



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:19 pm GMT

PDB ID : 2VC5  
Title : Structural basis for natural lactonase and promiscuous phosphotriesterase activities  
Authors : Elias, M.; Dupuy, J.; Merone, L.; Mandrich, L.; Moniot, S.; Lecomte, C.; Rossi, M.; Masson, P.; Manco, G.; Chabriere, E.  
Deposited on : 2007-09-18  
Resolution : 2.60 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

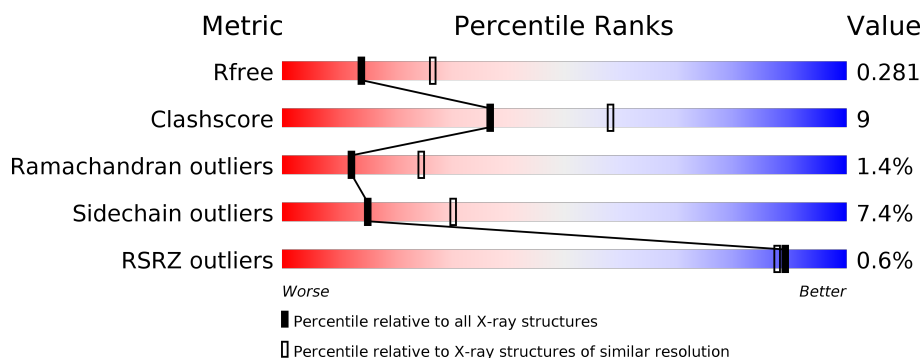
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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  $\geq 3$ , 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>84%</div> <div>13%</div> <div>.</div> </div>
1	B	314	<div> <div>%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>
1	C	314	<div> <div>%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
1	D	314	<div> <div>%</div> <div>75%</div> <div>21%</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	B	1321	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10475 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	314	Total	C	N	O	S	0	3	0
			2527	1619	429	472	7			
1	B	314	Total	C	N	O	S	0	4	0
			2537	1626	428	476	7			
1	C	314	Total	C	N	O	S	0	5	0
			2546	1630	434	475	7			
1	D	314	Total	C	N	O	S	0	1	0
			2519	1616	426	470	7			

- 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		
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:  $C_2H_6O_2$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	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	64	Total	O	0	0
			64	64		

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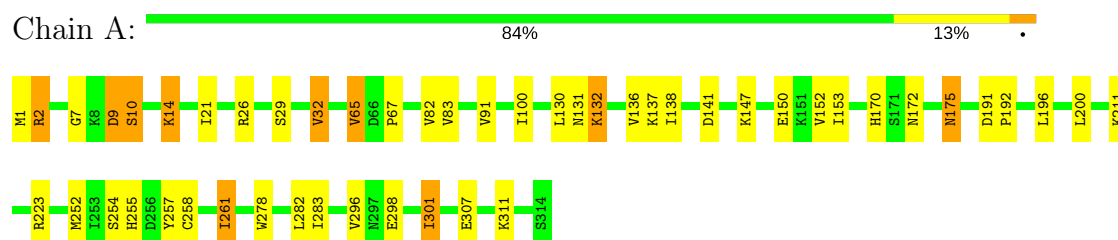
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	62	Total 62	O 62	0	0
6	C	55	Total 55	O 55	0	0
6	D	61	Total 61	O 61	0	0

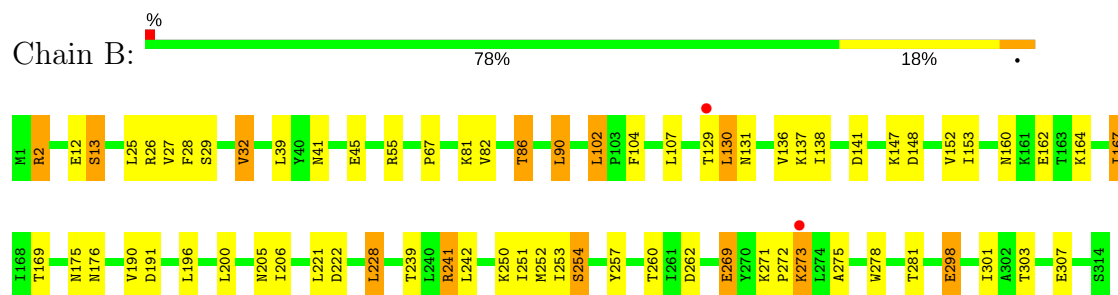
### 3 Residue-property plots [i](#)

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.

