



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 03:43 AM GMT

PDB ID : 2VC5  
Title : STRUCTURAL BASIS FOR NATURAL LACTONASE AND PROMISCU-  
OUS 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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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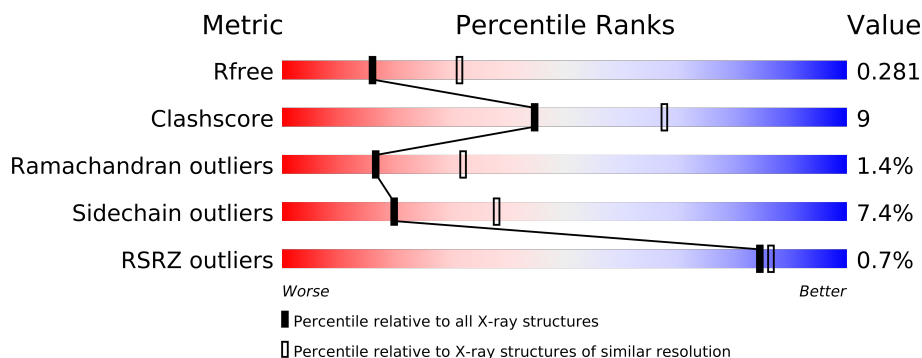
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	C	314	
1	D	314	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	B	1321	-	X
4	EDO	B	1324	-	X
4	EDO	C	1317	-	X
4	EDO	D	1320	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	A	1321	-	X
5	GOL	B	1318	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10475 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

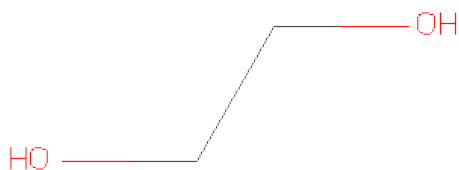
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



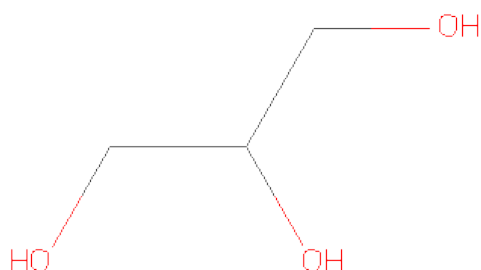
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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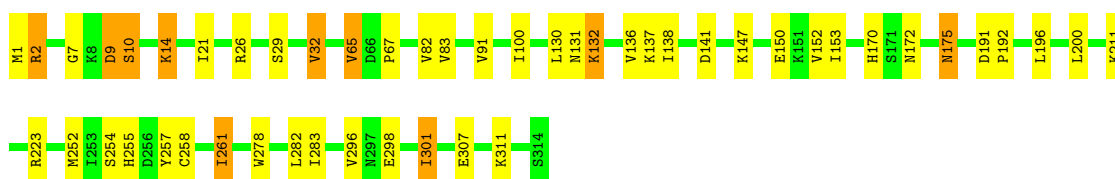
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	62	Total 62	O 62	0	0
6	C	55	Total 55	O 55	0	0
6	D	61	Total 61	O 61	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

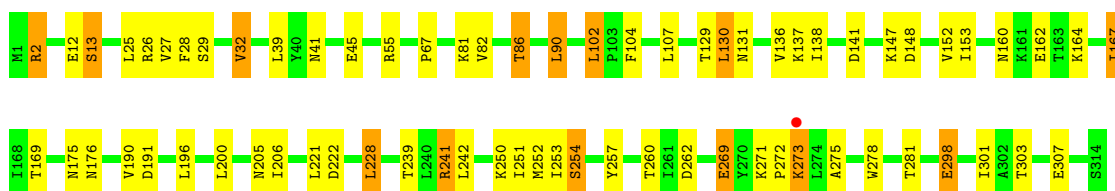
#### • Molecule 1: ARYLDIALKYLPHOSPHATASE

Chain A:



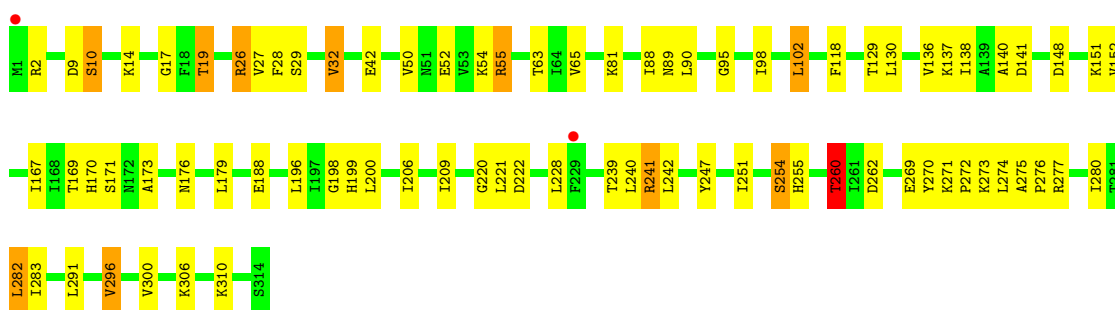
#### • Molecule 1: ARYLDIALKYLPHOSPHATASE

