Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 11:28 AM EDT

PDB ID	:	4KET
Title	:	Crystal structure of SsoPox W263I
Authors	:	Gotthard, G.; Hiblot, J.; Chabriere, E.; Elias, M.
Deposited on	:	2013-04-26
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

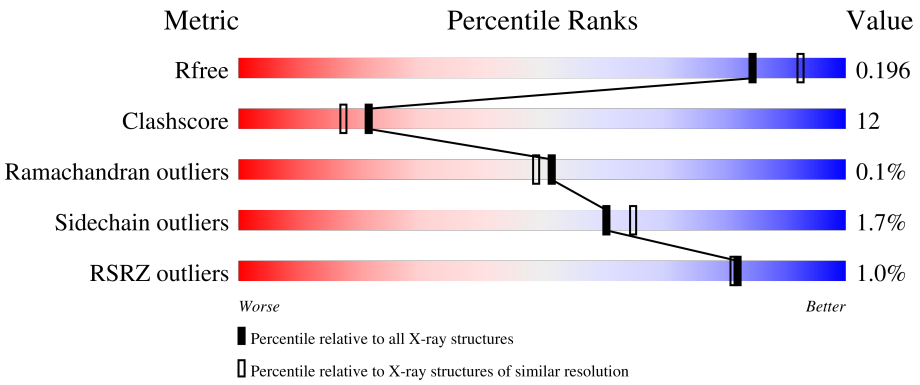
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	89% 10% •
1	B	314	2% 80% 19% •
1	C	314	2% 81% 17% •
1	D	314	% 83% 16% •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	405	-	-	X	-
6	PEG	B	407[B]	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11163 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
			Total	C	N	O	S			
1	A	314	2517	1615	426	469	7	0	2	0
1	B	314	2539	1631	430	471	7	0	6	0
1	C	314	2538	1631	429	471	7	0	6	0
1	D	314	2527	1621	429	470	7	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	ILE	TRP	ENGINEERED MUTATION	UNP Q97VT7
B	263	ILE	TRP	ENGINEERED MUTATION	UNP Q97VT7
C	263	ILE	TRP	ENGINEERED MUTATION	UNP Q97VT7
D	263	ILE	TRP	ENGINEERED MUTATION	UNP Q97VT7

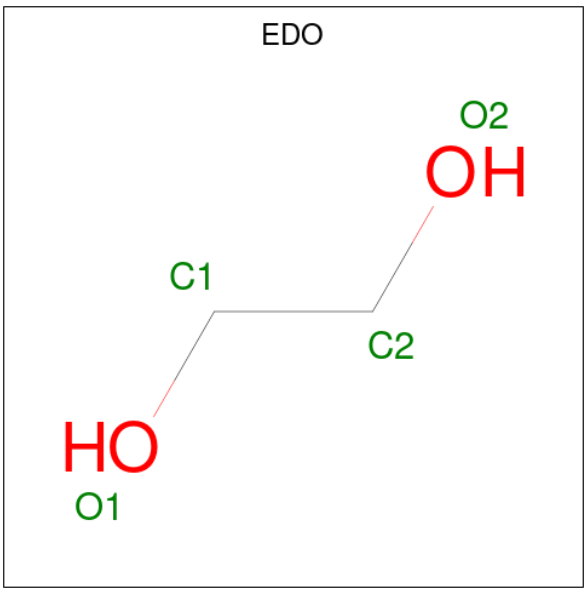
- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

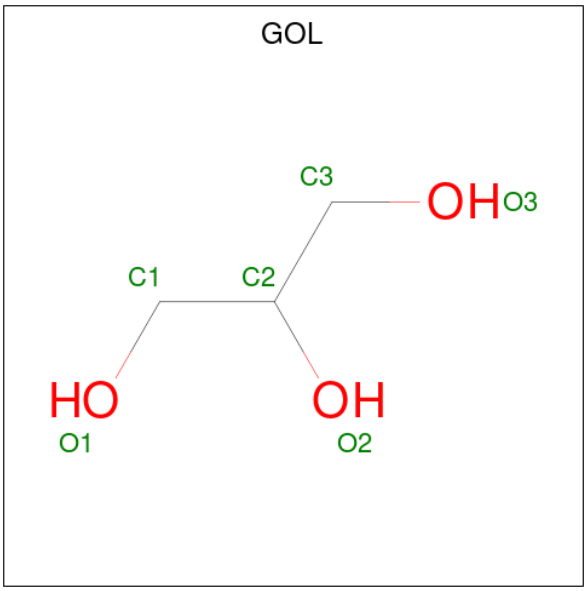
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co 1 1	0	0
3	B	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0
3	D	1	Total Co 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



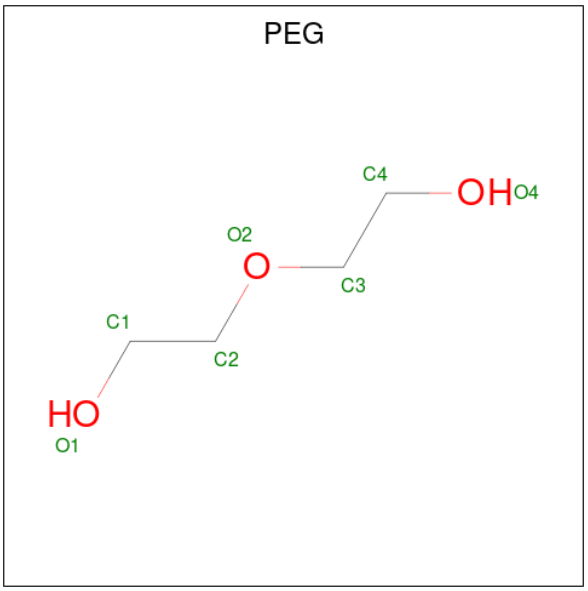
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