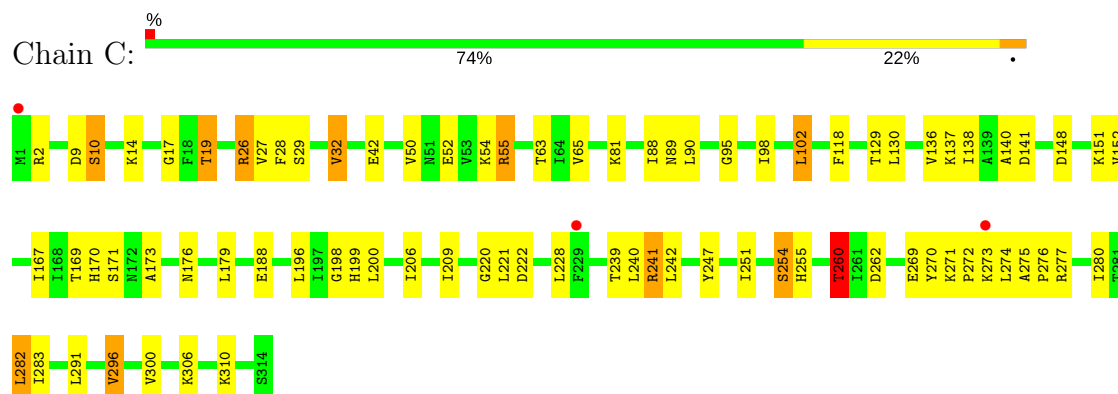
#### • Molecule 1: ARYLDIALKYLPHOSPHATASE



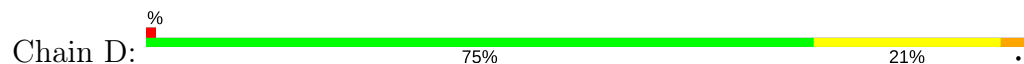
#### • Molecule 1: ARYLDIALKYLPHOSPHATASE



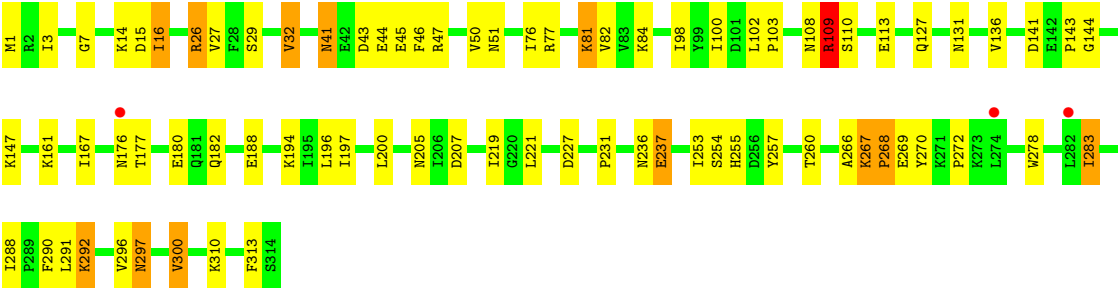
#### • Molecule 1: ARYLDIALKYLPHOSPHATASE



#### • Molecule 1: ARYLDIALKYLPHOSPHATASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.16Å 104.82Å 155.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.90 – 2.60 44.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.90-2.60) 99.4 (44.52-2.60)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.222 , 0.282 0.222 , 0.281	Depositor DCC
$R_{free}$ test set	2234 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10475	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.34	0/2565	0.50	0/3464
1	B	0.35	0/2578	0.53	1/3482 (0.0%)
1	C	0.41	1/2587 (0.0%)	0.53	0/3493
1	D	0.36	1/2560 (0.0%)	0.53	0/3457
All	All	0.37	2/10290 (0.0%)	0.53	1/13896 (0.0%)

