2.11	0.51
1:A:219:ILE:HG12	1:A:250:LYS:O	2.12	0.50
1:C:79:MET:O	1:C:83:VAL:HG23	2.11	0.50
1:A:141:ASP:O	1:A:144:GLY:N	2.44	0.50
1:D:277:ARG:NH1	1:D:286:ASP:OD2	2.42	0.50
1:D:23:GLU:OE1	1:D:254:SER:OG	2.30	0.50
1:D:142:GLU:HB2	1:D:143:PRO:HD3	1.94	0.50
1:D:225:GLY:HA3	1:D:278:TRP:HD1	1.77	0.50
1:A:240:LEU:HD11	1:A:244:LYS:HE3	1.92	0.50
1:C:28:PHE:CG	1:C:33:ARG:HD3	2.47	0.50
1:C:219:ILE:HD11	1:C:251:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:CD1	1:D:106:PHE:HB2	2.42	0.49
1:D:288:ILE:HB	1:D:289:PRO:HD3	1.93	0.49
1:A:107:LEU:O	1:A:109:ARG:N	2.45	0.49
1:B:257:TYR:HA	1:B:278:TRP:CZ2	2.48	0.49
1:B:98:ILE:HD13	1:B:102:LEU:HB3	1.95	0.49
1:A:102:LEU:HG	1:A:106:PHE:HB2	1.94	0.48
1:A:94:THR:O	1:A:136:VAL:HA	2.13	0.48
1:C:296:VAL:HG13	1:C:300:VAL:HG11	1.95	0.48
1:A:102:LEU:HD23	1:A:102:LEU:H	1.78	0.48
1:A:142:GLU:HB2	1:A:143:PRO:HD3	1.95	0.48
1:B:161:LYS:HE3	1:B:188:GLU:O	2.13	0.48
1:B:223:ARG:HB2	1:B:235:ARG:NH1	2.29	0.48
1:A:3:ILE:HD11	1:A:313:PHE:HB3	1.95	0.48
1:B:76:ILE:HD12	1:B:77:ARG:HD2	1.96	0.48
1:C:108:ASN:C	1:C:109:ARG:HG3	2.34	0.47
1:A:127:GLN:HA	1:D:37:PRO:HD2	1.96	0.47
1:D:150:GLU:OE1	1:D:154:ARG:NH1	2.47	0.47
1:B:297:ASN:OD1	1:B:299:GLU:N	2.48	0.47
1:C:169:THR:OG1	1:C:197:ILE:HA	2.14	0.47
1:B:219:ILE:HG22	1:B:250:LYS:O	2.14	0.47
1:D:55:ARG:HD2	1:D:281:THR:HG21	1.97	0.47
1:A:16:ILE:HG22	1:A:19:THR:OG1	2.14	0.47
1:B:75:ASP:HA	1:B:127:GLN:HE22	1.79	0.47
1:D:26:ARG:HD3	1:D:28:PHE:HD2	1.80	0.47
1:C:98:ILE:HD13	1:C:102:LEU:HB3	1.96	0.47
1:C:176:ASN:O	1:C:180:GLU:HG2	2.15	0.47
1:C:26:ARG:HD3	1:C:28:PHE:CE2	2.51	0.46
1:C:99:TYR:CD1	1:C:141:ASP:HB2	2.50	0.46
1:D:183:ARG:HD2	1:D:187:GLU:OE1	2.14	0.46
1:D:274:LEU:O	1:D:276:PRO:HD3	2.15	0.46
1:B:194:LYS:HG3	5:B:404:GOL:H11	1.96	0.46
1:C:14:LYS:HA	1:C:310:LYS:CD	2.41	0.46
1:A:137:KCX:OQ1	1:A:170:HIS:HB2	2.14	0.46
1:A:35:GLN:HA	1:D:127:GLN:HE21	1.81	0.46
1:D:197:ILE:HD12	1:D:212:ILE:HG23	1.97	0.46
1:B:176:ASN:O	1:B:180[B]:GLU:HG2	2.16	0.46
1:B:183:ARG:HH22	1:B:184:ILE:HG12	1.81	0.46
1:B:136:VAL:CG1	1:B:167:ILE:HG12	2.47	0.45
1:D:272:PRO:HA	1:D:275:ALA:HB3	1.98	0.45
1:A:35:GLN:NE2	1:D:74:ARG:HB3	2.27	0.45
1:D:242:LEU:HB3	1:D:251:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:NH1	1:B:127:GLN:O	2.50	0.45
1:B:192:PRO:HB2	1:B:216:GLY:HA3	1.99	0.45
1:B:79:MET:O	1:B:83:VAL:HG23	2.16	0.45
1:A:28:PHE:O	1:A:29:SER:CB	2.65	0.45
1:A:296:VAL:HG13	1:A:300:VAL:CG1	2.46	0.45
1:D:136:VAL:HG13	1:D:167:ILE:HG12	1.99	0.45
1:A:70:MET:HG2	1:D:31:ALA:HB1	1.98	0.44
