Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 11:14 AM EDT

PDB ID	:	4KES
Title	:	Crystal structure of SsoPox W263T
Authors	:	Gotthard, G.; Hiblot, J.; Chabriere, E.; Elias, M.
Deposited on	:	2013-04-26
Resolution	:	2.10 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:

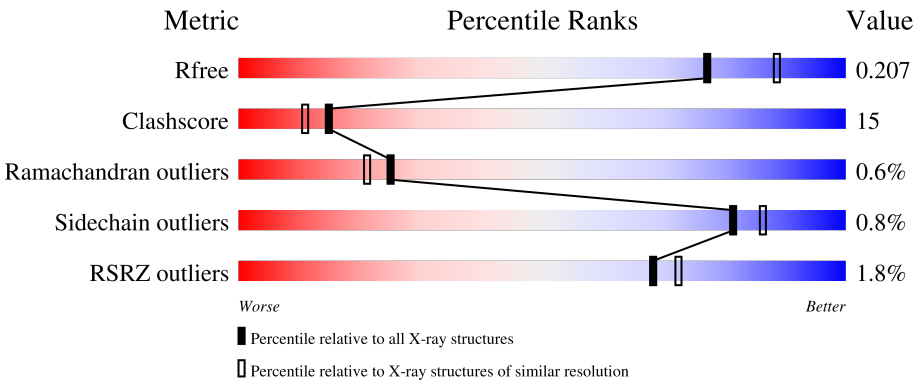
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	2% 80% 19% •
1	B	314	% 79% 20% •
1	C	314	3% 77% 21% •
1	D	314	2% 73% 26%

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	A	409	-	-	X	-
5	GOL	D	406	-	-	X	-
6	EDO	D	407	-	-	X	-
6	EDO	D	408	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10859 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	2533	1621	433	471	8	0	3	0
1	B	314	2544	1627	437	472	8	0	4	0
1	C	314	2514	1610	428	469	7	0	1	0
1	D	314	2543	1627	435	474	7	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

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

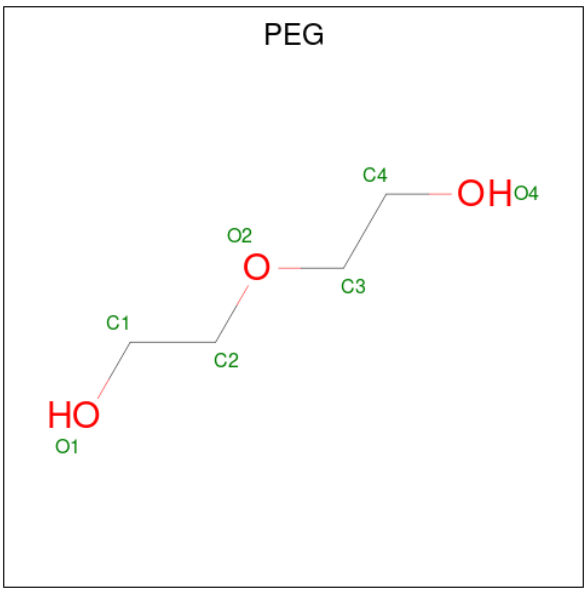
- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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).

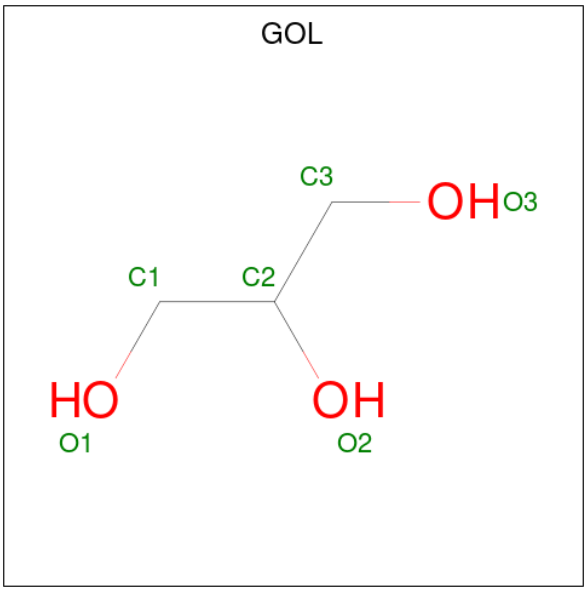
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Co 1 1	0	0
3	B	1	Total Co 1 1	0	0
3	C	1	Total Co 1 1	0	0
3	D	1	Total Co 1 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



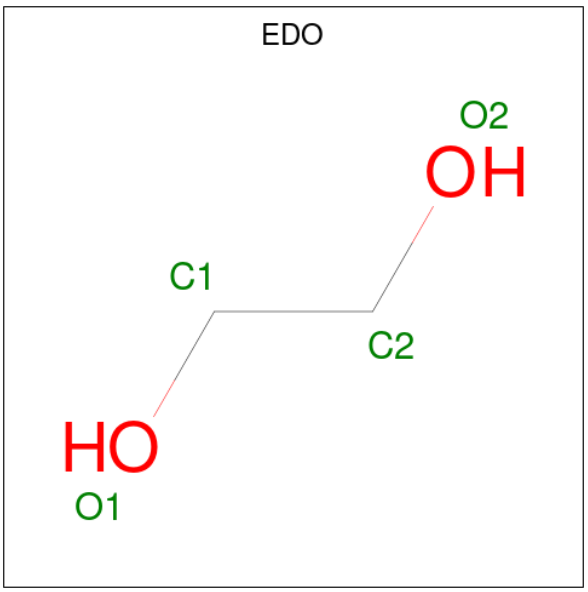
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- 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	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	B	1	6	3	3	0	0
5	B	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
5	D	1	6	3	3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	150	150	150	0	0