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	B	1	0
1	C	1	0
1	D	0	1
All	All	2	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	260	THR	CB-OG1	9.77	1.62	1.43
1	D	268	PRO	N-CD	5.58	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	LEU	CA-CB-CG	5.02	126.85	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	86	THR	CB
1	C	260	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	292	LYS	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	2527	0	2550	26	0
1	B	2537	0	2558	41	0
1	C	2546	0	2569	45	0
1	D	2519	0	2547	64	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
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	18	1	0
4	B	20	0	30	2	0
4	C	12	0	18	0	0
4	D	16	0	24	1	0
5	A	12	0	16	2	0
5	B	18	0	24	2	0
5	D	6	0	8	1	0
6	A	64	0	0	0	0
6	B	62	0	0	0	0
6	C	55	0	0	0	0
6	D	61	0	0	0	0
All	All	10475	0	10362	176	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 (176) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:PHE:HA	1:C:262:ASP:HB2	1.42	1.00
1:B:221:LEU:HD13	1:B:239:THR:HG22	1.53	0.89
1:D:14:LYS:HA	1:D:310:LYS:HD2	1.58	0.86
1:D:253:ILE:HG22	1:D:283:ILE:HD11	1.59	0.85
1:B:28:PHE:HA	1:B:262:ASP:HB2	1.58	0.83
1:C:271:LYS:HB3	1:C:272:PRO:HD3	1.60	0.83
1:D:182:GLN:HB2	1:D:197:ILE:HD11	1.60	0.82
1:D:176:ASN:O	1:D:180[B]:GLU:HG2	1.81	0.80
1:B:175:ASN:O	1:B:176:ASN:HB2	1.84	0.76
1:A:258:CYS:HB2	1:A:261:ILE:HG12	1.68	0.76
1:C:271:LYS:HB3	1:C:272:PRO:CD	2.17	0.74
1:C:221:LEU:HD13	1:C:239:THR:HG22	1.70	0.73
1:B:12:GLU:O	1:B:13:SER:CB	2.37	0.72
1:B:102:LEU:HD22	1:B:148:ASP:HB3	1.70	0.71
1:C:28:PHE:HA	1:C:262:ASP:CB	2.19	0.71
1:B:82:VAL:O	1:B:86:THR:HB	1.91	0.70
1:D:41:ASN:ND2	1:D:44:GLU:H	1.91	0.69
1:B:129:THR:O	1:B:130:LEU:HB2	1.92	0.68
1:D:16:ILE:HD11	1:D:310:LYS:HD3	1.76	0.68
1:C:199:HIS:O	1:C:200:LEU:HG	1.93	0.68
1:C:270:TYR:HB3	1:C:274:LEU:HD12	1.76	0.68
1:C:270:TYR:O	1:C:274:LEU:HB2	1.94	0.67
1:A:100:ILE:H	4:A:1317:EDO:H12	1.59	0.67
1:D:26:ARG:HH11	1:D:26:ARG:HG2	1.60	0.66
1:D:29:SER:HB2	1:D:32:VAL:HG13	1.78	0.64
1:D:291:LEU:O	1:D:292:LYS:HG2	1.98	0.64
1:D:26:ARG:HH11	1:D:26:ARG:CG	2.10	0.64
1:D:236:ASN:O	1:D:237:GLU:CB	2.45	0.63
1:D:76:ILE:HG13	1:D:127:GLN:HE21	1.64	0.63
1:A:196:LEU:HD13	1:A:252:MET:HE3	1.80	0.63
1:C:17:GLY:HA2	1:C:306:LYS:HE3	1.80	0.63
1:B:104:PHE:CD1	4:B:1324:EDO:O2	2.52	0.62
1:C:240:LEU:O	1:C:241:ARG:CB	2.48	0.62
1:C:240:LEU:O	1:C:241:ARG:HB3	2.00	0.62
1:D:176:ASN:O	1:D:180[B]:GLU:CG	2.48	0.62
1:D:269:GLU:O	1:D:272:PRO:HD2	1.99	0.62
1:A:14:LYS:HD2	1:A:14:LYS:H	1.65	0.61
1:D:253:ILE:CG2	1:D:283:ILE:HD11	2.31	0.60
1:B:196:LEU:HD13	1:B:252:MET:HE3	1.83	0.60
1:D:292:LYS:HB2	1:D:296:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:PRO:O	1:B:273:LYS:HB3	2.01	0.59
1:D:194:LYS:HG3	5:D:1319:GOL:H11	1.86	0.58
1:D:297:ASN:H	1:D:297:ASN:ND2	2.03	0.57
1:D:43:ASP:O	1:D:47:ARG:HG3	2.05	0.57
1:A:7:GLY:H	1:A:131:ASN:ND2	2.03	0.57
1:D:177:THR:HA	1:D:180[B]:GLU:HG3	1.87	0.57