1:D:273:LYS:HD2	1:D:273:LYS:H	1.82	0.44
1:A:100:ILE:H	4:A:404:EDO:H12	1.82	0.44
1:A:1:MET:N	1:A:10:SER:OG	2.46	0.44
1:D:180[A]:GLU:CD	1:D:183:ARG:HH11	2.21	0.44
1:D:225:GLY:HA3	1:D:278:TRP:CD1	2.52	0.44
1:A:26:ARG:HD3	1:A:28:PHE:CD1	2.53	0.44
1:D:102:LEU:HB2	1:D:103:PRO:HD2	1.99	0.44
1:B:236:ASN:HD22	1:B:236:ASN:HA	1.62	0.44
1:B:46:PHE:O	1:B:50:VAL:HG23	2.18	0.44
1:D:291:LEU:O	1:D:296:VAL:HG23	2.17	0.44
1:A:79:MET:O	1:A:83:VAL:HG23	2.17	0.44
1:B:1:MET:N	1:B:10:SER:OG	2.50	0.44
1:B:77:ARG:O	1:B:81:LYS:HB2	2.17	0.44
1:B:94:THR:O	1:B:137:KCX:N	2.51	0.44
1:C:194:LYS:HG3	5:C:404:GOL:H11	1.99	0.44
1:C:197:ILE:HD12	1:C:212:ILE:HG23	2.00	0.44
1:B:26:ARG:HG2	1:B:27:ALA:N	2.32	0.44
1:C:236:ASN:O	1:C:239:THR:OG1	2.19	0.44
1:B:76:ILE:HG13	1:B:127:GLN:NE2	2.29	0.43
1:D:172:ASN:HB3	1:D:175:ASN:OD1	2.17	0.43
1:A:98:ILE:HD13	1:A:102:LEU:HB3	2.00	0.43
1:C:292:LYS:HA	1:C:296:VAL:H	1.82	0.43
1:B:118:PHE:O	1:B:122:ILE:HG13	2.18	0.43
1:B:75:ASP:O	1:B:79:MET:HG3	2.18	0.43
1:D:182:GLN:HE21	1:D:217:SER:CB	2.32	0.43
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.54	0.43
1:D:2:ARG:NH1	1:D:13:SER:HB3	2.34	0.43
1:B:253:ILE:CG2	1:B:283:ILE:HD11	2.48	0.43
1:C:3:ILE:HD11	1:C:313:PHE:HB3	2.01	0.43
1:D:94:THR:O	1:D:137:KCX:N	2.51	0.43
1:A:28:PHE:O	1:A:29:SER:HB3	2.18	0.43
1:D:121:ASP:HA	1:D:125:GLY:O	2.19	0.43
1:C:95:GLY:HA2	1:C:118:PHE:CE1	2.54	0.43
1:C:205:ASN:O	1:C:207:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASN:HA	1:C:54:LYS:HG2	2.00	0.43
1:D:25:LEU:HD13	1:D:82:VAL:HG11	2.01	0.43
1:D:197:ILE:HD12	1:D:212:ILE:CG2	2.49	0.42
1:D:226:LEU:HD21	1:D:278:TRP:CZ2	2.55	0.42
1:D:6:VAL:HG21	1:D:90:LEU:HD12	2.01	0.42
1:B:223:ARG:HB2	1:B:235:ARG:HH12	1.84	0.42
1:D:77:ARG:O	1:D:81:LYS:HB2	2.18	0.42
1:D:137:KCX:HE3	1:D:170:HIS:HB2	2.02	0.42
1:B:222:ASP:O	1:B:256:ASP:HB2	2.20	0.42
1:C:118:PHE:O	1:C:122:ILE:HG13	2.19	0.42
1:D:224:TYR:HE1	1:D:236:ASN:OD1	2.02	0.42
1:B:100:ILE:H	4:B:403:EDO:H12	1.85	0.42
1:A:26:ARG:HE	1:A:45:GLU:CD	2.24	0.41
1:B:50:VAL:O	1:B:54:LYS:HG2	2.20	0.41
1:D:51:ASN:HA	1:D:54:LYS:HG2	2.02	0.41
1:A:102:LEU:HD22	1:A:148:ASP:HB3	2.02	0.41
1:A:136:VAL:HG13	1:A:167:ILE:HG12	2.02	0.41
1:B:209:ILE:HG23	1:B:219:ILE:CD1	2.50	0.41
1:D:59:PHE:CD2	1:D:284:PHE:CB	3.03	0.41
1:B:236:ASN:HD21	1:B:287:THR:HB	1.86	0.41
1:C:1:MET:N	1:C:10:SER:OG	2.51	0.41
1:A:77:ARG:NH1	1:A:127:GLN:O	2.50	0.41
1:A:76:ILE:HD12	1:A:77:ARG:N	2.36	0.41
1:B:164:LYS:HB2	1:B:164:LYS:HE3	1.78	0.41
1:D:76:ILE:H	1:D:76:ILE:HG13	1.71	0.41
