



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:14 AM UTC

PDB ID : 5W3W / pdb_00005w3w
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

<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

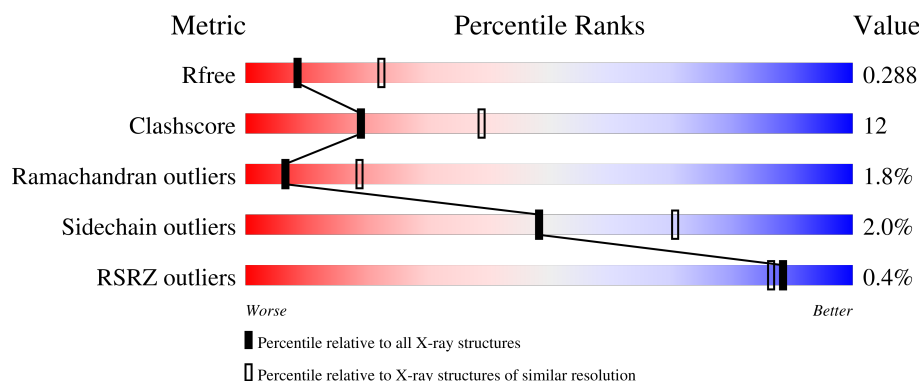
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 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 (II) ION (CCD ID: FE2) (formula: Fe).

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

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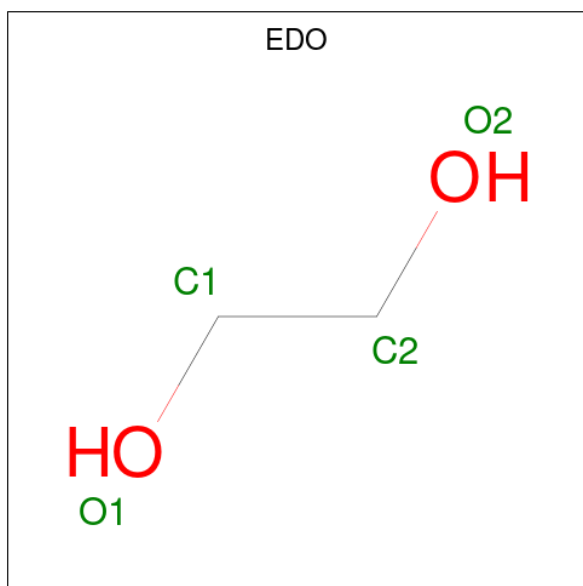
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

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

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

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

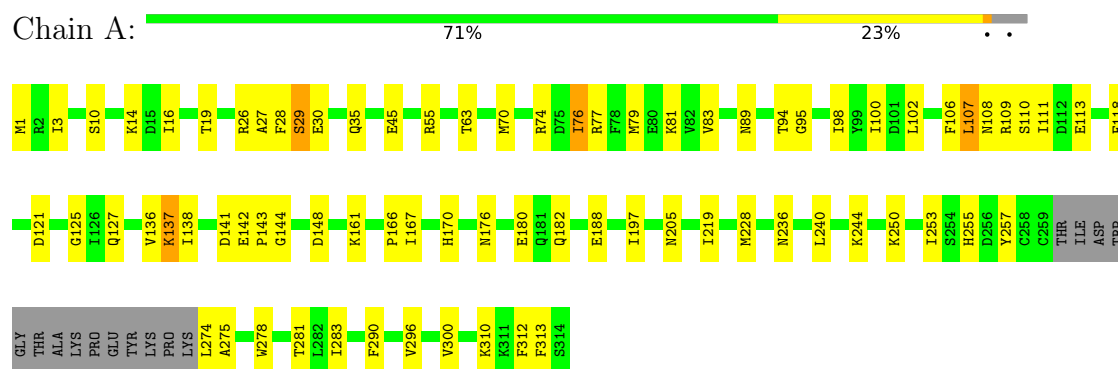
- Molecule 6 is water.