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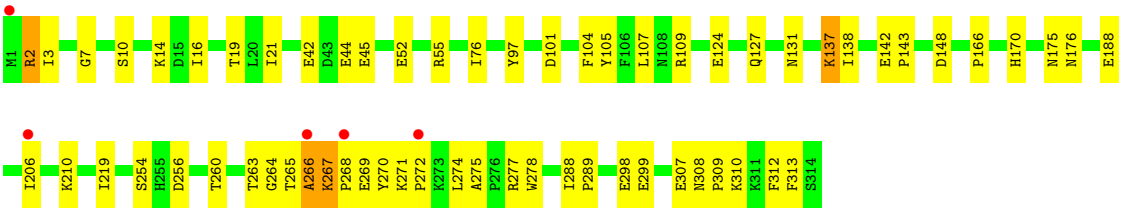
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	168	168	168	0	0
			Total	O		
7	C	138	138	138	0	0
			Total	O		
7	D	123	123	123	0	0

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.

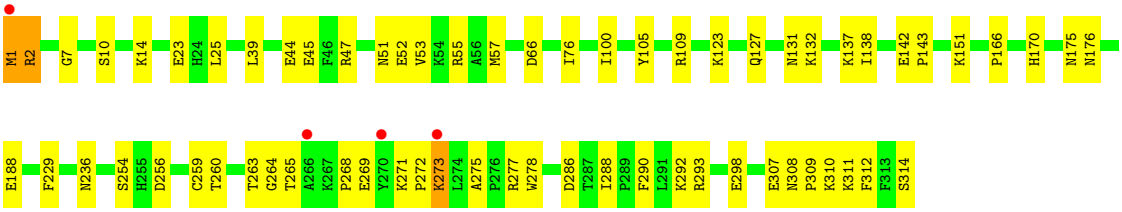
• Molecule 1: Aryldialkylphosphatase

Chain A:



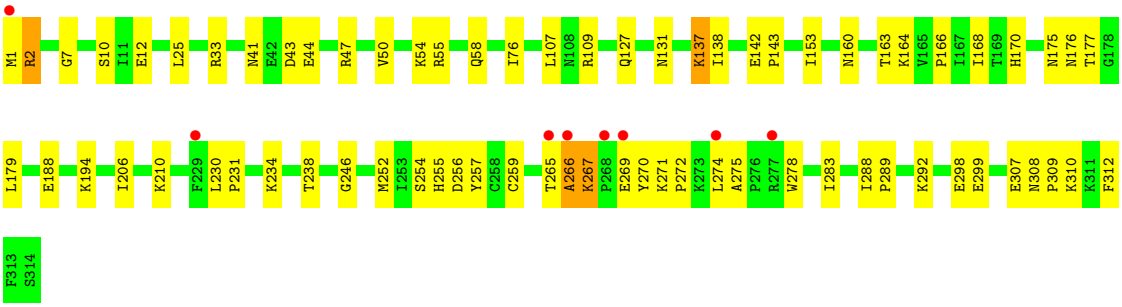
• Molecule 1: Aryldialkylphosphatase

Chain B:



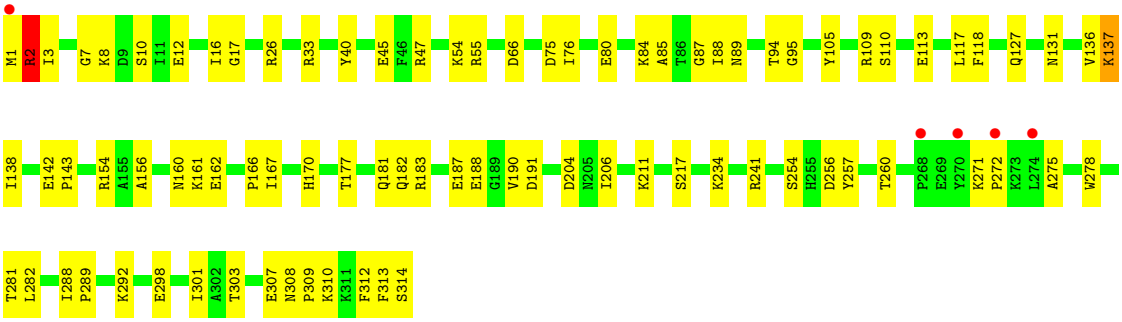
• Molecule 1: Aryldialkylphosphatase

Chain C:



• Molecule 1: Aryldialkylphosphatase

Chain D:


M1 R2 I3 G7 K8 D9 S10 I11 E12 I16 G17 R26 R33 Y40 E45 F46 R47 K54 R55 D66 D75 I76 E80 K84 A85 T86 G87 I88 N89 T94 G95 Y105 R109 S110 E113 L117 F118 Q127 N131 V136 K137
I138 E142 P143 R154 A155 A156 N160 K161 E162 P166 I167 H170 T177 Q181 Q182 R183 E187 E188 G189 V190 D191 D204 N205 I206 K211 S217 K234 R241 S254 H255 D256 Y257 T260 P268 E269 Y270 K271 P272 K273 L274 A275 W278
T281 L282 I288 P289 K292 E298 I301 A302 T303 E307 N308 P309 K310 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	84.20Å 103.60Å 151.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.10 49.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.52-2.10) 99.9 (49.52-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.163 , 0.205 0.163 , 0.207	Depositor DCC
R_{free} test set	3903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.2	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	0.97	EDS
Total number of atoms	10859	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: PEG, GOL, FE2, KCX, EDO, CO

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	0.37	0/2572	0.48	1/3470 (0.0%)
1	B	0.37	0/2583	0.47	1/3484 (0.0%)
1	C	0.36	0/2553	0.46	1/3446 (0.0%)
1	D	0.36	0/2582	0.46	1/3483 (0.0%)
All	All	0.36	0/10290	0.47	4/13883 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	256	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	256	ASP	CB-CG-OD1	6.08	123.77	118.30
1	C	256	ASP	CB-CG-OD1	5.42	123.18	118.30
1	D	256	ASP	CB-CG-OD1	5.30	123.07	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2533	0	2574	67	0
1	B	2544	0	2586	90	0
1	C	2514	0	2551	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2543	0	2580	91	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	7	0	10	0	0
4	B	7	0	10	1	0
5	A	30	0	40	11	0
5	B	30	0	40	3	0
5	C	6	0	8	3	0
5	D	18	0	24	7	0
6	A	12	0	18	5	0
6	B	8	0	12	3	0
6	C	8	0	12	3	0
6	D	12	0	18	19	0
7	A	150	0	0	15	0
7	B	168	0	0	17	0
7	C	138	0	0	10	0
7	D	123	0	0	9	0
All	All	10859	0	10483	316	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 15.