1:B:28:PHE:HA	1:B:262:ASP:CB	2.32	0.56
1:D:182:GLN:HB2	1:D:197:ILE:CD1	2.34	0.56
1:A:138:ILE:HD13	1:A:153:ILE:HG12	1.87	0.56
1:A:257:TYR:HA	1:A:278:TRP:CZ2	2.40	0.56
1:C:9:ASP:O	1:C:10:SER:CB	2.52	0.56
1:A:21:ILE:HA	1:A:65:VAL:HG13	1.87	0.56
1:D:100:ILE:H	4:D:1318:EDO:H12	1.71	0.56
1:A:223:ARG:NH2	5:A:1321:GOL:H32	2.21	0.56
1:D:46:PHE:O	1:D:50:VAL:HG23	2.07	0.55
1:A:9:ASP:O	1:A:10:SER:CB	2.53	0.55
1:B:271:LYS:HB3	1:B:272:PRO:HD3	1.89	0.55
1:C:291:LEU:O	1:C:296:VAL:HG13	2.07	0.55
1:C:136:VAL:HG13	1:C:167:ILE:HG12	1.90	0.54
1:D:41:ASN:HD22	1:D:44:GLU:H	1.55	0.54
1:C:169:THR:O	1:C:198:GLY:HA3	2.07	0.54
1:B:191:ASP:HB3	5:B:1318:GOL:H32	1.90	0.53
1:B:12:GLU:O	1:B:13:SER:HB3	2.08	0.53
1:D:26:ARG:NH1	1:D:26:ARG:HG2	2.22	0.53
1:D:292:LYS:HA	1:D:296:VAL:H	1.74	0.53
1:B:129:THR:HG23	1:B:131:ASN:H	1.73	0.52
1:D:236:ASN:O	1:D:237:GLU:HB2	2.10	0.52
1:B:257:TYR:HA	1:B:278:TRP:CZ2	2.44	0.52
1:B:29:SER:HB2	1:B:32:VAL:HG13	1.90	0.52
1:A:9:ASP:O	1:A:10:SER:HB2	2.09	0.52
1:C:255:HIS:CE1	1:C:283:ILE:HG12	2.45	0.52
1:C:228:LEU:HD21	1:C:274:LEU:HD13	1.91	0.52
1:B:12:GLU:O	1:B:13:SER:HB2	2.09	0.52
1:D:268:PRO:O	1:D:272:PRO:HD3	2.10	0.51
1:B:138:ILE:HD12	1:B:153:ILE:HG12	1.92	0.51
1:A:223:ARG:HH22	5:A:1321:GOL:H32	1.75	0.50
1:D:267:LYS:HD2	1:D:270:TYR:HE2	1.76	0.50
1:A:138:ILE:HG22	1:A:152:VAL:HG12	1.92	0.50
1:C:200:LEU:HD13	1:C:209:ILE:HG12	1.94	0.50
1:C:19:THR:HG22	1:C:63:THR:HB	1.94	0.50
1:D:291:LEU:O	1:D:292:LYS:CG	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176[A]:ASN:HD21	1:C:179:LEU:HD23	1.77	0.50
1:C:221:LEU:HD12	1:C:251:ILE:HG23	1.93	0.50
1:C:273:LYS:H	1:C:276:PRO:HG3	1.77	0.49
1:B:160:ASN:HD22	1:B:190:VAL:HG22	1.77	0.49
1:D:136:VAL:HG13	1:D:167:ILE:HG12	1.94	0.48
1:D:161:LYS:HE3	1:D:188:GLU:O	2.12	0.48
1:B:164:LYS:HD2	5:B:1318:GOL:H12	1.94	0.48
1:D:26:ARG:HH11	1:D:26:ARG:HB3	1.78	0.48
1:C:271:LYS:CB	1:C:272:PRO:CD	2.89	0.48
1:C:148:ASP:HA	1:C:151:LYS:HD3	1.96	0.47
1:D:291:LEU:O	1:D:292:LYS:CB	2.60	0.47
1:C:29:SER:HB2	1:C:32:VAL:CG1	2.45	0.47
1:D:16:ILE:H	1:D:16:ILE:HG13	1.49	0.47
1:B:242:LEU:HB3	1:B:251:ILE:HD11	1.96	0.47
1:D:227:ASP:OD1	1:D:231:PRO:HA	2.15	0.47
1:D:41:ASN:C	1:D:41:ASN:HD22	2.18	0.47
1:C:9:ASP:O	1:C:10:SER:HB3	2.14	0.47
1:D:257:TYR:HA	1:D:278:TRP:CZ2	2.49	0.47
1:D:296:VAL:HG13	1:D:300:VAL:CG1	2.45	0.47
1:D:267:LYS:HA	1:D:268:PRO:HD3	1.80	0.47
1:A:82:VAL:HG12	1:A:83:VAL:H	1.80	0.46
1:B:45:GLU:HG2	1:B:260:THR:HG21	1.97	0.46
1:C:14:LYS:HA	1:C:310:LYS:HE2	1.97	0.46
1:C:138:ILE:HG22	1:C:152:VAL:HG12	1.96	0.46
1:B:55:ARG:HG2	1:B:281:THR:HG21	1.97	0.46
1:D:14:LYS:HA	1:D:310:LYS:CD	2.38	0.46
1:A:29[A]:SER:HB2	1:A:32:VAL:HG13	1.97	0.46
1:C:88:ILE:HG13	1:C:89:ASN:N	2.31	0.46
1:D:221:LEU:HB2	1:D:253:ILE:HD13	1.98	0.46
1:C:50:VAL:O	1:C:54[A]:LYS:HG2	2.15	0.46
1:D:255:HIS:CE1	1:D:283:ILE:HB	2.50	0.45
1:C:199:HIS:O	1:C:220:GLY:O	2.34	0.45
1:D:255:HIS:NE2	1:D:283:ILE:HB	2.31	0.45
1:D:76:ILE:HG13	1:D:127:GLN:NE2	2.30	0.45