1:A:255:HIS:NE2	1:A:283:ILE:HB	2.36	0.41
1:B:288:ILE:HB	1:B:289:PRO:HD3	2.01	0.41
1:B:311:LYS:HA	1:B:314:SER:OG	2.21	0.41
1:A:14:LYS:HA	1:A:310:LYS:CD	2.31	0.41
1:B:55:ARG:HD2	1:B:281:THR:HG21	2.03	0.41
1:A:236:ASN:HB3	1:A:290:PHE:CE1	2.56	0.41
1:B:290:PHE:O	1:B:293:ARG:HB3	2.21	0.41
1:A:63:THR:HA	1:A:89:ASN:HB2	2.02	0.40
1:B:224:TYR:OH	1:B:236:ASN:ND2	2.50	0.40
1:B:14:LYS:HA	1:B:310:LYS:CD	2.43	0.40
1:B:239:THR:O	1:B:243:ILE:HG13	2.21	0.40
1:C:253:ILE:CG2	1:C:283:ILE:HD11	2.52	0.40
1:D:283:ILE:HD13	1:D:283:ILE:HG21	1.78	0.40
1:B:33:ARG:NH1	1:B:40:TYR:CD2	2.90	0.40
1:D:224:TYR:CE1	1:D:236:ASN:OD1	2.74	0.40
1:D:306:LYS:O	1:D:310:LYS:HB2	2.21	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	296/314 (94%)	264 (89%)	26 (9%)	6 (2%)	9	36
1	B	295/314 (94%)	268 (91%)	23 (8%)	4 (1%)	13	46
1	C	293/314 (93%)	263 (90%)	25 (8%)	5 (2%)	11	41
1	D	298/314 (95%)	266 (89%)	26 (9%)	6 (2%)	9	36
All	All	1182/1256 (94%)	1061 (90%)	100 (8%)	21 (2%)	10	39

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	107	LEU
1	A	108	ASN
1	A	205	ASN
1	A	275	ALA
1	B	294	ASN
1	C	109	ARG
1	D	276	PRO
1	B	205	ASN
1	C	108	ASN
1	C	110	SER
1	C	206	ILE
1	D	205	ASN
1	C	276	PRO
1	D	275	ALA
1	D	295	GLY
1	A	111	ILE
1	D	143	PRO
1	B	103	PRO
1	D	100	ILE

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Mol	Chain	Res	Type
1	B	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	260/271 (96%)	259 (100%)	1 (0%)	93	98
1	B	259/271 (96%)	255 (98%)	4 (2%)	70	90
1	C	257/271 (95%)	252 (98%)	5 (2%)	62	87
1	D	262/271 (97%)	256 (98%)	6 (2%)	56	84
All	All	1038/1084 (96%)	1022 (98%)	16 (2%)	70	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	B	26	ARG
1	B	200	LEU
1	B	235	ARG
1	B	236	ASN
1	C	109	ARG
1	C	110	SER
1	C	142	GLU
1	C	200	LEU
1	C	228	MET
1	D	1	MET
1	D	102	LEU
1	D	196	LEU
1	D	200	LEU
1	D	228	MET
1	D	297	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	B	127	GLN
1	B	236	ASN
1	B	294	ASN
1	C	127	GLN
1	D	38	HIS
1	D	297	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	A	137	1,3,2	8,11,12	0.68	0	6,12,14	1.51	1 (16%)
1	KCX	B	137	1,3,2	8,11,12	0.80	0	6,12,14	1.08	0
1	KCX	C	137	1,3,2	8,11,12	0.72	0	6,12,14	1.54	1 (16%)
1	KCX	D	137	1,3,2	8,11,12	0.98	1 (12%)	6,12,14	1.51	1 (16%)

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	A	137	1,3,2	-	0/6/10/12	0/0/0/0
1	KCX	B	137	1,3,2	-	0/6/10/12	0/0/0/0
1	KCX	C	137	1,3,2	-	0/6/10/12	0/0/0/0