All (316) 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:1[A]:MET:N	1:B:1[A]:MET:CE	1.89	1.35
1:B:1[A]:MET:N	1:B:1[A]:MET:HE2	0.95	1.25
1:A:16:ILE:HG23	7:A:650:HOH:O	1.38	1.19
1:B:51:ASN:HB3	7:B:579:HOH:O	1.42	1.17
1:D:2[A]:ARG:HH11	1:D:2[A]:ARG:HG2	1.06	1.16
1:B:2[B]:ARG:HG2	1:B:2[B]:ARG:HH21	1.00	1.15
1:D:84:LYS:HG3	6:D:408:EDO:O1	0.99	1.15
1:A:124:GLU:HG3	7:A:610:HOH:O	1.48	1.13
1:D:84:LYS:CG	6:D:408:EDO:O1	1.93	1.13
1:B:1[A]:MET:O	1:B:2[A]:ARG:HG2	1.44	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2[A]:ARG:HG3	1:B:2[A]:ARG:HH11	1.13	1.13
1:B:1[A]:MET:CE	1:B:1[A]:MET:H2	1.55	1.12
1:B:2[B]:ARG:HH21	1:B:2[B]:ARG:CG	1.63	1.12
1:B:151:LYS:NZ	7:B:667:HOH:O	1.76	1.12
1:D:2[A]:ARG:HH11	1:D:2[A]:ARG:CG	1.61	1.11
1:B:1[B]:MET:HE2	1:B:1[B]:MET:HA	1.21	1.10
1:B:2[A]:ARG:HH11	1:B:2[A]:ARG:CG	1.62	1.10
1:B:272:PRO:O	1:B:273:LYS:HB2	1.53	1.08
1:B:1[A]:MET:HE2	1:B:1[A]:MET:CA	1.84	1.08
1:C:33:ARG:HH21	6:C:404:EDO:H12	1.21	1.05
1:A:298:GLU:HG3	7:A:635:HOH:O	1.57	1.03
1:B:14:LYS:HA	1:B:310:LYS:HE2	1.40	1.02
1:D:2[B]:ARG:HH22	1:D:314:SER:HA	1.26	0.98
1:D:80:GLU:HA	6:D:408:EDO:H21	1.46	0.98
1:B:1[B]:MET:HA	1:B:1[B]:MET:CE	1.94	0.98
1:C:43:ASP:HB3	7:C:585:HOH:O	1.63	0.97
1:A:298:GLU:OE2	6:B:401:EDO:H22	1.67	0.93
1:D:7:GLY:HA3	6:D:408:EDO:H22	1.51	0.92
1:B:1[A]:MET:CE	1:B:1[A]:MET:H1	1.68	0.92
1:B:1[B]:MET:HE2	1:B:1[B]:MET:CA	2.00	0.91
1:D:2[A]:ARG:HG2	1:D:2[A]:ARG:NH1	1.81	0.89
1:B:1[A]:MET:HE1	7:B:633:HOH:O	1.71	0.89
1:B:1[A]:MET:HB3	1:B:10:SER:OG	1.73	0.89
1:C:266:ALA:O	1:C:267:LYS:HB3	1.73	0.88
1:A:206:ILE:HD11	1:A:210:LYS:HE3	1.56	0.87
1:B:1[A]:MET:HE2	1:B:1[A]:MET:H1	1.06	0.87
1:B:2[A]:ARG:HH11	1:B:2[A]:ARG:CB	1.86	0.87
1:A:16:ILE:CG2	7:A:650:HOH:O	2.04	0.87
1:D:7:GLY:HA3	6:D:408:EDO:C2	2.04	0.86
1:D:80:GLU:HG2	6:D:408:EDO:O2	1.75	0.86
1:B:52:GLU:OE1	1:B:55:ARG:NH2	2.08	0.86
1:D:84:LYS:HG3	6:D:408:EDO:HO1	1.34	0.86
1:B:188:GLU:OE2	4:B:408:PEG:H21	1.75	0.85
1:B:2[A]:ARG:CB	1:B:2[A]:ARG:NH1	2.39	0.84
1:B:2[B]:ARG:HG2	1:B:2[B]:ARG:NH2	1.78	0.84
1:B:1[B]:MET:CB	1:B:10:SER:OG	2.25	0.83
1:A:97:TYR:OH	6:A:407:EDO:H12	1.78	0.83
1:A:107:LEU:HD12	5:A:409:GOL:C3	2.06	0.83
1:B:1[B]:MET:CE	1:B:1[B]:MET:CA	2.56	0.82
5:B:404:GOL:H11	7:B:610:HOH:O	1.78	0.82
1:D:84:LYS:HE3	6:D:408:EDO:C1	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:SER:HB3	5:A:410:GOL:H11	1.60	0.82
1:B:2[A]:ARG:HG3	1:B:2[A]:ARG:NH1	1.89	0.81
1:A:104:PHE:O	1:A:107:LEU:HD13	1.79	0.81
1:D:47[B]:ARG:HD3	7:D:550:HOH:O	1.80	0.80
1:B:271:LYS:HB3	1:B:272:PRO:HD3	1.62	0.79
1:D:2[B]:ARG:NH2	1:D:314:SER:HA	1.96	0.79
1:A:104:PHE:HA	1:A:107:LEU:CD1	2.13	0.79
1:D:136:VAL:HG22	1:D:167:ILE:HG12	1.65	0.78
1:B:263:THR:HG22	1:B:265:THR:H	1.45	0.78
1:C:234:LYS:HD2	7:C:608:HOH:O	1.82	0.78
1:D:105:TYR:O	1:D:109:ARG:HD2	1.84	0.77
1:D:161:LYS:HE3	1:D:188:GLU:O	1.84	0.77
1:A:107:LEU:HD12	5:A:409:GOL:H31	1.65	0.77
1:D:80:GLU:CA	6:D:408:EDO:H21	2.14	0.77