Chain B:



#### • Molecule 1: ARYLDIALKYLPHOSPHATASE

Chain C:

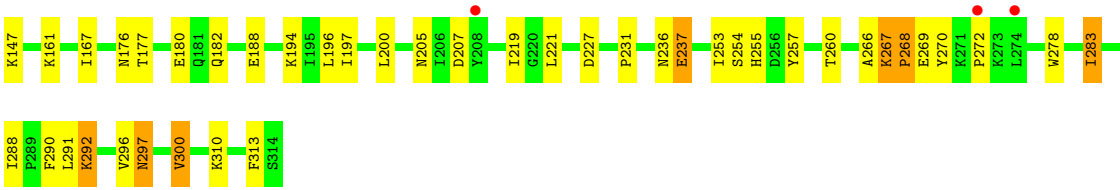


#### • Molecule 1: ARYLDIALKYLPHOSPHATASE

Chain D:







## 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 0.223 , 0.281	Depositor DCC
$R_{free}$ test set	2234 reflections (5.30%)	DCC
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 , 17.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 44355 reflections (0.002%)	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (176) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:292:LYS:HB2	1:D:296:VAL:O	2.02	0.59
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:D:177:THR:HA	1:D:180[B]:GLU:HG3	1.87	0.57
1:A:7:GLY:H	1:A:131:ASN:ND2	2.03	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:D:100:ILE:H	4:D:1318:EDO:H12	1.71	0.56
1:A:21:ILE:HA	1:A:65:VAL:HG13	1.87	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:D:41:ASN:HD22	1:D:44:GLU:H	1.55	0.54
1:C:136:VAL:HG13	1:C:167:ILE:HG12	1.90	0.54
1:C:169:THR:O	1:C:198:GLY:HA3	2.07	0.54
1:B:12:GLU:O	1:B:13:SER:HB3	2.08	0.53
1:B:191:ASP:HB3	5:B:1318:GOL:H32	1.90	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:29:SER:HB2	1:B:32:VAL:HG13	1.90	0.52
1:B:257:TYR:HA	1:B:278:TRP:CZ2	2.44	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	Distance(Å)	Clash(Å)
1:C:221:LEU:HD12	1:C:251:ILE:HG23	1.93	0.50
1:C:176[A]:ASN:HD21	1:C:179:LEU:HD23	1.77	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:161:LYS:HE3	1:D:188:GLU:O	2.12	0.48
1:D:136:VAL:HG13	1:D:167:ILE:HG12	1.94	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:D:291:LEU:O	1:D:292:LYS:CB	2.60	0.47
1:C:148:ASP:HA	1:C:151:LYS:HD3	1.96	0.47
1:D:16:ILE:HG13	1:D:16:ILE:H	1.49	0.47
1:C:29:SER:HB2	1:C:32:VAL:CG1	2.45	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:D:296:VAL:HG13	1:D:300:VAL:CG1	2.45	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: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: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:45:GLU:HG2	1:B:260:THR:HG21	1.97	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:C:88:ILE:HG13	1:C:89:ASN:N	2.31	0.46
1:A:29[A]:SER:HB2	1:A:32:VAL:HG13	1.97	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:D:255:HIS:NE2	1:D:283:ILE:HB	2.31	0.45
1:C:199:HIS:O	1:C:220:GLY:O	2.34	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:C:296:VAL:HG23	1:C:300:VAL:HB	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:B:138:ILE:HG12	1:B:167:ILE:CD1	2.47	0.45
1:A:307:GLU:HG3	1:A:311:LYS:HE3	1.98	0.45
1:B:138:ILE:HG22	1:B:152:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:26:ARG:CB	1:D:26:ARG:HH11	2.31	0.44
1:A:298:GLU:O	1:A:301:ILE:HD13	2.18	0.44
1:D:267:LYS:HD2	1:D:270:TYR:CE2	2.52	0.44
1:C:129:THR:HG22	1:C:130:LEU:H	1.83	0.43
1:B:222:ASP:HA	1:B:254:SER: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:D:236:ASN:HB3	1:D:290:PHE:CE2	2.53	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:C:29:SER:HB2	1:C:32:VAL:HG12	2.01	0.43
1:A:2:ARG:HA	1:A:2:ARG:NE	2.34	0.43
1:D:267:LYS:HB3	1:D:270:TYR:CE2	2.54	0.42
1:B:269:GLU:HG3	1:B:269:GLU:H	1.73	0.42
1:B:67:PRO:HB2	1:B:137:KCX:HG2	2.01	0.42
1:C:95:GLY:HA2	1:C:118:PHE:CE1	2.55	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:25:LEU:HD13	1:B:82:VAL:HG11	2.00	0.42
1:B:275:ALA:HB1	1:B:278:TRP:HB2	2.01	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:D:108:ASN:O	1:D:109:ARG:O	2.38	0.41
1:A:255:HIS:CE1	1:A:283:ILE:HG12	2.56	0.41
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:277:ARG:O	1:C:282:LEU:HG	2.21	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