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

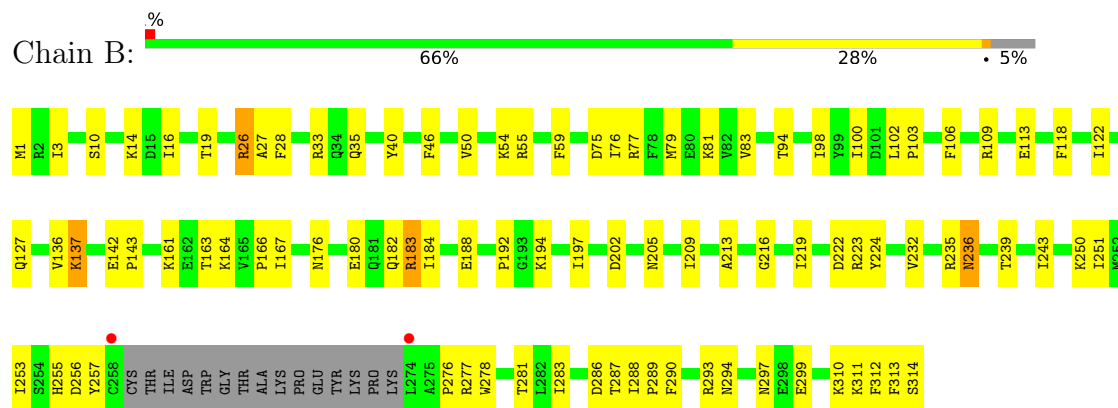
3 Residue-property plots

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.

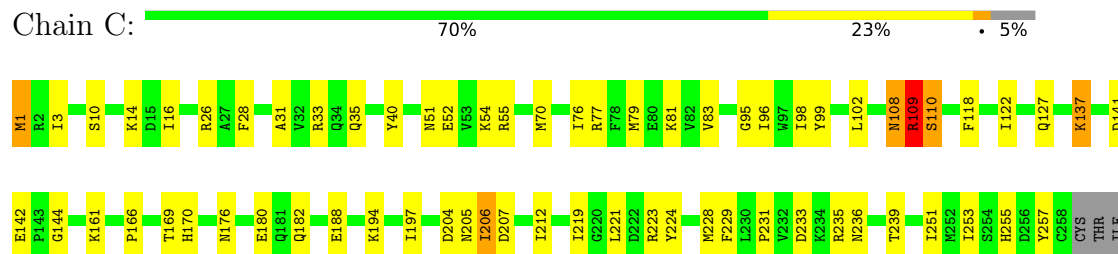
• Molecule 1: Aryldialkylphosphatase



• Molecule 1: Aryldialkylphosphatase

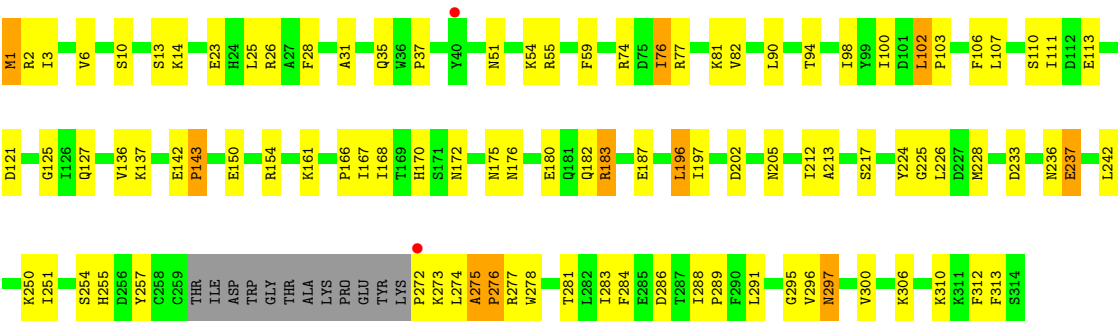


• Molecule 1: Aryldialkylphosphatase





● 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	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 , 0.288	Depositor DCC
R_{free} test set	1409 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 80.7	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: CO, KCX, EDO, GOL, FE2