1:D:3:ILE:HD11	1:D:313:PHE:HB3	1.65	0.77
1:A:52:GLU:OE1	1:A:55:ARG:NH2	2.16	0.77
1:B:45:GLU:HG2	1:B:260:THR:HG21	1.68	0.75
1:B:272:PRO:O	1:B:273:LYS:CB	2.31	0.75
1:A:264:GLY:N	1:C:109:ARG:NH1	2.35	0.74
1:D:76:ILE:H	1:D:127:GLN:HE22	1.36	0.73
1:C:50:VAL:O	1:C:54:LYS:HG2	1.88	0.73
1:A:76:ILE:H	1:A:127:GLN:HE22	1.37	0.73
1:D:47[A]:ARG:HD3	7:D:602:HOH:O	1.87	0.72
1:B:1[B]:MET:HB3	1:B:10:SER:OG	1.89	0.71
1:B:2[A]:ARG:NH2	1:B:314:SER:HA	2.05	0.71
1:A:104:PHE:CD2	7:A:633:HOH:O	2.44	0.70
1:D:191:ASP:N	5:D:406:GOL:O3	2.23	0.70
1:B:1[A]:MET:O	1:B:2[A]:ARG:CG	2.32	0.70
1:C:7:GLY:H	1:C:131:ASN:ND2	1.90	0.70
1:C:33:ARG:NH2	6:C:404:EDO:H12	2.03	0.70
1:A:270:TYR:HB3	1:A:274:LEU:HD22	1.74	0.69
1:D:75:ASP:HB3	6:D:407:EDO:H22	1.74	0.69
1:C:292:LYS:NZ	7:C:507:HOH:O	2.25	0.69
6:D:407:EDO:H12	7:D:524:HOH:O	1.92	0.69
1:D:136:VAL:HG21	1:D:156:ALA:HB1	1.76	0.68
1:D:76:ILE:H	1:D:127:GLN:NE2	1.92	0.68
1:C:160:ASN:HD21	5:C:403:GOL:H11	1.59	0.68
6:B:410:EDO:H21	7:B:553:HOH:O	1.92	0.68
1:A:275:ALA:HB1	1:A:278:TRP:HB2	1.76	0.68
1:B:292:LYS:NZ	1:B:298:GLU:OE1	2.28	0.67
1:C:275:ALA:HB1	1:C:278:TRP:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:GLY:H	1:D:131:ASN:ND2	1.94	0.66
1:B:14:LYS:CA	1:B:310:LYS:HE2	2.21	0.66
6:A:406:EDO:H12	1:B:292:LYS:HD2	1.78	0.65
1:D:84:LYS:HE3	6:D:408:EDO:H11	1.77	0.65
1:A:7:GLY:H	1:A:131:ASN:ND2	1.94	0.65
1:A:277:ARG:CD	7:B:601:HOH:O	2.44	0.65
1:B:123:LYS:O	1:B:132:LYS:HE3	1.97	0.65
1:D:162:GLU:HG2	7:D:574:HOH:O	1.97	0.65
1:B:277[B]:ARG:NH2	1:B:286:ASP:OD2	2.28	0.64
1:C:2[B]:ARG:HH21	1:C:2[B]:ARG:HB2	1.62	0.64
1:D:1:MET:HB2	1:D:12:GLU:HG3	1.77	0.64
1:B:2[B]:ARG:CG	1:B:2[B]:ARG:NH2	2.35	0.64
1:A:271:LYS:HB3	1:A:272:PRO:HD3	1.80	0.63
1:C:271:LYS:HB3	1:C:272:PRO:HD3	1.79	0.63
1:B:76:ILE:H	1:B:127:GLN:HE22	1.45	0.63
1:B:76:ILE:H	1:B:127:GLN:NE2	1.97	0.62
1:B:1[B]:MET:CE	1:B:1[B]:MET:N	2.63	0.62
1:C:266:ALA:O	1:C:267:LYS:CB	2.45	0.62
1:C:206:ILE:HG22	1:C:210:LYS:HE3	1.81	0.62
1:A:104:PHE:HA	1:A:107:LEU:HD13	1.81	0.62
1:B:307:GLU:HG3	1:B:311:LYS:NZ	2.15	0.62
1:B:1[A]:MET:HE3	7:B:666:HOH:O	1.99	0.62
1:D:2[A]:ARG:CG	1:D:2[A]:ARG:NH1	2.34	0.62
1:A:264:GLY:N	1:C:109:ARG:HH12	1.98	0.61
1:A:264:GLY:CA	1:C:109:ARG:NH1	2.63	0.61
1:D:7:GLY:CA	6:D:408:EDO:O2	2.48	0.61
1:D:12:GLU:OE1	1:D:12:GLU:N	2.25	0.61
1:A:76:ILE:H	1:A:127:GLN:NE2	1.97	0.61
1:A:307:GLU:HG2	7:A:629:HOH:O	2.01	0.61
1:B:1[B]:MET:N	1:B:1[B]:MET:HE3	2.16	0.61
1:D:275:ALA:HB1	1:D:278:TRP:HB2	1.81	0.61
1:B:311:LYS:HE2	7:B:531:HOH:O	2.01	0.60
1:D:191:ASP:H	5:D:406:GOL:HO3	1.49	0.60
1:A:268:PRO:HA	7:A:640:HOH:O	2.00	0.60
1:D:110:SER:OG	1:D:113:GLU:HG3	2.02	0.60
1:B:1[A]:MET:HE2	1:B:1[A]:MET:H2	0.77	0.60
1:C:142:GLU:HB2	1:C:143:PRO:HD3	1.84	0.60
1:B:2[A]:ARG:CG	1:B:2[A]:ARG:NH1	2.34	0.60
1:D:160:ASN:OD1	5:D:406:GOL:H31	2.02	0.59
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.38	0.59