1:B:2:ARG:HB2	1:B:12:GLU:O	2.15	0.45
1:D:3:ILE:HD11	1:D:313:PHE:HB3	1.98	0.45
1:A:82:VAL:O	1:A:83:VAL:HB	2.16	0.45
1:B:303:THR:HA	1:B:307:GLU:HB2	1.99	0.45
1:C:296:VAL:HG23	1:C:300:VAL:HB	1.98	0.45
1:A:307:GLU:HG3	1:A:311:LYS:HE3	1.98	0.45
1:B:138:ILE:HG12	1:B:167:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:HG22	1:B:152:VAL:HG12	1.98	0.45
1:B:55:ARG:NH1	1:B:281:THR:OG1	2.50	0.45
1:D:102:LEU:HB2	1:D:103:PRO:HD2	1.98	0.44
1:D:288:ILE:O	1:D:291:LEU:O	2.35	0.44
1:D:76:ILE:HD12	1:D:77:ARG:HD2	1.98	0.44
1:D:77:ARG:O	1:D:81:LYS:HB2	2.17	0.44
1:D:110:SER:HB3	1:D:113:GLU:HG3	1.98	0.44
1:A:172:ASN:HB3	1:A:175:ASN:ND2	2.32	0.44
1:C:26:ARG:HB2	1:C:260:THR:HG22	1.99	0.44
1:C:173:ALA:HB2	1:C:200:LEU:HA	1.99	0.44
1:A:298:GLU:O	1:A:301:ILE:HD13	2.18	0.44
1:D:26:ARG:CB	1:D:26:ARG:HH11	2.31	0.44
1:D:267:LYS:HD2	1:D:270:TYR:CE2	2.52	0.44
1:B:222:ASP:HA	1:B:254:SER:H	1.83	0.43
1:C:129:THR:HG22	1:C:130:LEU:H	1.83	0.43
1:D:3:ILE:CD1	1:D:313:PHE:HB3	2.48	0.43
1:D:7:GLY:H	1:D:131:ASN:ND2	2.17	0.43
1:D:267:LYS:HB3	1:D:270:TYR:CD2	2.53	0.43
1:A:67:PRO:HB2	1:A:137:KCX:HG2	2.00	0.43
1:C:52:GLU:HG3	1:C:280:ILE:CG2	2.48	0.43
1:B:298[B]:GLU:OE1	1:B:301:ILE:HD11	2.19	0.43
1:D:200:LEU:HD11	1:D:219:ILE:HB	2.01	0.43
1:D:236:ASN:HB3	1:D:290:PHE:CE2	2.53	0.43
1:A:2:ARG:NE	1:A:2:ARG:HA	2.34	0.43
1:C:29:SER:HB2	1:C:32:VAL:HG12	2.01	0.43
1:B:67:PRO:HB2	1:B:137:KCX:HG2	2.01	0.42
1:B:269:GLU:HG3	1:B:269:GLU:H	1.73	0.42
1:C:95:GLY:HA2	1:C:118:PHE:CE1	2.55	0.42
1:D:267:LYS:HB3	1:D:270:TYR:CE2	2.54	0.42
1:A:65:VAL:HB	1:A:91:VAL:HB	2.01	0.42
1:B:104:PHE:H	4:B:1324:EDO:H12	1.84	0.42
1:B:206:ILE:HD13	1:B:241:ARG:HD3	2.00	0.42
1:B:275:ALA:HB1	1:B:278:TRP:HB2	2.01	0.42
1:B:25:LEU:HD13	1:B:82:VAL:HG11	2.00	0.42
1:C:98:ILE:HD13	1:C:102:LEU:HD13	2.02	0.42
1:B:167:ILE:HD11	1:B:169:THR:HG22	2.02	0.41
1:C:242:LEU:O	1:C:247:TYR:HB2	2.20	0.41
1:C:137:KCX:OQ1	1:C:170:HIS:HB2	2.20	0.41
1:A:137:KCX:OQ1	1:A:170:HIS:HB2	2.20	0.41
1:A:255:HIS:CE1	1:A:283:ILE:HG12	2.56	0.41
1:D:108:ASN:O	1:D:109:ARG:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ASP:HA	1:C:254:SER:H	1.85	0.41
1:B:25:LEU:HD11	1:B:90:LEU:HD11	2.03	0.41
1:C:277:ARG:O	1:C:282:LEU:HG	2.21	0.41
1:D:236:ASN:O	1:D:237:GLU:HB3	2.20	0.41
1:D:297:ASN:H	1:D:297:ASN:HD22	1.68	0.41
1:B:29:SER:HB2	1:B:32:VAL:CG1	2.51	0.41
1:A:130:LEU:O	1:A:132:LYS:HD2	2.21	0.41
1:D:45:GLU:HG2	1:D:260:THR:HG21	2.03	0.40
1:A:191:ASP:HA	1:A:192:PRO:HD2	1.90	0.40
1:C:140:ALA:O	1:C:171:SER:HA	2.21	0.40
1:D:98:ILE:HD13	1:D:102:LEU:HB3	2.03	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	313/314 (100%)	293 (94%)	18 (6%)	2 (1%)	27	51
1	B	314/314 (100%)	299 (95%)	10 (3%)	5 (2%)	11	21
1	C	315/314 (100%)	290 (92%)	21 (7%)	4 (1%)	13	27
1	D	312/314 (99%)	284 (91%)	21 (7%)	7 (2%)	7	13
All	All	1254/1256 (100%)	1166 (93%)	70 (6%)	18 (1%)	12	24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	B	2	ARG
1	B	13	SER
1	C	10	SER