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/314 (100%)	293 (94%)	18 (6%)	2 (1%)	33	63
1	B	314/314 (100%)	299 (95%)	10 (3%)	5 (2%)	14	28
1	C	315/314 (100%)	290 (92%)	21 (7%)	4 (1%)	18	35
1	D	312/314 (99%)	284 (91%)	21 (7%)	7 (2%)	10	18
All	All	1254/1256 (100%)	1166 (93%)	70 (6%)	18 (1%)	16	32

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
1	C	55	ARG
1	C	241	ARG
1	D	109	ARG
1	D	237	GLU
1	B	205	ASN

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Mol	Chain	Res	Type
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%)	22	42
1	B	275/272 (101%)	250 (91%)	25 (9%)	14	25
1	C	276/272 (102%)	255 (92%)	21 (8%)	19	36
1	D	273/272 (100%)	253 (93%)	20 (7%)	20	38
All	All	1098/1088 (101%)	1013 (92%)	85 (8%)	20	35

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
1	A	136	VAL
1	A	141	ASP
1	A	147	LYS
1	A	150	GLU
1	A	175	ASN
1	A	200	LEU

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Mol	Chain	Res	Type
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
1	C	32	VAL
1	C	42	GLU
1	C	65	VAL
1	C	81	LYS
1	C	90	LEU
1	C	102	LEU

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Mol	Chain	Res	Type
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
1	A	175	ASN
1	A	236	ASN
1	B	41	ASN
1	B	160	ASN
1	C	160	ASN
1	C	236	ASN

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Mol	Chain	Res	Type
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 chains 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	11,11,12	5.55	2 (18%)	10,12,14	1.54	2 (20%)
1	KCX	B	137	1,3,2	11,11,12	5.47	2 (18%)	10,12,14	1.37	2 (20%)
1	KCX	C	137	1,3,2	11,11,12	5.53	2 (18%)	10,12,14	1.58	4 (40%)
1	KCX	D	137	1,3,2	11,11,12	5.46	2 (18%)	10,12,14	1.44	2 (20%)