1:C:12:GLU:HG3	7:C:583:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LYS:HA	1:A:310:LYS:HE2	1.84	0.59
1:A:16:ILE:HG22	7:A:595:HOH:O	2.02	0.59
1:A:107:LEU:CD1	5:A:409:GOL:H31	2.33	0.58
1:B:1[B]:MET:HB2	1:B:10:SER:OG	2.04	0.58
1:D:190:VAL:HA	5:D:406:GOL:O3	2.04	0.58
5:A:408:GOL:H32	7:B:586:HOH:O	2.04	0.58
1:B:2[A]:ARG:HH22	1:B:314:SER:HA	1.65	0.58
1:C:179:LEU:HD12	7:C:614:HOH:O	2.03	0.57
1:A:263:THR:C	1:C:109:ARG:HH12	2.08	0.57
1:A:206:ILE:CD1	1:A:210:LYS:HE3	2.29	0.57
1:B:138:ILE:C	1:B:138:ILE:HD12	2.24	0.57
1:A:148:ASP:OD1	5:A:409:GOL:H2	2.05	0.57
1:B:7:GLY:H	1:B:131:ASN:ND2	2.02	0.57
1:C:267:LYS:CD	1:C:269:GLU:OE2	2.52	0.56
1:D:75:ASP:HB3	6:D:407:EDO:C2	2.34	0.56
1:D:105:TYR:O	1:D:109:ARG:CD	2.52	0.56
6:D:407:EDO:C1	7:D:524:HOH:O	2.52	0.56
1:D:138:ILE:C	1:D:138:ILE:HD12	2.27	0.55
1:B:273:LYS:HG3	7:B:648:HOH:O	2.06	0.55
6:A:411:EDO:H11	7:A:574:HOH:O	2.06	0.55
1:B:275:ALA:HB1	1:B:278:TRP:HB2	1.89	0.55
1:D:2[A]:ARG:HH11	1:D:2[A]:ARG:HG3	1.61	0.55
1:A:105:TYR:O	1:A:109:ARG:HD2	2.06	0.55
1:D:3:ILE:CD1	1:D:313:PHE:HB3	2.34	0.55
1:A:104:PHE:CA	1:A:107:LEU:HD13	2.36	0.55
1:C:270:TYR:HB3	1:C:274:LEU:HD22	1.87	0.55
1:D:161:LYS:CE	1:D:188:GLU:O	2.54	0.54
1:C:206:ILE:CD1	1:C:238:THR:HG23	2.37	0.54
1:D:95:GLY:HA2	1:D:118:PHE:CE1	2.42	0.54
1:B:268:PRO:HG2	1:B:269:GLU:OE1	2.07	0.54
1:C:76:ILE:H	1:C:127:GLN:NE2	2.06	0.54
1:D:136:VAL:CG2	1:D:167:ILE:HG12	2.36	0.54
1:D:204:ASP:OD2	1:D:234:LYS:HE2	2.08	0.54
1:B:137:KCX:OQ1	1:B:170:HIS:HB2	2.07	0.54
1:B:298:GLU:HG3	7:B:650:HOH:O	2.08	0.54
1:B:293:ARG:NH2	7:B:552:HOH:O	2.34	0.54
1:C:299:GLU:HB2	7:C:613:HOH:O	2.08	0.53
1:B:271:LYS:HB3	1:B:272:PRO:CD	2.36	0.53
1:D:288:ILE:HG22	1:D:292:LYS:HE2	1.90	0.53
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.42	0.53
1:B:272:PRO:O	7:B:648:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ASN:HD21	5:D:406:GOL:H31	1.74	0.53
1:C:267:LYS:HD3	1:C:269:GLU:OE2	2.09	0.53
1:D:26:ARG:HH11	6:D:407:EDO:H22	1.73	0.53
1:C:55:ARG:HD3	7:C:635:HOH:O	2.07	0.53
1:B:263:THR:HG22	1:B:265:THR:N	2.21	0.53
1:B:2[A]:ARG:NH1	1:B:2[A]:ARG:HB3	2.20	0.52
1:D:160:ASN:OD1	5:D:406:GOL:C3	2.57	0.52
1:B:1[A]:MET:CE	1:B:1[A]:MET:CA	2.63	0.52
1:D:33:ARG:HA	1:D:40:TYR:CE1	2.44	0.52
1:C:298:GLU:HG2	7:C:606:HOH:O	2.09	0.52
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.44	0.52
1:C:274:LEU:N	1:C:274:LEU:CD1	2.73	0.52
1:C:270:TYR:O	1:C:274:LEU:HD13	2.09	0.51
1:C:33:ARG:HH21	6:C:404:EDO:C1	2.07	0.51
1:B:229:PHE:CD1	5:B:406:GOL:H12	2.45	0.51
1:D:7:GLY:HA3	6:D:408:EDO:O2	2.10	0.51
1:C:1:MET:HA	1:C:10:SER:OG	2.10	0.51
1:C:137:KCX:OQ2	1:C:170:HIS:HB2	2.09	0.51
1:C:274:LEU:N	1:C:274:LEU:HD12	2.26	0.51
1:A:104:PHE:C	1:A:107:LEU:HD13	2.31	0.51
1:A:188:GLU:OE1	1:A:188:GLU:HA	2.11	0.51
1:C:76:ILE:H	1:C:127:GLN:HE22	1.56	0.51
1:C:7:GLY:H	1:C:131:ASN:HD21	1.58	0.51
1:A:101:ASP:HB2	7:A:574:HOH:O	2.10	0.50
1:D:16:ILE:CG2	1:D:17:GLY:N	2.73	0.50
1:A:265:THR:O	1:A:266:ALA:O	2.29	0.50