1	KCX	D	137	1,3,2	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	137	KCX	CB-CA	-2.12	1.50	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	KCX	CE-NZ-CX	-3.12	119.53	123.35
1	A	137	KCX	CB-CA-C	-2.99	106.73	111.65
1	D	137	KCX	CB-CA-C	-2.65	107.28	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	137	KCX	1	0
1	B	137	KCX	1	0
1	C	137	KCX	1	0
1	D	137	KCX	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	$\# Z > 2$
4	EDO	A	403	-	3,3,3	0.56	0	2,2,2	0.65	0
4	EDO	A	404	-	3,3,3	0.51	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	405	-	5,5,5	0.11	0	5,5,5	0.24	0
4	EDO	B	403	-	3,3,3	0.53	0	2,2,2	0.06	0
5	GOL	B	404	-	5,5,5	0.18	0	5,5,5	0.46	0
4	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	C	403	-	3,3,3	0.58	0	2,2,2	0.08	0
5	GOL	C	404	-	5,5,5	0.28	0	5,5,5	0.24	0
4	EDO	C	405	-	3,3,3	0.48	0	2,2,2	0.33	0
4	EDO	D	403	-	3,3,3	0.57	0	2,2,2	0.33	0
4	EDO	D	404	-	3,3,3	0.55	0	2,2,2	0.09	0
5	GOL	D	405	-	5,5,5	0.30	0	5,5,5	0.54	0
4	EDO	D	406	-	3,3,3	0.59	0	2,2,2	0.12	0
5	GOL	D	407	-	5,5,5	0.79	0	5,5,5	0.66	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
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
5	GOL	A	405	-	-	0/4/4/4	0/0/0/0
4	EDO	B	403	-	-	0/1/1/1	0/0/0/0
5	GOL	B	404	-	-	0/4/4/4	0/0/0/0
4	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	EDO	C	403	-	-	0/1/1/1	0/0/0/0
5	GOL	C	404	-	-	0/4/4/4	0/0/0/0
4	EDO	C	405	-	-	0/1/1/1	0/0/0/0
4	EDO	D	403	-	-	0/1/1/1	0/0/0/0
4	EDO	D	404	-	-	0/1/1/1	0/0/0/0
5	GOL	D	405	-	-	0/4/4/4	0/0/0/0
4	EDO	D	406	-	-	0/1/1/1	0/0/0/0
5	GOL	D	407	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	EDO	1	0
4	B	403	EDO	1	0
5	B	404	GOL	1	0
5	C	404	GOL	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	299/314 (95%)	0.37	5 (1%)	70 51	52, 95, 151, 256	0
1	B	298/314 (94%)	0.58	24 (8%)	13 7	54, 113, 167, 194	0
1	C	297/314 (94%)	1.05	59 (19%)	1 1	79, 141, 196, 217	0
1	D	301/314 (95%)	0.21	5 (1%)	70 51	42, 79, 123, 185	0
All	All	1195/1256 (95%)	0.55	93 (7%)	14 7	42, 105, 178, 256	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.4
1	B	229	PHE	6.1
1	C	197	ILE	6.0
1	B	99	TYR	5.5
1	C	184	ILE	5.3
1	C	212	ILE	5.1
1	C	104	PHE	5.1
1	C	209	ILE	4.9
1	C	200	LEU	4.8
1	B	230	LEU	4.7
1	A	259	CYS	4.0
1	C	206	ILE	3.9
1	C	277	ARG	3.9
1	B	100	ILE	3.9
1	C	208	TYR	3.8
1	C	276	PRO	3.7
1	B	278	TRP	3.6
1	C	103	PRO	3.5
1	B	104	PHE	3.4
1	C	182	GLN	3.4
1	C	253	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	242	LEU	3.3
1	C	136	VAL	3.3
1	A	278	TRP	3.3
1	A	257	TYR	3.3
1	B	200	LEU	3.2
1	C	221	LEU	3.2
1	C	153	ILE	3.2
1	D	40	TYR	3.2