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Mol	Chain	Res	Type
1	C	55	ARG
1	C	241	ARG
1	D	109	ARG
1	D	237	GLU
1	B	205	ASN
1	D	205	ASN
1	D	266	ALA
1	A	2	ARG
1	B	273	LYS
1	C	275	ALA
1	D	144	GLY
1	D	267	LYS
1	B	130	LEU
1	D	143	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	274/272 (101%)	255 (93%)	19 (7%)	17	34
1	B	275/272 (101%)	250 (91%)	25 (9%)	10	20
1	C	276/272 (102%)	255 (92%)	21 (8%)	14	28
1	D	273/272 (100%)	253 (93%)	20 (7%)	15	31
All	All	1098/1088 (101%)	1013 (92%)	85 (8%)	15	27

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ASP
1	A	14	LYS
1	A	26	ARG
1	A	32	VAL
1	A	65	VAL
1	A	132	LYS

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Mol	Chain	Res	Type
1	A	136	VAL
1	A	141	ASP
1	A	147	LYS
1	A	150	GLU
1	A	175	ASN
1	A	200	LEU
1	A	211	LYS
1	A	254	SER
1	A	261	ILE
1	A	282	LEU
1	A	296	VAL
1	A	301	ILE
1	B	26	ARG
1	B	27	VAL
1	B	32	VAL
1	B	39	LEU
1	B	41	ASN
1	B	81	LYS
1	B	86	THR
1	B	90	LEU
1	B	102	LEU
1	B	107	LEU
1	B	136	VAL
1	B	141	ASP
1	B	147	LYS
1	B	162[A]	GLU
1	B	162[B]	GLU
1	B	167	ILE
1	B	200	LEU
1	B	228	LEU
1	B	241	ARG
1	B	250	LYS
1	B	253	ILE
1	B	254	SER
1	B	269	GLU
1	B	298[A]	GLU
1	B	298[B]	GLU
1	C	2[A]	ARG
1	C	2[B]	ARG
1	C	19	THR
1	C	26	ARG
1	C	27	VAL