1:A:137:KCX:OQ2	1:A:170:HIS:HB2	2.12	0.50
1:C:307:GLU:OE2	1:C:310:LYS:NZ	2.40	0.50
1:D:7:GLY:H	1:D:131:ASN:HD21	1.57	0.49
1:A:264:GLY:HA2	1:C:109:ARG:NH1	2.26	0.49
1:A:267:LYS:HG2	1:A:269:GLU:OE1	2.12	0.49
1:C:206:ILE:CG2	1:C:210:LYS:HE3	2.42	0.49
1:C:163:THR:O	1:C:164:LYS:HB2	2.13	0.49
1:D:3:ILE:HD12	1:D:313:PHE:CD2	2.48	0.49
1:C:308:ASN:HB2	1:C:309:PRO:HD3	1.93	0.49
1:D:137:KCX:OQ2	1:D:170:HIS:HB2	2.12	0.49
1:D:271:LYS:N	1:D:272:PRO:CD	2.76	0.49
1:D:16:ILE:HG23	1:D:17:GLY:N	2.27	0.48
1:B:53:VAL:O	1:B:57:MET:HG3	2.13	0.48
1:C:175:ASN:O	1:C:176:ASN:HB3	2.13	0.48
1:B:2[A]:ARG:HB3	1:B:2[A]:ARG:CZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:CD	1:A:269:GLU:H	2.15	0.48
1:D:161:LYS:HB2	7:D:574:HOH:O	2.13	0.48
1:D:177:THR:O	1:D:181:GLN:HG3	2.13	0.48
1:B:264:GLY:HA2	1:D:109:ARG:NH1	2.28	0.48
1:D:166:PRO:HB2	1:D:312:PHE:CZ	2.49	0.48
1:D:288:ILE:HB	1:D:289:PRO:HD3	1.96	0.48
1:B:45:GLU:CG	1:B:260:THR:HG21	2.42	0.48
1:C:288:ILE:HB	1:C:289:PRO:HD3	1.95	0.48
1:B:175:ASN:O	1:B:176:ASN:HB2	2.15	0.47
1:B:229:PHE:HD1	5:B:406:GOL:H12	1.79	0.47
1:D:298:GLU:HG3	7:D:562:HOH:O	2.15	0.47
1:A:299:GLU:HB3	7:A:598:HOH:O	2.13	0.47
1:A:138:ILE:HD12	1:A:138:ILE:C	2.34	0.47
1:C:175:ASN:O	1:C:176:ASN:CB	2.62	0.47
1:D:88:ILE:HG13	1:D:89:ASN:N	2.30	0.47
1:B:105:TYR:O	1:B:109[A]:ARG:HD2	2.14	0.47
1:A:289:PRO:HB3	5:A:408:GOL:H31	1.97	0.46
6:B:410:EDO:C2	7:B:553:HOH:O	2.55	0.46
1:C:255:HIS:NE2	1:C:283:ILE:HG23	2.29	0.46
1:D:160:ASN:ND2	5:D:406:GOL:H31	2.30	0.46
1:B:307:GLU:HG3	1:B:311:LYS:HZ1	1.79	0.46
1:D:75:ASP:N	6:D:407:EDO:H21	2.31	0.46
1:D:84:LYS:CD	6:D:408:EDO:O1	2.62	0.46
1:A:55:ARG:HD3	6:A:406:EDO:H11	1.97	0.46
1:D:1:MET:N	1:D:10:SER:C	2.69	0.46
1:D:8:LYS:NZ	1:D:87:GLY:O	2.47	0.46
1:A:104:PHE:HA	1:A:107:LEU:HD11	1.93	0.46
1:A:45:GLU:HG2	1:A:260:THR:HG21	1.98	0.46
1:B:39:LEU:HD11	1:D:117:LEU:HD21	1.98	0.45
1:B:269:GLU:CD	1:B:269:GLU:H	2.19	0.45
5:A:404:GOL:H11	7:A:545:HOH:O	2.15	0.45
1:C:246:GLY:HA2	7:C:580:HOH:O	2.15	0.45
1:A:44:GLU:HG3	7:A:625:HOH:O	2.17	0.45
1:A:308:ASN:HB2	1:A:309:PRO:HD3	1.97	0.45
1:A:107:LEU:CD1	5:A:409:GOL:C3	2.87	0.45
1:A:267:LYS:HD2	1:A:269:GLU:OE2	2.16	0.45
1:C:265:THR:O	1:C:266:ALA:O	2.34	0.45
1:C:206:ILE:HD12	1:C:238:THR:HG23	1.98	0.45
1:B:288:ILE:HG22	1:B:292:LYS:HE2	1.97	0.45
1:C:54:LYS:O	1:C:58:GLN:HG3	2.17	0.45
1:A:3:ILE:HD11	1:A:313:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HD2	7:B:601:HOH:O	2.12	0.44
1:D:257:TYR:HA	1:D:278:TRP:CZ2	2.53	0.44
1:C:252:MET:CE	1:C:309:PRO:HG3	2.47	0.44
1:A:7:GLY:H	1:A:131:ASN:HD21	1.65	0.44
1:C:138:ILE:HD12	1:C:153:ILE:HG12	1.99	0.44
1:A:16:ILE:HG12	1:A:19:THR:OG1	2.18	0.44
1:A:288:ILE:HB	1:A:289:PRO:HD3	1.99	0.44
1:B:236:ASN:HB3	1:B:290:PHE:CE2	2.53	0.44
1:C:206:ILE:O	1:C:210:LYS:HG3	2.18	0.43
1:A:124:GLU:CG	7:A:610:HOH:O	2.30	0.43
1:D:206:ILE:CD1	1:D:241:ARG:HG2	2.49	0.43
1:B:44:GLU:HG2	1:B:47:ARG:HH12	1.83	0.43
1:D:282:LEU:C	1:D:282:LEU:HD13	2.39	0.43