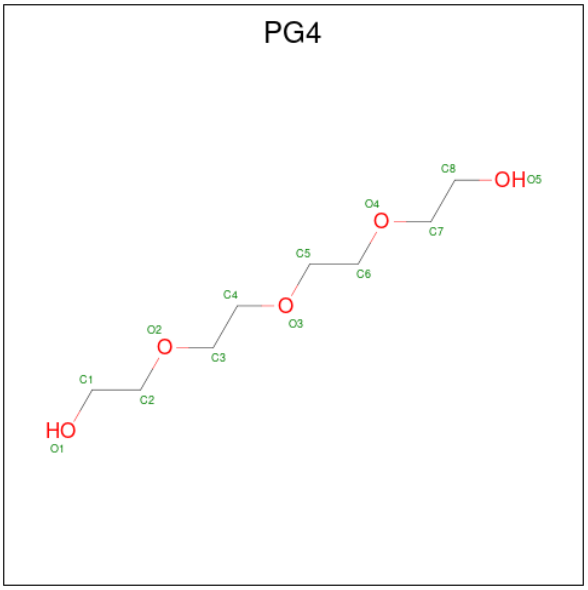
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
5	A	1	6	3	3	0	0
5	A	1	6	3	3	0	0
5	B	1	6	3	3	0	0
5	B	1	6	3	3	0	0
5	B	1	6	3	3	0	0
5	C	1	6	3	3	0	0
5	C	1	6	3	3	0	0
5	C	1	6	3	3	0	0
5	D	1	6	3	3	0	0
5	D	1	6	3	3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	14	8	6	0	1

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	13	8	5	0	0
			Total	C	O		
7	D	1	13	8	5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	220	220	220	0	0
			Total	O		
8	B	235	235	235	0	0
			Total	O		
8	C	222	222	222	0	0
			Total	O		
8	D	223	223	223	0	0

3 Residue-property plots (i)

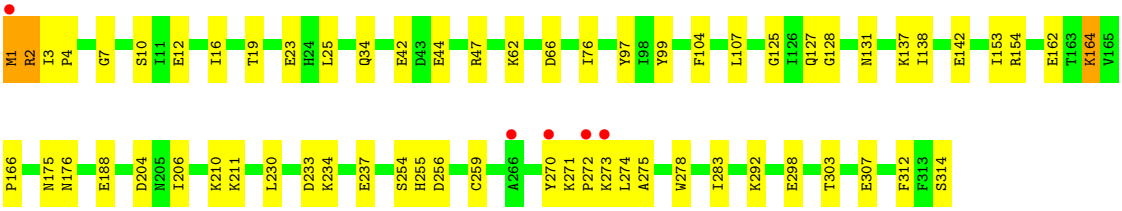
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Aryldialkylphosphatase

Chain A:

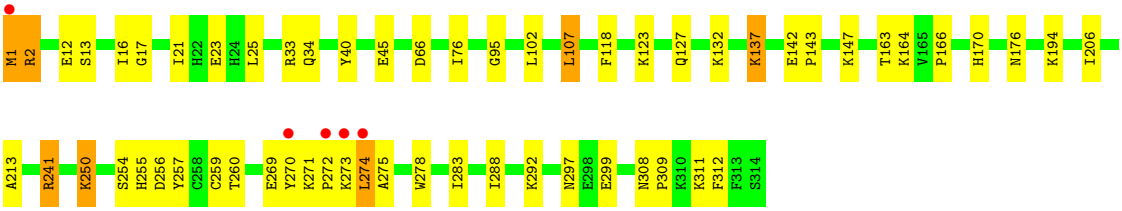
- Molecule 1: Aryldialkylphosphatase

Chain B:



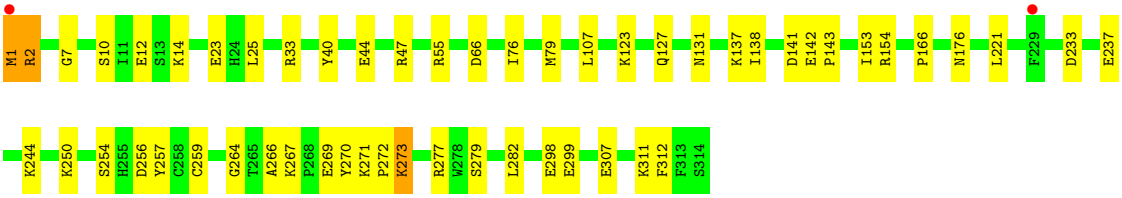
- Molecule 1: Aryldialkylphosphatase

Chain C:



- Molecule 1: Aryldialkylphosphatase

Chain D:


M1
R2
G7
S10
I11
E12
S13
K14
E23
H24
L25
R33
Y40
E44
R47
R55
D66
I76
M79
L107
K123
Q127
N131
K137
I138
D141
E142
P143
I153
R154
P166
N176
L221
F229
D233
E237
K244
K250
S254
H255
D256
Y257
C258
C259
G264
T265
A266
K267
P268
E269
Y270
K271
P272
K273
R277
W278
S279
L282
E298
E299
E307
K311
F312
F313
S314

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.40Å 103.90Å 150.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.66 – 2.00 44.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.66-2.00) 99.6 (44.66-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.190 0.151 , 0.196	Depositor DCC
R_{free} test set	4637 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11163	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PG4, FE2, CO, KCX, GOL, PEG, EDO