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Mol	Chain	Res	Type
1	C	32	VAL
1	C	42	GLU
1	C	65	VAL
1	C	81	LYS
1	C	90	LEU
1	C	102	LEU
1	C	141	ASP
1	C	188[A]	GLU
1	C	188[B]	GLU
1	C	196	LEU
1	C	206	ILE
1	C	254	SER
1	C	260	THR
1	C	269	GLU
1	C	282	LEU
1	C	296	VAL
1	D	1	MET
1	D	15	ASP
1	D	16	ILE
1	D	26	ARG
1	D	27	VAL
1	D	32	VAL
1	D	41	ASN
1	D	51	ASN
1	D	81	LYS
1	D	82	VAL
1	D	84	LYS
1	D	109	ARG
1	D	141	ASP
1	D	147	LYS
1	D	196	LEU
1	D	207	ASP
1	D	254	SER
1	D	283	ILE
1	D	297	ASN
1	D	300	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	160	ASN

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Mol	Chain	Res	Type
1	A	175	ASN
1	A	236	ASN
1	B	41	ASN
1	B	160	ASN
1	C	160	ASN
1	C	236	ASN
1	D	41	ASN
1	D	58	GLN
1	D	127	GLN
1	D	131	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	A	137	1,3,2	8,11,12	1.09	2 (25%)	6,12,14	0.90	0
1	KCX	B	137	1,3,2	8,11,12	1.13	1 (12%)	6,12,14	0.81	0
1	KCX	C	137	1,3,2	8,11,12	1.01	0	6,12,14	0.98	0
1	KCX	D	137	1,3,2	8,11,12	1.13	1 (12%)	6,12,14	0.83	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
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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	KCX	CE-NZ	2.01	1.50	1.45
1	A	137	KCX	CA-C	2.04	1.52	1.50
1	D	137	KCX	CA-C	2.31	1.53	1.50
1	B	137	KCX	CA-C	2.44	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 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	1317	-	3,3,3	0.44	0	2,2,2	0.37	0
5	GOL	A	1318	-	5,5,5	0.38	0	5,5,5	0.27	0
4	EDO	A	1319	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	A	1320	-	3,3,3	0.45	0	2,2,2	0.45	0
5	GOL	A	1321	-	5,5,5	0.37	0	5,5,5	0.19	0
4	EDO	B	1317	-	3,3,3	0.47	0	2,2,2	0.37	0
5	GOL	B	1318	-	5,5,5	0.36	0	5,5,5	0.42	0
5	GOL	B	1319	-	5,5,5	0.34	0	5,5,5	0.35	0
5	GOL	B	1320	-	5,5,5	0.37	0	5,5,5	0.23	0
4	EDO	B	1321	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	B	1322	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	B	1323	-	3,3,3	0.48	0	2,2,2	0.36	0
4	EDO	B	1324	-	3,3,3	0.83	0	2,2,2	0.63	0
4	EDO	C	1317	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	C	1318	-	3,3,3	0.49	0	2,2,2	0.32	0
4	EDO	C	1319	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	D	1317	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	D	1318	-	3,3,3	0.45	0	2,2,2	0.40	0
5	GOL	D	1319	-	5,5,5	0.35	0	5,5,5	0.32	0
4	EDO	D	1320	-	3,3,3	0.48	0	2,2,2	0.38	0
4	EDO	D	1321	-	3,3,3	0.48	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
4	EDO	A	1317	-	-	0/1/1/1	0/0/0/0
5	GOL	A	1318	-	-	0/4/4/4	0/0/0/0
4	EDO	A	1319	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1320	-	-	0/1/1/1	0/0/0/0
5	GOL	A	1321	-	-	0/4/4/4	0/0/0/0
4	EDO	B	1317	-	-	0/1/1/1	0/0/0/0
5	GOL	B	1318	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1319	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1320	-	-	0/4/4/4	0/0/0/0