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	0.80	0/2440	0.83	0/3291
1	B	0.67	0/2434	0.78	0/3283
1	C	0.63	0/2417	0.80	0/3260
1	D	0.84	0/2457	0.83	0/3313
All	All	0.74	0/9748	0.81	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	58	0
1	B	2398	0	2421	62	0
1	C	2384	0	2404	49	0
1	D	2420	0	2447	72	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	230	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 12.

All (230) 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:H	1:D:297:ASN:HD22	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:108:ASN:C	1:C:109:ARG:HG3	2.34	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:A:74:ARG:HB3	1:D:35:GLN:OE1	2.11	0.51
1:C:287:THR:O	1:C:291:LEU:HG	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:228:MET:HE2	1:A:274:LEU:O	2.12	0.50
1:A:240:LEU:HD11	1:A:244:LYS:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:180[A]:GLU:CD	1:D:183:ARG:HH11	2.21	0.49
1:B:98:ILE:HD13	1:B:102:LEU:HB3	1.95	0.49
1:A:94:THR:O	1:A:136:VAL:HA	2.13	0.48
1:A:102:LEU:HG	1:A:106:PHE:HB2	1.94	0.48
1:C:296:VAL:HG13	1:C:300:VAL:HG11	1.95	0.48
1:A:102:LEU:H	1:A:102:LEU:HD23	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: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:C:236:ASN:O	1:C:239:THR:OG1	2.19	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:A:26:ARG:HE	1:A:45:GLU:CD	2.24	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:35:GLN:HA	1:D:127:GLN:HE21	1.81	0.46
1:A:137:KCX:OQ1	1:A:170:HIS:HB2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:77:ARG:NH1	1:B:127:GLN:O	2.50	0.45
1:B:79:MET:O	1:B:83:VAL:HG23	2.16	0.45
1:B:192:PRO:HB2	1:B:216:GLY:HA3	1.99	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:H	1:D:273:LYS:HD2	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: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:46:PHE:O	1:B:50:VAL:HG23	2.18	0.44
1:B:236:ASN:HD22	1:B:236:ASN:HA	1.62	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: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: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:A:138:ILE:HD12	1:A:138:ILE:C	2.44	0.43
1:C:292:LYS:HA	1:C:296:VAL:H	1.82	0.43
1:B:75:ASP:O	1:B:79:MET:HG3	2.18	0.43
1:B:118:PHE:O	1:B:122:ILE:HG13	2.18	0.43
1:D:182:GLN:HE21	1:D:217:SER:CB	2.32	0.43
1:A:30:GLU:CD	1:A:30:GLU:H	2.27	0.43
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.54	0.43
1:C:70:MET:HE2	1:C:96:ILE:HG23	2.01	0.43
1:B:1:MET:N	1:B:10:SER:OG	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:51:ASN:HA	1:C:54:LYS:HG2	2.00	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
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:6:VAL:HG21	1:D:90:LEU:HD12	2.01	0.42
1:D:226:LEU:HD21	1:D:278:TRP:CZ2	2.55	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:106:PHE:O	1:D:107:LEU:C	2.62	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:B:50:VAL:O	1:B:54:LYS:HG2	2.20	0.41
1:C:204:ASP:C	1:C:206:ILE:H	2.28	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:HE3	1:B:164:LYS:HB2	1.78	0.41
1:D:76:ILE:H	1:D:76:ILE:HG13	1.71	0.41
1:A:14:LYS:HA	1:A:310:LYS:CD	2.31	0.41
1:A:255:HIS:NE2	1:A:283:ILE:HB	2.36	0.41
1:B:55:ARG:HD2	1:B:281:THR:HG21	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG21	1:D:283:ILE:HD13	1.78	0.40
1:D:2:ARG:C	1:D:3:ILE:HD13	2.46	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%)	6	16
1	B	295/314 (94%)	268 (91%)	23 (8%)	4 (1%)	9	24
1	C	293/314 (93%)	263 (90%)	25 (8%)	5 (2%)	7	20
1	D	298/314 (95%)	266 (89%)	26 (9%)	6 (2%)	6	16
All	All	1182/1256 (94%)	1061 (90%)	100 (8%)	21 (2%)	6	19