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	0.39	0/2559	0.50	1/3455 (0.0%)
1	B	0.39	0/2592	0.51	2/3493 (0.1%)
1	C	0.39	0/2591	0.49	1/3493 (0.0%)
1	D	0.38	0/2572	0.49	1/3470 (0.0%)
All	All	0.39	0/10314	0.50	5/13911 (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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	256	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	256	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	256	ASP	CB-CG-OD1	6.35	124.01	118.30
1	C	256	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	256	ASP	CB-CG-OD2	-5.32	113.51	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	221	LEU	Peptide

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	2517	0	2559	38	0
1	B	2539	0	2602	80	0
1	C	2538	0	2600	55	1
1	D	2527	0	2574	56	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	8	0	12	4	0
4	B	4	0	6	0	0
4	C	4	0	6	3	0
4	D	12	0	18	5	0
5	A	18	0	24	1	0
5	B	18	0	24	10	0
5	C	18	0	24	0	0
5	D	12	0	16	2	0
6	B	14	0	20	14	0
7	C	13	0	18	2	0
7	D	13	0	18	4	0
8	A	220	0	0	19	0
8	B	235	0	0	24	1
8	C	222	0	0	15	0
8	D	223	0	0	30	0
All	All	11163	0	10521	250	1

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 (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2[B]:ARG:HH11	1:B:2[B]:ARG:CB	1.21	1.48
1:B:2[B]:ARG:NH1	1:B:2[B]:ARG:HB3	1.24	1.42
7:D:404:PG4:H31	8:D:704:HOH:O	1.35	1.20
1:B:16[A]:ILE:HG23	8:B:719:HOH:O	1.40	1.20
1:D:307:GLU:HB2	8:D:713:HOH:O	1.35	1.19
4:D:403:EDO:H12	8:D:719:HOH:O	1.42	1.17
1:A:2:ARG:HG2	8:A:704:HOH:O	1.40	1.17
1:C:176:ASN:HB3	8:C:710:HOH:O	1.44	1.14
4:C:406:EDO:H21	8:C:706:HOH:O	1.51	1.09
1:D:1:MET:SD	1:D:1:MET:N	2.26	1.09
1:B:292:LYS:HE2	1:B:298:GLU:OE1	1.57	1.04
1:B:237:GLU:HG2	8:B:658:HOH:O	1.58	1.03
5:B:405:GOL:H32	8:B:722:HOH:O	1.59	1.02
1:B:3:ILE:CD1	1:B:16[C]:ILE:HD11	1.88	1.02
1:B:16[A]:ILE:CG2	8:B:719:HOH:O	2.00	1.01
1:D:1:MET:HG2	8:D:647:HOH:O	1.60	0.99
1:C:1:MET:SD	1:C:1:MET:N	2.36	0.99
1:B:62[A]:LYS:HE2	8:B:717:HOH:O	1.60	0.99
1:B:44:GLU:HG2	8:B:600:HOH:O	1.60	0.98
1:C:271:LYS:HA	8:C:707:HOH:O	1.61	0.98
1:B:128:GLY:H	6:B:407[B]:PEG:H12	1.27	0.96
1:B:128:GLY:N	6:B:407[B]:PEG:H12	1.86	0.90
1:B:2[B]:ARG:HH11	1:B:2[B]:ARG:CG	1.83	0.89
1:C:102:LEU:O	4:C:406:EDO:H22	1.73	0.88
1:A:194:LYS:HD2	8:A:705:HOH:O	1.75	0.86
1:B:42:GLU:HG2	8:B:724:HOH:O	1.77	0.84
1:A:194:LYS:CD	8:A:705:HOH:O	2.24	0.84
1:D:277:ARG:HD2	8:D:581:HOH:O	1.78	0.84
1:B:128:GLY:H	6:B:407[B]:PEG:C1	1.90	0.83
1:B:2[B]:ARG:NH2	1:B:314[B]:SER:HA	1.95	0.81
1:A:142:GLU:HG2	8:A:586:HOH:O	1.79	0.81
1:B:128:GLY:HA2	6:B:407[A]:PEG:H12	1.62	0.81
1:B:292:LYS:CE	1:B:298:GLU:OE1	2.30	0.80
1:B:16[A]:ILE:HG22	8:B:590:HOH:O	1.83	0.78
1:C:297:ASN:HD22	1:C:299:GLU:H	1.28	0.78
1:A:273:LYS:HG3	8:A:701:HOH:O	1.83	0.77
1:B:2[B]:ARG:CB	1:B:2[B]:ARG:NH1	2.05	0.77
1:A:16[B]:ILE:HD12	1:A:17:GLY:N	2.00	0.76
1:B:3:ILE:HD11	1:B:16[C]:ILE:HD11	1.67	0.76
1:C:311:LYS:HG3	8:C:589:HOH:O	1.85	0.76
6:B:407[B]:PEG:H31	8:B:656:HOH:O	1.85	0.76
1:B:1:MET:HE1	8:C:679:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:MET:HE3	8:D:514:HOH:O	1.87	0.74
1:D:79:MET:CE	8:D:514:HOH:O	2.35	0.74
1:B:162:GLU:HG2	8:B:611:HOH:O	1.88	0.73
1:D:299:GLU:HG3	8:D:551:HOH:O	1.88	0.73
1:B:164[B]:LYS:HE3	8:B:732:HOH:O	1.89	0.73
5:B:405:GOL:H12	8:B:729:HOH:O	1.89	0.73
5:D:407:GOL:H31	8:D:706:HOH:O	1.89	0.72
5:A:406:GOL:H12	8:A:711:HOH:O	1.88	0.72
1:C:273:LYS:HG3	1:C:274:LEU:HD13	1.72	0.71
1:C:1:MET:HE2	1:C:12:GLU:OE1	1.89	0.71
1:A:2:ARG:CB	8:A:547:HOH:O	2.38	0.70
1:B:128:GLY:CA	6:B:407[A]:PEG:H12	2.21	0.70
4:D:403:EDO:C1	8:D:719:HOH:O	2.17	0.70
1:B:107:LEU:HD12	8:B:575:HOH:O	1.91	0.70
1:D:250:LYS:HE3	4:D:408:EDO:H22	1.71	0.70
1:C:270:TYR:HB3	1:C:274:LEU:HD22	1.73	0.70
1:D:270:TYR:HA	1:D:273[B]:LYS:HE2	1.74	0.70
1:B:2[B]:ARG:HH11	1:B:2[B]:ARG:HB3	0.55	0.69
1:C:16[A]:ILE:HD12	1:C:17:GLY:N	2.08	0.69
1:B:104:PHE:HA	1:B:107:LEU:HD13	1.75	0.68
1:D:250:LYS:CE	4:D:408:EDO:H22	2.23	0.67