1:D:142:GLU:HB2	1:D:143:PRO:HD3	1.99	0.43
1:C:25:LEU:O	1:C:259:CYS:HB2	2.18	0.43
1:D:303:THR:HA	1:D:307:GLU:HB3	2.01	0.43
6:A:411:EDO:H21	7:A:511:HOH:O	2.19	0.43
1:B:100:ILE:HB	7:B:592:HOH:O	2.18	0.43
1:A:175:ASN:O	1:A:176:ASN:CB	2.66	0.43
1:B:273:LYS:CG	7:B:648:HOH:O	2.66	0.43
1:D:154:ARG:NH2	1:D:188:GLU:OE2	2.44	0.43
1:A:21:ILE:O	1:A:21:ILE:HG13	2.18	0.43
1:A:264:GLY:HA3	1:C:107:LEU:O	2.19	0.43
1:D:142:GLU:N	1:D:143:PRO:CD	2.81	0.43
1:C:137:KCX:HA	1:C:168:ILE:O	2.19	0.42
1:C:265:THR:C	1:C:266:ALA:O	2.57	0.42
1:C:269:GLU:H	1:C:269:GLU:CD	2.23	0.42
1:B:142:GLU:HB2	1:B:143:PRO:HD3	2.02	0.42
1:C:230:LEU:HA	1:C:231:PRO:HD3	1.91	0.42
1:B:25:LEU:O	1:B:259:CYS:HB2	2.19	0.42
1:B:307:GLU:HG3	1:B:311:LYS:HZ2	1.82	0.42
1:D:45:GLU:HG2	1:D:260:THR:HG21	2.01	0.42
1:C:188:GLU:OE2	1:C:188:GLU:HA	2.18	0.42
1:D:1:MET:SD	1:D:12:GLU:OE2	2.77	0.42
1:A:107:LEU:HD12	5:A:409:GOL:O3	2.20	0.42
1:D:211:LYS:HD2	7:D:608:HOH:O	2.19	0.42
1:D:301:ILE:HB	7:D:562:HOH:O	2.20	0.42
1:A:219:ILE:O	1:A:219:ILE:HG13	2.20	0.42
1:D:55:ARG:HD2	1:D:281:THR:HG21	2.02	0.41
1:D:94:THR:O	1:D:136:VAL:HA	2.20	0.41
1:D:66:ASP:C	1:D:66:ASP:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2[B]:ARG:HH21	1:B:2[B]:ARG:HG3	1.69	0.41
1:A:142:GLU:HB3	1:A:143:PRO:HD3	2.02	0.41
1:D:2[A]:ARG:NH1	1:D:2[A]:ARG:HG3	2.29	0.41
1:D:182:GLN:NE2	1:D:217:SER:HB2	2.35	0.41
1:B:1[B]:MET:CG	1:B:10:SER:OG	2.68	0.41
1:C:194:LYS:HG3	5:C:403:GOL:H12	2.02	0.41
1:B:2[A]:ARG:NH1	1:B:2[A]:ARG:HB2	2.29	0.41
1:B:23:GLU:O	1:B:66:ASP:HA	2.20	0.41
1:C:175:ASN:OD1	1:C:177:THR:HG23	2.21	0.41
1:C:47:ARG:NH1	7:C:585:HOH:O	2.52	0.41
1:C:164:LYS:HG3	5:C:403:GOL:O1	2.20	0.41
1:D:54[B]:LYS:NZ	1:D:85:ALA:O	2.54	0.41
1:D:308:ASN:HB2	1:D:309:PRO:HD3	2.03	0.41
1:A:148:ASP:OD1	5:A:409:GOL:C2	2.68	0.41
1:C:257:TYR:HA	1:C:278:TRP:CZ2	2.56	0.41
1:B:308:ASN:HB2	1:B:309:PRO:HD3	2.02	0.40
1:D:183:ARG:O	1:D:187[A]:GLU:HG3	2.21	0.40
1:D:310:LYS:HB2	1:D:310:LYS:HE3	1.63	0.40
1:C:41:ASN:ND2	1:C:44:GLU:HG3	2.36	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%)	300 (96%)	9 (3%)	4 (1%)	12 7
1	B	314/314 (100%)	302 (96%)	11 (4%)	1 (0%)	41 41
1	C	312/314 (99%)	294 (94%)	14 (4%)	4 (1%)	12 7
1	D	315/314 (100%)	302 (96%)	11 (4%)	2 (1%)	25 21
All	All	1254/1256 (100%)	1198 (96%)	45 (4%)	11 (1%)	25 12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ALA
1	B	273	LYS
1	C	266	ALA
1	D	2[A]	ARG
1	D	2[B]	ARG
1	A	2[A]	ARG
1	A	2[B]	ARG
1	A	267	LYS
1	C	267	LYS
1	C	2[A]	ARG
1	C	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	275/272 (101%)	271 (98%)	4 (2%)	65	71
1	B	276/272 (102%)	271 (98%)	5 (2%)	59	65
1	C	273/272 (100%)	272 (100%)	1 (0%)	91	94
1	D	276/272 (102%)	273 (99%)	3 (1%)	73	79
All	All	1100/1088 (101%)	1087 (99%)	13 (1%)	81	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2[A]	ARG
1	A	2[B]	ARG
1	A	42	GLU
1	A	254	SER
1	B	1[A]	MET
1	B	1[B]	MET
1	B	2[A]	ARG
1	B	2[B]	ARG
1	B	254	SER