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

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Mol	Chain	Res	Type
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
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%)	84	92
1	B	259/271 (96%)	256 (99%)	3 (1%)	63	79
1	C	257/271 (95%)	250 (97%)	7 (3%)	39	64
1	D	262/271 (97%)	252 (96%)	10 (4%)	29	55
All	All	1038/1084 (96%)	1017 (98%)	21 (2%)	48	71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ILE
1	B	26	ARG
1	B	183	ARG
1	B	236	ASN
1	C	1	MET
1	C	16	ILE
1	C	76	ILE
1	C	109	ARG

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Mol	Chain	Res	Type
1	C	110	SER
1	C	142	GLU
1	C	228	MET
1	D	1	MET
1	D	76	ILE
1	D	102	LEU
1	D	161	LYS
1	D	183	ARG
1	D	196	LEU
1	D	202	ASP
1	D	228	MET
1	D	237	GLU
1	D	297	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	35	GLN
1	A	294	ASN
1	B	127	GLN
1	B	205	ASN
1	B	236	ASN
1	B	294	ASN
1	C	127	GLN
1	D	41	ASN
1	D	205	ASN
1	D	294	ASN
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	C	137	3,1,2	10,11,12	0.60	0	6,12,14	1.21	1 (16%)
1	KCX	D	137	3,1,2	10,11,12	0.80	0	6,12,14	0.65	0
1	KCX	B	137	3,1,2	10,11,12	1.77	1 (10%)	6,12,14	1.01	1 (16%)
1	KCX	A	137	3,1,2	10,11,12	0.66	0	6,12,14	1.00	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	C	137	3,1,2	-	4/9/10/12	-
1	KCX	D	137	3,1,2	-	4/9/10/12	-
1	KCX	B	137	3,1,2	-	3/9/10/12	-
1	KCX	A	137	3,1,2	-	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	OQ1-CX	4.71	1.30	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	KCX	OQ1-CX-NZ	-2.21	121.56	124.92
1	A	137	KCX	OQ1-CX-NZ	-2.20	121.58	124.92
1	B	137	KCX	OQ1-CX-NZ	-2.12	121.70	124.92

There are no chirality outliers.