1:B:76:ILE:H	1:B:127:GLN:NE2	1.92	0.67
1:B:107:LEU:CD1	8:B:575:HOH:O	2.42	0.67
1:C:288:ILE:HG22	1:C:292:LYS:HE2	1.76	0.67
1:A:7:GLY:H	1:A:131:ASN:ND2	1.92	0.67
1:B:76:ILE:H	1:B:127:GLN:HE22	1.43	0.66
1:B:125:GLY:CA	6:B:407[B]:PEG:H22	2.25	0.66
1:B:142:GLU:HB3	8:B:633:HOH:O	1.94	0.66
1:A:1:MET:HB3	1:A:10:SER:OG	1.96	0.66
1:D:269:GLU:O	1:D:273[B]:LYS:NZ	2.23	0.65
1:C:16[A]:ILE:HD12	1:C:17:GLY:O	1.96	0.65
1:C:76:ILE:H	1:C:127:GLN:NE2	1.93	0.65
1:D:44:GLU:HG2	1:D:47:ARG:NH2	2.11	0.64
5:B:405:GOL:C1	8:B:729:HOH:O	2.45	0.64
1:C:76:ILE:H	1:C:127:GLN:HE22	1.45	0.64
1:C:1:MET:CE	1:C:12:GLU:OE1	2.46	0.64
4:A:407:EDO:H21	7:C:404:PG4:H11	1.80	0.63
1:D:1:MET:O	1:D:2[A]:ARG:HB2	1.96	0.63
5:D:407:GOL:C3	8:D:706:HOH:O	2.47	0.63
1:B:44:GLU:CG	8:B:600:HOH:O	2.30	0.63
1:B:154:ARG:NH2	1:B:188:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ARG:HD3	8:D:717:HOH:O	1.97	0.62
1:A:194:LYS:HD3	8:A:705:HOH:O	1.94	0.62
1:A:292:LYS:CE	8:A:608:HOH:O	2.46	0.62
5:B:405:GOL:H11	8:B:685:HOH:O	1.99	0.62
1:A:16[A]:ILE:HG22	8:A:595:HOH:O	1.99	0.62
1:B:1:MET:HB2	1:B:12:GLU:HG2	1.81	0.62
1:C:147[A]:LYS:HE2	8:C:722:HOH:O	1.99	0.62
1:C:107:LEU:HD13	4:C:406:EDO:O2	1.99	0.61
1:A:107:LEU:HD13	8:A:645:HOH:O	2.00	0.61
1:D:272:PRO:HB2	1:D:273[A]:LYS:HD3	1.83	0.61
1:B:125:GLY:O	6:B:407[B]:PEG:H11	2.00	0.61
1:D:76:ILE:H	1:D:127:GLN:HE22	1.49	0.61
1:A:271:LYS:HB3	1:A:272:PRO:HD3	1.83	0.60
1:C:147[A]:LYS:HE2	1:C:147[A]:LYS:HA	1.81	0.60
1:D:76:ILE:H	1:D:127:GLN:NE2	2.00	0.60
1:D:307:GLU:CB	8:D:713:HOH:O	2.15	0.60
1:B:271:LYS:HB3	1:B:272:PRO:HD3	1.84	0.60
1:A:16[B]:ILE:HG13	8:A:595:HOH:O	2.00	0.59
1:B:1:MET:SD	1:B:1:MET:N	2.68	0.59
1:B:7:GLY:H	1:B:131:ASN:ND2	2.00	0.59
1:B:125:GLY:C	6:B:407[B]:PEG:H22	2.22	0.59
1:D:123:LYS:NZ	8:D:644:HOH:O	2.35	0.59
1:D:272:PRO:HD2	1:D:273[B]:LYS:NZ	2.18	0.59
1:B:2[B]:ARG:NH1	1:B:2[B]:ARG:CG	2.50	0.59
1:B:47:ARG:NH2	8:B:600:HOH:O	2.34	0.58
1:B:128:GLY:CA	6:B:407[B]:PEG:H12	2.33	0.58
1:B:230:LEU:HD11	1:B:234:LYS:HE3	1.84	0.58
1:C:271:LYS:HB3	1:C:272:PRO:HD3	1.85	0.58
1:B:16[C]:ILE:HG22	1:B:19:THR:OG1	2.04	0.57
1:D:7:GLY:H	1:D:131:ASN:ND2	2.02	0.57
1:D:266:ALA:HA	7:D:404:PG4:H72	1.85	0.57
1:B:34:GLN:NE2	8:B:694:HOH:O	2.16	0.57
1:B:97:TYR:OH	5:B:404:GOL:H31	2.04	0.57
1:D:44:GLU:HG2	1:D:47:ARG:HH22	1.70	0.57
1:D:1:MET:HA	1:D:10:SER:OG	2.04	0.57
1:C:273:LYS:CG	1:C:274:LEU:HD13	2.34	0.56
1:C:297:ASN:ND2	1:C:299:GLU:H	2.01	0.56
1:D:298:GLU:HG3	8:D:723:HOH:O	2.05	0.56
1:D:107:LEU:CD1	8:D:650:HOH:O	2.53	0.56
4:A:403:EDO:H12	8:A:706:HOH:O	2.06	0.55
4:A:407:EDO:H21	7:C:404:PG4:C1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:O	1:D:2[B]:ARG:HB2	2.05	0.55
1:A:2:ARG:HB2	8:A:547:HOH:O	2.03	0.55
1:D:166:PRO:HB2	1:D:312:PHE:CZ	2.42	0.55
1:C:257:TYR:HD1	8:C:689:HOH:O	1.88	0.55
1:B:2[B]:ARG:HH21	1:B:314[B]:SER:HA	1.69	0.55
1:D:307:GLU:HG3	1:D:311:LYS:HE3	1.89	0.55
1:C:123:LYS:O	1:C:132:LYS:HE3	2.08	0.54
1:B:3:ILE:HD13	1:B:16[C]:ILE:HD11	1.85	0.54
1:B:2[B]:ARG:HH22	1:B:314[B]:SER:HA	1.72	0.53
1:C:206:ILE:HD13	1:C:241:ARG:HH11	1.73	0.53
1:B:273:LYS:HG3	8:B:668:HOH:O	2.08	0.53
4:D:406:EDO:H22	8:D:718:HOH:O	2.08	0.52
1:D:14:LYS:HE2	8:D:719:HOH:O	2.09	0.52
5:B:405:GOL:C3	8:B:722:HOH:O	2.36	0.52
1:C:147[A]:LYS:CE	8:C:722:HOH:O	2.57	0.52
1:A:2:ARG:CG	8:A:704:HOH:O	2.22	0.52
1:C:16[A]:ILE:HG13	8:C:708:HOH:O	2.09	0.52
1:C:206:ILE:CD1	1:C:241:ARG:NH1	2.73	0.52
1:D:79:MET:HE2	8:D:514:HOH:O	2.04	0.52
1:D:244:LYS:HE2	8:D:572:HOH:O	2.09	0.52
1:C:269:GLU:HG3	8:C:703:HOH:O	2.09	0.51
1:B:275:ALA:HB1	1:B:278:TRP:HB2	1.92	0.51
1:C:147[A]:LYS:HG2	8:C:575:HOH:O	2.11	0.51
1:C:16[B]:ILE:HG22	8:C:708:HOH:O	2.10	0.51
1:C:206:ILE:HD13	1:C:241:ARG:NH1	2.26	0.51
1:D:25:LEU:O	1:D:259:CYS:HB2	2.11	0.50
1:A:13:SER:O	1:A:16[B]:ILE:HG13	2.12	0.50
1:A:275:ALA:HB1	1:A:278:TRP:HB2	1.92	0.50
1:C:45:GLU:HG2	1:C:260:THR:HG21	1.94	0.50
1:C:255:HIS:NE2	1:C:283:ILE:HG23	2.25	0.50