4	EDO	B	1321	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1322	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1323	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1324	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1317	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1318	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	1319	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1317	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1318	-	-	0/1/1/1	0/0/0/0
5	GOL	D	1319	-	-	0/4/4/4	0/0/0/0
4	EDO	D	1320	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1321	-	-	0/1/1/1	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.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1317	EDO	1	0
5	A	1321	GOL	2	0
5	B	1318	GOL	2	0
4	B	1324	EDO	2	0
4	D	1318	EDO	1	0
5	D	1319	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	313/314 (99%)	-0.20	0 <b>100</b> <b>100</b>	24, 32, 45, 50	1 (0%)
1	B	313/314 (99%)	-0.16	2 (0%) <b>89</b> <b>88</b>	24, 37, 48, 53	1 (0%)
1	C	313/314 (99%)	-0.10	3 (0%) <b>82</b> <b>79</b>	27, 38, 50, 56	1 (0%)
1	D	313/314 (99%)	0.12	3 (0%) <b>82</b> <b>79</b>	28, 46, 56, 59	0
All	All	1252/1256 (99%)	-0.08	8 (0%) <b>89</b> <b>88</b>	24, 38, 53, 59	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	LYS	2.3
1	D	176	ASN	2.3
1	D	274	LEU	2.2
1	B	273	LYS	2.2
1	C	229	PHE	2.2
1	B	129	THR	2.1
1	D	282	LEU	2.1
1	C	1	MET	2.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	D	137	12/13	0.93	0.17	39,40,41,41	0
1	KCX	C	137	12/13	0.95	0.14	26,28,30,31	0
1	KCX	A	137	12/13	0.97	0.14	24,25,25,25	0
1	KCX	B	137	12/13	0.98	0.15	27,29,30,30	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	1321	4/4	0.65	0.44	77,77,77,77	0
4	EDO	C	1318	4/4	0.72	0.27	45,45,45,45	0
4	EDO	B	1324	4/4	0.72	0.39	76,76,76,76	0
4	EDO	D	1320	4/4	0.77	0.19	48,48,48,48	0
4	EDO	B	1323	4/4	0.78	0.28	44,45,45,45	0
4	EDO	C	1319	4/4	0.80	0.19	51,51,51,51	0
4	EDO	B	1317	4/4	0.82	0.20	44,44,44,44	0
5	GOL	D	1319	6/6	0.86	0.18	61,61,61,61	0
4	EDO	D	1318	4/4	0.89	0.19	39,40,40,40	0
4	EDO	A	1319	4/4	0.89	0.13	46,46,46,46	0
5	GOL	B	1318	6/6	0.89	0.24	46,46,46,46	0
5	GOL	A	1321	6/6	0.90	0.37	45,45,45,45	0
4	EDO	C	1317	4/4	0.90	0.24	50,50,50,50	0
4	EDO	D	1321	4/4	0.90	0.14	46,46,47,47	0
4	EDO	D	1317	4/4	0.90	0.16	45,45,45,46	0
4	EDO	A	1320	4/4	0.91	0.15	49,49,49,50	0
4	EDO	B	1322	4/4	0.91	0.18	47,47,47,47	0
5	GOL	B	1320	6/6	0.94	0.26	50,50,50,50	0
4	EDO	A	1317	4/4	0.94	0.16	35,35,36,36	0
5	GOL	A	1318	6/6	0.94	0.18	43,43,43,43	0
5	GOL	B	1319	6/6	0.94	0.21	32,32,33,33	0
2	FE	A	1315	1/1	0.98	0.11	20,20,20,20	0
2	FE	C	1315	1/1	0.99	0.11	25,25,25,25	0
3	CO	B	1316	1/1	0.99	0.13	29,29,29,29	0
3	CO	C	1316	1/1	0.99	0.11	28,28,28,28	0
3	CO	D	1316	1/1	0.99	0.10	33,33,33,33	0
2	FE	D	1315	1/1	0.99	0.10	34,34,34,34	0
3	CO	A	1316	1/1	1.00	0.09	28,28,28,28	0
2	FE	B	1315	1/1	1.00	0.09	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.