1	C	180	GLU	3.2
1	C	152	VAL	3.2
1	B	140	ALA	3.0
1	B	232	VAL	3.0
1	C	196	LEU	2.9
1	C	202	ASP	2.9
1	B	207	ASP	2.9
1	C	313	PHE	2.9
1	C	140	ALA	2.9
1	C	151	LYS	2.9
1	C	130	LEU	2.8
1	B	204	ASP	2.8
1	C	275	ALA	2.8
1	C	195	ILE	2.8
1	C	282	LEU	2.8
1	C	177	THR	2.8
1	C	228	MET	2.7
1	C	139	ALA	2.7
1	C	149	VAL	2.7
1	C	64	ILE	2.7
1	B	226	LEU	2.7
1	C	181	GLN	2.7
1	C	138	ILE	2.6
1	C	203	THR	2.6
1	C	224	TYR	2.6
1	C	257	TYR	2.6
1	C	185	LEU	2.6
1	C	1	MET	2.6
1	C	176	ASN	2.4
1	C	278	TRP	2.4
1	D	272	PRO	2.4
1	A	37	PRO	2.4
1	D	277	ARG	2.4
1	C	155	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	2.4
1	C	99	TYR	2.3
1	B	240	LEU	2.3
1	C	178	GLY	2.3
1	B	234	LYS	2.3
1	C	156	ALA	2.3
1	C	217	SER	2.3
1	D	275	ALA	2.3
1	C	167	ILE	2.3
1	C	304	ILE	2.3
1	B	231	PRO	2.3
1	B	274	LEU	2.2
1	C	114	ILE	2.2
1	C	241	ARG	2.2
1	C	107	LEU	2.2
1	C	227	ASP	2.2
1	C	90	LEU	2.2
1	C	296	VAL	2.2
1	B	203	THR	2.2
1	D	1	MET	2.2
1	B	224	TYR	2.2
1	B	300	VAL	2.2
1	C	299	GLU	2.2
1	C	219	ILE	2.1
1	B	60	GLY	2.0
1	C	51	ASN	2.0
1	C	279	SER	2.0
1	B	228	MET	2.0
1	B	206	ILE	2.0
1	B	314	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	KCX	C	137	12/13	0.97	0.23	-	95,113,118,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	KCX	A	137	12/13	0.97	0.20	-	46,53,64,66	0
1	KCX	D	137	12/13	0.96	0.20	-	39,44,49,52	0
1	KCX	B	137	12/13	0.97	0.14	-	50,54,62,70	0

6.3 Carbohydrates

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	D	403	4/4	0.83	0.56	8.45	45,48,48,49	0
5	GOL	C	404	6/6	0.76	0.64	7.70	109,111,114,116	0
4	EDO	C	405	4/4	0.29	0.91	6.56	111,113,114,121	0
4	EDO	B	403	4/4	-0.12	1.28	5.75	137,137,138,139	0
4	EDO	D	406	4/4	0.79	0.48	4.34	64,68,69,70	0
4	EDO	A	404	4/4	0.80	0.46	4.16	91,91,94,100	0
4	EDO	B	405	4/4	0.77	0.35	3.12	84,84,86,87	0
4	EDO	A	403	4/4	0.94	0.29	1.98	33,34,35,36	0
5	GOL	B	404	6/6	0.89	0.31	1.95	65,66,73,77	0
5	GOL	D	405	6/6	0.92	0.21	0.22	41,42,46,53	0
5	GOL	A	405	6/6	0.89	0.20	-0.42	56,60,65,67	0
5	GOL	D	407	6/6	0.89	0.16	-0.81	56,58,62,65	0
3	CO	B	402	1/1	0.98	0.05	-2.55	49,49,49,49	0
3	CO	C	402	1/1	0.96	0.05	-3.25	66,66,66,66	0
3	CO	D	402	1/1	0.98	0.04	-3.33	28,28,28,28	0
3	CO	A	402	1/1	0.98	0.04	-7.05	13,13,13,13	0
2	FE	B	401	1/1	0.95	0.05	-	44,44,44,44	0
2	FE	D	401	1/1	0.98	0.04	-	19,19,19,19	0
2	FE	C	401	1/1	0.97	0.07	-	50,50,50,50	0
4	EDO	C	403	4/4	-0.03	0.87	-	109,116,120,125	0
4	EDO	D	404	4/4	0.89	0.38	-	75,75,77,80	0
2	FE	A	401	1/1	0.96	0.05	-	13,13,13,13	0

6.5 Other polymers

There are no such residues in this entry.