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	-	0/8/10/12	0/0/0/0
1	KCX	B	137	1,3,2	-	0/8/10/12	0/0/0/0
1	KCX	C	137	1,3,2	-	0/8/10/12	0/0/0/0
1	KCX	D	137	1,3,2	-	0/8/10/12	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	KCX	O-C	18.01	1.23	1.11
1	C	137	KCX	O-C	18.00	1.23	1.11
1	B	137	KCX	O-C	17.75	1.23	1.11
1	D	137	KCX	O-C	17.71	1.23	1.11
1	B	137	KCX	CA-C	2.75	1.53	1.48
1	D	137	KCX	CA-C	2.67	1.53	1.48
1	A	137	KCX	CA-C	2.49	1.52	1.48
1	C	137	KCX	CA-C	2.40	1.52	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	KCX	OQ2-CX-OQ1	-2.85	118.60	122.17
1	A	137	KCX	OQ2-CX-NZ	2.72	119.72	116.33
1	C	137	KCX	C-CA-N	-2.70	111.13	113.83
1	D	137	KCX	OQ2-CX-OQ1	-2.57	118.95	122.17
1	C	137	KCX	OQ2-CX-NZ	2.54	119.49	116.33
1	D	137	KCX	OQ2-CX-NZ	2.48	119.41	116.33
1	C	137	KCX	OQ2-CX-OQ1	-2.46	119.09	122.17
1	B	137	KCX	OQ2-CX-OQ1	-2.45	119.11	122.17
1	B	137	KCX	OQ2-CX-NZ	2.27	119.15	116.33
1	C	137	KCX	OQ1-CX-NZ	-2.12	121.42	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.51	0	2,2,2	0.38	0
5	GOL	A	1318	-	5,5,5	0.36	0	5,5,5	0.24	0
4	EDO	A	1319	-	3,3,3	0.54	0	2,2,2	0.34	0
4	EDO	A	1320	-	3,3,3	0.52	0	2,2,2	0.46	0
5	GOL	A	1321	-	5,5,5	0.35	0	5,5,5	0.20	0
4	EDO	B	1317	-	3,3,3	0.54	0	2,2,2	0.38	0
5	GOL	B	1318	-	5,5,5	0.34	0	5,5,5	0.38	0
5	GOL	B	1319	-	5,5,5	0.31	0	5,5,5	0.37	0
5	GOL	B	1320	-	5,5,5	0.33	0	5,5,5	0.28	0
4	EDO	B	1321	-	3,3,3	0.55	0	2,2,2	0.38	0
4	EDO	B	1322	-	3,3,3	0.54	0	2,2,2	0.37	0
4	EDO	B	1323	-	3,3,3	0.55	0	2,2,2	0.37	0
4	EDO	B	1324	-	3,3,3	0.87	0	2,2,2	0.64	0
4	EDO	C	1317	-	3,3,3	0.52	0	2,2,2	0.41	0
4	EDO	C	1318	-	3,3,3	0.56	0	2,2,2	0.33	0
4	EDO	C	1319	-	3,3,3	0.55	0	2,2,2	0.38	0
4	EDO	D	1317	-	3,3,3	0.53	0	2,2,2	0.36	0
4	EDO	D	1318	-	3,3,3	0.52	0	2,2,2	0.41	0
5	GOL	D	1319	-	5,5,5	0.33	0	5,5,5	0.31	0
4	EDO	D	1320	-	3,3,3	0.55	0	2,2,2	0.39	0
4	EDO	D	1321	-	3,3,3	0.55	0	2,2,2	0.37	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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	314/314 (100%)	-0.18	0 100 100	24, 32, 45, 50	1 (0%)
1	B	314/314 (100%)	-0.12	1 (0%) 91 92	24, 37, 48, 53	1 (0%)
1	C	314/314 (100%)	-0.07	2 (0%) 86 89	27, 38, 50, 56	1 (0%)
1	D	314/314 (100%)	0.18	5 (1%) 68 69	28, 46, 56, 59	0
All	All	1256/1256 (100%)	-0.05	8 (0%) 84 89	24, 38, 53, 59	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	LEU	3.2
1	B	273	LYS	2.9
1	D	108	ASN	2.6
1	D	1	MET	2.6
1	C	1	MET	2.5
1	D	272	PRO	2.2
1	D	208	TYR	2.2
1	C	229	PHE	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. 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	C	137	12/13	0.14	-0.31	26,28,30,31	0
1	KCX	D	137	12/13	0.16	-0.52	39,40,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	B	137	12/13	0.14	-0.70	27,29,30,30	0
1	KCX	A	137	12/13	0.12	-1.02	24,25,25,25	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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	1321	6/6	0.34	7.51	45,45,45,45	0
4	EDO	B	1321	4/4	0.55	7.06	77,77,77,77	0
4	EDO	C	1317	4/4	0.22	3.70	50,50,50,50	0
4	EDO	B	1324	4/4	0.33	3.34	76,76,76,76	0
5	GOL	B	1318	6/6	0.24	2.52	46,46,46,46	0
4	EDO	D	1320	4/4	0.20	2.37	48,48,48,48	0
5	GOL	A	1318	6/6	0.19	1.92	43,43,43,43	0
5	GOL	B	1320	6/6	0.26	1.91	50,50,50,50	0
4	EDO	B	1323	4/4	0.27	1.70	44,45,45,45	0
4	EDO	C	1318	4/4	0.24	1.37	45,45,45,45	0
4	EDO	C	1319	4/4	0.23	0.92	51,51,51,51	0
5	GOL	B	1319	6/6	0.20	0.82	32,32,33,33	0
4	EDO	A	1320	4/4	0.20	0.56	49,49,49,50	0
5	GOL	D	1319	6/6	0.22	0.32	61,61,61,61	0
4	EDO	B	1317	4/4	0.19	-0.04	44,44,44,44	0
3	CO	B	1316	1/1	0.14	-0.41	29,29,29,29	0
4	EDO	A	1317	4/4	0.15	-0.68	35,35,36,36	0
4	EDO	B	1322	4/4	0.19	-0.81	47,47,47,47	0
2	FE	A	1315	1/1	0.12	-1.31	20,20,20,20	0
4	EDO	D	1317	4/4	0.14	-1.55	45,45,45,46	0
2	FE	C	1315	1/1	0.11	-1.65	25,25,25,25	0
4	EDO	D	1321	4/4	0.12	-2.04	46,46,47,47	0
3	CO	A	1316	1/1	0.09	-2.46	28,28,28,28	0
4	EDO	A	1319	4/4	0.11	-2.54	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE	D	1315	1/1	0.11	-2.66	34,34,34,34	0
3	CO	C	1316	1/1	0.10	-2.92	28,28,28,28	0
4	EDO	D	1318	4/4	0.15	-3.32	39,40,40,40	0
3	CO	D	1316	1/1	0.11	-3.35	33,33,33,33	0
2	FE	B	1315	1/1	0.10	-4.57	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.