All (14) 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

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

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
5	GOL	D	407	-	5,5,5	0.84	0	5,5,5	0.70	0
4	EDO	D	404	-	3,3,3	0.53	0	2,2,2	0.12	0
5	GOL	B	404	-	5,5,5	0.19	0	5,5,5	0.53	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	0.14	0	5,5,5	0.28	0
4	EDO	D	403	-	3,3,3	0.55	0	2,2,2	0.34	0
5	GOL	C	404	-	5,5,5	0.30	0	5,5,5	0.29	0
4	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.62	0
4	EDO	C	405	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	C	403	-	3,3,3	0.55	0	2,2,2	0.10	0
4	EDO	B	403	-	3,3,3	0.51	0	2,2,2	0.04	0
4	EDO	A	404	-	3,3,3	0.49	0	2,2,2	0.26	0
5	GOL	D	405	-	5,5,5	0.24	0	5,5,5	0.66	0
4	EDO	D	406	-	3,3,3	0.57	0	2,2,2	0.11	0
4	EDO	B	405	-	3,3,3	0.39	0	2,2,2	0.36	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	D	407	-	-	2/4/4/4	-
4	EDO	D	404	-	-	1/1/1/1	-
5	GOL	B	404	-	-	2/4/4/4	-
5	GOL	A	405	-	-	2/4/4/4	-
4	EDO	D	403	-	-	1/1/1/1	-
5	GOL	C	404	-	-	2/4/4/4	-
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
5	GOL	D	405	-	-	2/4/4/4	-
4	EDO	D	406	-	-	0/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	404	GOL	O1-C1-C2-C3
5	C	404	GOL	O1-C1-C2-C3
5	D	405	GOL	O1-C1-C2-C3
5	D	407	GOL	C1-C2-C3-O3
5	D	407	GOL	O2-C2-C3-O3
5	A	405	GOL	O1-C1-C2-O2
5	B	404	GOL	O1-C1-C2-O2
5	C	404	GOL	O1-C1-C2-O2
5	D	405	GOL	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2
4	D	404	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
4	A	403	EDO	O1-C1-C2-O2
4	D	403	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	GOL	1	0
5	C	404	GOL	1	0
4	B	403	EDO	1	0
4	A	404	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 [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	299/314 (95%)	-0.03	0 100 100	52, 94, 151, 256	1 (0%)
1	B	298/314 (94%)	0.03	2 (0%) 84 80	54, 112, 167, 194	1 (0%)
1	C	297/314 (94%)	0.10	1 (0%) 90 88	79, 141, 196, 217	0
1	D	301/314 (95%)	-0.21	2 (0%) 84 80	42, 79, 123, 185	1 (0%)
All	All	1195/1256 (95%)	-0.03	5 (0%) 88 86	42, 105, 178, 256	3 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	CYS	2.6
1	D	40	TYR	2.4
1	C	275	ALA	2.4
1	B	274	LEU	2.2
1	D	272	PRO	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	A	137	12/13	0.95	0.09	46,53,64,66	0
1	KCX	C	137	12/13	0.95	0.09	95,113,118,122	0
1	KCX	B	137	12/13	0.96	0.07	50,54,62,70	0
1	KCX	D	137	12/13	0.96	0.08	39,44,49,52	0

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(Å ²)	Q<0.9
4	EDO	C	403	4/4	0.15	0.20	109,116,120,125	0
4	EDO	B	405	4/4	0.66	0.15	84,84,86,87	0
4	EDO	B	403	4/4	0.67	0.13	137,137,138,139	0
4	EDO	D	404	4/4	0.74	0.18	75,75,77,80	0
4	EDO	C	405	4/4	0.78	0.15	111,113,114,121	0
4	EDO	A	404	4/4	0.78	0.18	91,91,94,100	0
5	GOL	C	404	6/6	0.79	0.10	109,111,114,116	0
5	GOL	B	404	6/6	0.84	0.14	65,66,73,77	0
5	GOL	A	405	6/6	0.86	0.13	56,60,65,67	0
5	GOL	D	407	6/6	0.86	0.18	56,58,62,65	0
5	GOL	D	405	6/6	0.87	0.14	41,42,46,53	0
4	EDO	D	403	4/4	0.88	0.20	45,48,48,49	0
4	EDO	A	403	4/4	0.92	0.13	33,34,35,36	0
4	EDO	D	406	4/4	0.93	0.15	64,68,69,70	0
2	FE2	C	401	1/1	0.97	0.11	50,50,50,50	0
3	CO	C	402	1/1	0.97	0.10	66,66,66,66	0
3	CO	D	402	1/1	0.99	0.12	28,28,28,28	0
2	FE2	A	401	1/1	0.99	0.11	13,13,13,13	0
3	CO	A	402	1/1	0.99	0.12	13,13,13,13	0
3	CO	B	402	1/1	0.99	0.10	49,49,49,49	0
2	FE2	B	401	1/1	0.99	0.10	44,44,44,44	0
2	FE2	D	401	1/1	1.00	0.12	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.