1:D:55:ARG:CG	8:D:718:HOH:O	2.59	0.49
1:D:14:LYS:CE	8:D:719:HOH:O	2.60	0.49
1:A:307:GLU:OE2	8:A:674:HOH:O	2.20	0.49
1:B:138:ILE:HD12	1:B:153:ILE:HG12	1.95	0.49
1:A:33:ARG:HA	1:A:40:TYR:CE1	2.48	0.49
1:B:292:LYS:NZ	1:B:298:GLU:OE1	2.46	0.49
1:C:275:ALA:HB1	1:C:278:TRP:HB2	1.95	0.48
1:D:270:TYR:HA	1:D:273[B]:LYS:CE	2.41	0.48
1:C:163:THR:O	1:C:164:LYS:HB2	2.13	0.48
1:B:125:GLY:HA3	6:B:407[B]:PEG:H22	1.94	0.48
1:B:125:GLY:C	6:B:407[B]:PEG:H11	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ILE:HG22	1:A:292:LYS:HE2	1.94	0.48
4:A:403:EDO:C1	8:A:706:HOH:O	2.62	0.48
1:B:204:ASP:O	1:B:206:ILE:HD12	2.14	0.48
1:D:264:GLY:O	1:D:267:LYS:HG3	2.13	0.48
1:A:2:ARG:CD	8:A:704:HOH:O	2.57	0.47
1:B:211:LYS:HE2	8:B:726:HOH:O	2.14	0.47
1:B:175:ASN:O	1:B:176:ASN:HB2	2.14	0.47
5:B:405:GOL:C1	8:B:685:HOH:O	2.57	0.47
1:B:303:THR:HA	1:B:307:GLU:HB2	1.96	0.47
1:A:215:LYS:HG2	8:A:691:HOH:O	2.14	0.47
1:C:16[A]:ILE:CD1	1:C:17:GLY:O	2.61	0.47
1:D:272:PRO:HD2	1:D:273[B]:LYS:HZ2	1.79	0.47
1:B:125:GLY:O	6:B:407[B]:PEG:C1	2.63	0.47
1:D:271:LYS:N	1:D:272:PRO:CD	2.77	0.46
1:D:107:LEU:HD12	8:D:650:HOH:O	2.15	0.46
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.51	0.46
1:D:55:ARG:HG3	8:D:718:HOH:O	2.16	0.46
1:B:255:HIS:CE1	1:B:283:ILE:HG12	2.51	0.45
1:C:273:LYS:HG3	1:C:274:LEU:CD1	2.44	0.45
1:C:34:GLN:HG2	8:C:643:HOH:O	2.16	0.45
1:D:282:LEU:HD12	1:D:282:LEU:O	2.17	0.45
1:A:137:KCX:OQ2	1:A:170:HIS:HB2	2.16	0.45
1:B:1:MET:HB3	8:C:642:HOH:O	2.15	0.45
1:B:128:GLY:H	6:B:407[A]:PEG:C1	2.30	0.45
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.51	0.45
1:D:55:ARG:HG2	8:D:718:HOH:O	2.16	0.45
1:C:147[A]:LYS:HE2	1:C:147[A]:LYS:CA	2.47	0.44
1:D:244:LYS:HD3	1:D:244:LYS:HA	1.65	0.44
1:D:176:ASN:HB3	8:D:630:HOH:O	2.17	0.44
1:B:104:PHE:HA	1:B:107:LEU:CD1	2.46	0.44
1:C:2[B]:ARG:NH1	1:C:13:SER:OG	2.50	0.44
1:B:97:TYR:HH	1:B:99:TYR:HH	1.66	0.44
1:D:2[B]:ARG:HB2	1:D:12[B]:GLU:HA	1.99	0.44
1:C:2[B]:ARG:HH11	1:C:13:SER:H	1.65	0.44
1:C:137:KCX:OQ1	1:C:170:HIS:HB2	2.18	0.44
1:A:16[B]:ILE:HD12	1:A:17:GLY:O	2.19	0.43
1:B:206:ILE:CG2	1:B:210:LYS:HE3	2.48	0.43
1:C:308:ASN:HB2	1:C:309:PRO:HD3	1.99	0.43
1:A:176[B]:ASN:OD1	1:A:180:GLU:HG2	2.19	0.43
1:C:25:LEU:O	1:C:259:CYS:HB2	2.19	0.43
7:D:404:PG4:H21	8:D:704:HOH:O	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:SER:HB3	5:B:405:GOL:H11	2.01	0.42
1:C:292:LYS:HE3	8:C:527:HOH:O	2.19	0.42
1:B:23:GLU:O	1:B:66:ASP:HA	2.18	0.42
1:C:21:ILE:HG13	1:C:21:ILE:O	2.19	0.42
1:D:33:ARG:HA	1:D:40:TYR:CE1	2.54	0.42
1:C:33:ARG:HA	1:C:40:TYR:CE1	2.54	0.42
1:B:16[C]:ILE:CG2	1:B:19:THR:OG1	2.67	0.42
1:D:23:GLU:O	1:D:66:ASP:HA	2.20	0.42
1:D:142:GLU:N	1:D:143:PRO:CD	2.81	0.42
1:D:154:ARG:HD3	8:D:555:HOH:O	2.20	0.42
1:B:233:ASP:O	1:B:237:GLU:HG3	2.20	0.42
1:D:138:ILE:HD12	1:D:153:ILE:HG12	2.01	0.42
7:D:404:PG4:C3	8:D:704:HOH:O	2.19	0.42
1:B:16[A]:ILE:HG12	1:B:19:THR:OG1	2.20	0.41
1:D:233:ASP:O	1:D:237:GLU:HG3	2.20	0.41
1:B:25:LEU:O	1:B:259:CYS:HB2	2.20	0.41
1:B:44:GLU:HG2	1:B:47:ARG:NH2	2.35	0.41
1:A:211:LYS:HE3	1:A:211:LYS:HB2	1.81	0.41
1:A:303:THR:HA	1:A:307:GLU:HB2	2.02	0.41
1:B:97:TYR:OH	5:B:404:GOL:C3	2.68	0.41
1:B:270:TYR:HB3	1:B:274:LEU:HD12	2.02	0.41
1:C:213:ALA:HB1	1:C:250:LYS:HG2	2.02	0.41
1:D:257:TYR:CE2	1:D:279:SER:HA	2.56	0.41
1:A:138:ILE:HD12	1:A:153:ILE:HG12	2.03	0.41
1:B:3:ILE:HD12	1:B:16[C]:ILE:HD11	1.91	0.41
1:A:7:GLY:H	1:A:131:ASN:HD21	1.68	0.41
1:C:23:GLU:O	1:C:66:ASP:HA	2.21	0.41
1:A:25:LEU:O	1:A:259:CYS:HB2	2.22	0.40
1:B:1:MET:HB2	1:B:12:GLU:CG	2.47	0.40
1:C:95:GLY:HA2	1:C:118:PHE:CE1	2.56	0.40
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.89	0.40
1:D:141:ASP:OD1	1:D:142:GLU:N	2.53	0.40
1:B:4:PRO:CB	5:B:405:GOL:H2	2.51	0.40
1:C:142:GLU:N	1:C:143:PRO:CD	2.85	0.40
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.57	0.40
1:D:123:LYS:CE	8:D:644:HOH:O	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:CE	8:B:723:HOH:O[3_654]	2.11	0.09

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%)	304 (97%)	9 (3%)	0	100	100
1	B	316/314 (101%)	303 (96%)	13 (4%)	0	100	100
1	C	316/314 (101%)	306 (97%)	10 (3%)	0	100	100
1	D	314/314 (100%)	302 (96%)	10 (3%)	2 (1%)	25	19
All	All	1259/1256 (100%)	1215 (96%)	42 (3%)	2 (0%)	51	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2[A]	ARG
1	D	2[B]	ARG

5.3.2 Protein sidechains (i)

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%)	270 (98%)	4 (2%)	65	69
1	B	278/272 (102%)	272 (98%)	6 (2%)	52	55
1	C	278/272 (102%)	270 (97%)	8 (3%)	42	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	275/272 (101%)	271 (98%)	4 (2%)	65	69
All	All	1105/1088 (102%)	1083 (98%)	22 (2%)	60	58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	107	LEU
1	A	254	SER
1	B	1	MET
1	B	2[A]	ARG
1	B	2[B]	ARG
1	B	164[A]	LYS
1	B	164[B]	LYS
1	B	254	SER
1	C	1	MET
1	C	2[A]	ARG
1	C	2[B]	ARG
1	C	107	LEU
1	C	241	ARG
1	C	250	LYS
1	C	254	SER
1	C	274	LEU
1	D	1	MET
1	D	254	SER
1	D	273[A]	LYS
1	D	273[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	294	ASN
1	B	51	ASN
1	B	58	GLN
1	B	127	GLN
1	B	131	ASN
1	B	176	ASN
1	B	294	ASN
1	C	51	ASN

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Mol	Chain	Res	Type
1	C	58	GLN
1	C	127	GLN
1	C	294	ASN
1	C	297	ASN
1	D	34	GLN
1	D	58	GLN
1	D	108	ASN
1	D	127	GLN
1	D	131	ASN
1	D	294	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	10,11,12	0.66	0	6,12,14	1.26	1 (16%)
1	KCX	D	137	3,1	10,11,12	2.11	1 (10%)	6,12,14	2.90	1 (16%)
1	KCX	B	137	3,1	10,11,12	2.09	1 (10%)	6,12,14	2.80	1 (16%)
1	KCX	A	137	3,1	10,11,12	2.23	1 (10%)	6,12,14	2.84	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	-	1/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	D	137	3,1	-	0/9/10/12	-
1	KCX	B	137	3,1	-	1/9/10/12	-
1	KCX	A	137	3,1	-	0/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	KCX	OQ1-CX	6.81	1.34	1.21
1	D	137	KCX	OQ1-CX	6.42	1.33	1.21
1	B	137	KCX	OQ1-CX	6.39	1.33	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	137	KCX	OQ1-CX-NZ	-6.83	114.55	124.92
1	B	137	KCX	OQ1-CX-NZ	-6.73	114.70	124.92
1	A	137	KCX	OQ1-CX-NZ	-6.72	114.72	124.92
1	C	137	KCX	CE-NZ-CX	2.75	126.64	121.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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	D	408	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	C	406	-	3,3,3	0.45	0	2,2,2	0.29	0
6	PEG	B	407[B]	-	6,6,6	0.45	0	5,5,5	0.30	0
4	EDO	B	401	-	3,3,3	0.49	0	2,2,2	0.34	0
5	GOL	A	404	-	5,5,5	0.32	0	5,5,5	0.30	0
6	PEG	B	407[A]	-	6,6,6	0.47	0	5,5,5	0.30	0
7	PG4	C	404	-	12,12,12	0.48	0	11,11,11	0.20	0
5	GOL	A	405	-	5,5,5	0.30	0	5,5,5	0.26	0
5	GOL	A	406	-	5,5,5	0.22	0	5,5,5	0.47	0
5	GOL	B	406	-	5,5,5	0.27	0	5,5,5	0.43	0
5	GOL	C	407	-	5,5,5	0.26	0	5,5,5	0.41	0
4	EDO	D	403	-	3,3,3	0.39	0	2,2,2	0.45	0
5	GOL	C	403	-	5,5,5	0.25	0	5,5,5	0.37	0
7	PG4	D	404	-	12,12,12	0.50	0	11,11,11	0.19	0
5	GOL	B	404	3	5,5,5	0.26	0	5,5,5	0.31	0
4	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.35	0
5	GOL	D	405	-	5,5,5	0.25	0	5,5,5	0.39	0
5	GOL	C	405	-	5,5,5	0.26	0	5,5,5	0.40	0
5	GOL	B	405	-	5,5,5	0.27	0	5,5,5	0.39	0
4	EDO	A	403	-	3,3,3	0.42	0	2,2,2	0.48	0
5	GOL	D	407	-	5,5,5	0.31	0	5,5,5	0.42	0
4	EDO	D	406	-	3,3,3	0.41	0	2,2,2	0.41	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	D	408	-	-	0/1/1/1	-
4	EDO	C	406	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	B	407[B]	-	-	3/4/4/4	-
4	EDO	B	401	-	-	1/1/1/1	-
5	GOL	A	404	-	-	2/4/4/4	-
6	PEG	B	407[A]	-	-	2/4/4/4	-
7	PG4	C	404	-	-	8/10/10/10	-
5	GOL	A	405	-	-	0/4/4/4	-
5	GOL	A	406	-	-	2/4/4/4	-
5	GOL	B	406	-	-	0/4/4/4	-
5	GOL	C	407	-	-	0/4/4/4	-
4	EDO	D	403	-	-	1/1/1/1	-
5	GOL	C	403	-	-	0/4/4/4	-
7	PG4	D	404	-	-	5/10/10/10	-
5	GOL	B	404	3	-	4/4/4/4	-
4	EDO	A	407	-	-	0/1/1/1	-
5	GOL	D	405	-	-	2/4/4/4	-
5	GOL	C	405	-	-	4/4/4/4	-
5	GOL	B	405	-	-	1/4/4/4	-
4	EDO	A	403	-	-	1/1/1/1	-
5	GOL	D	407	-	-	0/4/4/4	-
4	EDO	D	406	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	GOL	C1-C2-C3-O3
5	A	406	GOL	C1-C2-C3-O3
5	B	404	GOL	C1-C2-C3-O3
7	C	404	PG4	O2-C3-C4-O3
7	D	404	PG4	O2-C3-C4-O3
5	A	404	GOL	O2-C2-C3-O3
5	C	405	GOL	O2-C2-C3-O3
6	B	407[B]	PEG	O2-C3-C4-O4
7	D	404	PG4	O3-C5-C6-O4
6	B	407[A]	PEG	O2-C3-C4-O4
7	C	404	PG4	O4-C7-C8-O5
7	D	404	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
7	C	404	PG4	O3-C5-C6-O4
5	B	404	GOL	O1-C1-C2-C3
5	C	405	GOL	O1-C1-C2-C3
5	C	405	GOL	C1-C2-C3-O3
5	D	405	GOL	O1-C1-C2-C3
5	A	406	GOL	O2-C2-C3-O3
5	B	404	GOL	O2-C2-C3-O3
6	B	407[B]	PEG	O1-C1-C2-O2
4	A	403	EDO	O1-C1-C2-O2
4	D	403	EDO	O1-C1-C2-O2
4	D	406	EDO	O1-C1-C2-O2
5	C	405	GOL	O1-C1-C2-O2
5	D	405	GOL	O1-C1-C2-O2
4	C	406	EDO	O1-C1-C2-O2
7	C	404	PG4	O1-C1-C2-O2
5	B	405	GOL	O1-C1-C2-C3
6	B	407[B]	PEG	C1-C2-O2-C3
4	B	401	EDO	O1-C1-C2-O2
7	C	404	PG4	C5-C6-O4-C7
7	C	404	PG4	C8-C7-O4-C6
7	C	404	PG4	C3-C4-O3-C5
6	B	407[A]	PEG	O1-C1-C2-O2
7	D	404	PG4	C4-C3-O2-C2
5	B	404	GOL	O1-C1-C2-O2
7	D	404	PG4	C1-C2-O2-C3
7	C	404	PG4	C4-C3-O2-C2

There are no ring outliers.

14 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	408	EDO	2	0
4	C	406	EDO	3	0
6	B	407[B]	PEG	11	0
6	B	407[A]	PEG	3	0
7	C	404	PG4	2	0
5	A	406	GOL	1	0
4	D	403	EDO	2	0
7	D	404	PG4	4	0
5	B	404	GOL	2	0
4	A	407	EDO	2	0
5	B	405	GOL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	EDO	2	0
5	D	407	GOL	2	0
4	D	406	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	313/314 (99%)	-0.54	1 (0%)	94	93	12, 19, 38, 60	0
1	B	313/314 (99%)	-0.41	5 (1%)	72	70	12, 20, 39, 60	0
1	C	313/314 (99%)	-0.51	5 (1%)	72	70	12, 20, 38, 64	0
1	D	313/314 (99%)	-0.33	2 (0%)	89	88	13, 22, 40, 60	0
All	All	1252/1256 (99%)	-0.45	13 (1%)	82	81	12, 20, 39, 64	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	4.8
1	D	1	MET	4.1
1	A	1	MET	3.5
1	C	270	TYR	3.5
1	B	1	MET	3.2
1	B	270	TYR	2.5
1	C	274	LEU	2.5
1	C	272	PRO	2.3
1	B	272	PRO	2.2
1	D	229	PHE	2.2
1	B	266	ALA	2.2
1	C	273	LYS	2.1
1	B	273	LYS	2.0

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	C	137	12/13	0.97	0.09	13,14,16,16	0
1	KCX	B	137	12/13	0.98	0.09	10,11,12,14	0
1	KCX	D	137	12/13	0.98	0.07	13,14,17,17	0
1	KCX	A	137	12/13	0.99	0.08	11,12,15,15	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
5	GOL	D	405	6/6	0.74	0.18	53,60,63,69	0
4	EDO	B	401	4/4	0.79	0.14	43,44,50,53	0
7	PG4	D	404	13/13	0.80	0.16	50,52,57,58	0
4	EDO	D	408	4/4	0.82	0.21	41,43,44,50	0
4	EDO	C	406	4/4	0.83	0.39	33,40,45,48	0
6	PEG	B	407[B]	7/7	0.85	0.25	28,33,40,46	7
6	PEG	B	407[A]	7/7	0.85	0.25	32,41,46,51	7
5	GOL	D	407	6/6	0.88	0.18	31,36,42,42	0
7	PG4	C	404	13/13	0.88	0.16	45,53,61,63	0
5	GOL	B	404	6/6	0.88	0.14	49,53,55,64	0
4	EDO	A	407	4/4	0.90	0.18	43,45,46,50	0
4	EDO	D	406	4/4	0.90	0.12	40,47,51,60	0
5	GOL	C	405	6/6	0.90	0.20	33,42,51,56	0
5	GOL	C	403	6/6	0.91	0.15	36,43,48,52	0
5	GOL	A	406	6/6	0.94	0.18	33,47,52,55	0
4	EDO	A	403	4/4	0.95	0.11	39,49,51,58	0
5	GOL	A	405	6/6	0.95	0.12	25,30,33,40	0
5	GOL	B	406	6/6	0.96	0.12	23,26,31,38	0
5	GOL	A	404	6/6	0.96	0.15	23,30,37,56	0
4	EDO	D	403	4/4	0.96	0.13	26,44,46,63	0
5	GOL	C	407	6/6	0.96	0.11	27,33,37,39	0
5	GOL	B	405	6/6	0.96	0.14	18,25,37,45	0
2	FE2	D	401	1/1	0.99	0.07	14,14,14,14	0
3	CO	A	402	1/1	0.99	0.06	17,17,17,17	0
2	FE2	A	401	1/1	0.99	0.06	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	C	401	1/1	0.99	0.07	12,12,12,12	0
3	CO	C	402	1/1	1.00	0.06	16,16,16,16	0
3	CO	D	402	1/1	1.00	0.05	19,19,19,19	0
2	FE2	B	402	1/1	1.00	0.07	12,12,12,12	0
3	CO	B	403	1/1	1.00	0.06	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.