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Mol	Chain	Res	Type
1	C	254	SER
1	D	2[A]	ARG
1	D	2[B]	ARG
1	D	254	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	127	GLN
1	A	131	ASN
1	B	127	GLN
1	B	131	ASN
1	B	294	ASN
1	C	34	GLN
1	C	58	GLN
1	C	127	GLN
1	C	131	ASN
1	D	51	ASN
1	D	58	GLN
1	D	127	GLN
1	D	131	ASN
1	D	176	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	B	137	1,3	10,11,12	0.69	0	6,12,14	0.71	0
1	KCX	D	137	1,3	10,11,12	2.22	1 (10%)	6,12,14	2.86	2 (33%)
1	KCX	A	137	1,3	10,11,12	2.17	1 (10%)	6,12,14	2.47	1 (16%)
1	KCX	C	137	1,3	10,11,12	2.11	1 (10%)	6,12,14	2.71	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	B	137	1,3	-	0/9/10/12	-
1	KCX	D	137	1,3	-	3/9/10/12	-
1	KCX	A	137	1,3	-	0/9/10/12	-
1	KCX	C	137	1,3	-	1/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	137	KCX	OQ1-CX	6.81	1.34	1.21
1	A	137	KCX	OQ1-CX	6.63	1.33	1.21
1	C	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	-6.44	115.14	124.92
1	C	137	KCX	OQ1-CX-NZ	-6.34	115.29	124.92
1	A	137	KCX	OQ1-CX-NZ	-5.74	116.20	124.92
1	D	137	KCX	CE-NZ-CX	2.68	126.54	121.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	D	406	-	5,5,5	0.25	0	5,5,5	0.34	0
6	EDO	D	407	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	D	403	-	3,3,3	0.43	0	2,2,2	0.45	0
5	GOL	B	405	-	5,5,5	0.21	0	5,5,5	0.51	0
5	GOL	A	409	-	5,5,5	0.26	0	5,5,5	0.37	0
6	EDO	B	401	-	3,3,3	0.44	0	2,2,2	0.40	0
4	PEG	B	408	-	6,6,6	0.44	0	5,5,5	0.35	0
5	GOL	A	410	-	5,5,5	0.32	0	5,5,5	0.54	0
5	GOL	B	404	-	5,5,5	0.25	0	5,5,5	0.44	0
6	EDO	A	407	-	3,3,3	0.41	0	2,2,2	0.46	0
6	EDO	A	411	-	3,3,3	0.43	0	2,2,2	0.43	0
6	EDO	C	405	-	3,3,3	0.44	0	2,2,2	0.37	0
5	GOL	B	406	-	5,5,5	0.31	0	5,5,5	0.28	0
5	GOL	A	408	-	5,5,5	0.26	0	5,5,5	0.27	0
6	EDO	C	404	-	3,3,3	0.44	0	2,2,2	0.41	0
6	EDO	A	406	-	3,3,3	0.46	0	2,2,2	0.31	0
5	GOL	A	405	-	5,5,5	0.27	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	409	-	5,5,5	0.25	0	5,5,5	0.43	0
5	GOL	B	407	-	5,5,5	0.26	0	5,5,5	0.27	0
5	GOL	A	404	-	5,5,5	0.29	0	5,5,5	0.48	0
5	GOL	D	405	-	5,5,5	0.27	0	5,5,5	0.35	0
6	EDO	B	410	-	3,3,3	0.42	0	2,2,2	0.42	0
5	GOL	C	403	-	5,5,5	0.27	0	5,5,5	0.33	0
5	GOL	D	404	-	5,5,5	0.35	0	5,5,5	0.19	0
6	EDO	D	408	-	3,3,3	0.47	0	2,2,2	0.45	0
4	PEG	A	403	-	6,6,6	0.45	0	5,5,5	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	406	-	-	1/4/4/4	-
6	EDO	D	407	-	-	1/1/1/1	-
6	EDO	D	403	-	-	0/1/1/1	-
5	GOL	B	405	-	-	0/4/4/4	-
5	GOL	A	409	-	-	0/4/4/4	-
6	EDO	B	401	-	-	1/1/1/1	-
4	PEG	B	408	-	-	1/4/4/4	-
5	GOL	A	410	-	-	2/4/4/4	-
5	GOL	B	404	-	-	0/4/4/4	-
6	EDO	A	407	-	-	1/1/1/1	-
6	EDO	A	411	-	-	1/1/1/1	-
6	EDO	C	405	-	-	1/1/1/1	-
5	GOL	B	406	-	-	2/4/4/4	-
5	GOL	A	408	-	-	2/4/4/4	-
6	EDO	C	404	-	-	1/1/1/1	-
6	EDO	A	406	-	-	1/1/1/1	-
5	GOL	A	405	-	-	2/4/4/4	-
5	GOL	B	409	-	-	2/4/4/4	-
5	GOL	B	407	-	-	2/4/4/4	-
5	GOL	A	404	-	-	1/4/4/4	-
5	GOL	D	405	-	-	3/4/4/4	-
6	EDO	B	410	-	-	0/1/1/1	-
5	GOL	C	403	-	-	0/4/4/4	-
5	GOL	D	404	-	-	0/4/4/4	-
6	EDO	D	408	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	403	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	407	GOL	C1-C2-C3-O3
4	A	403	PEG	O1-C1-C2-O2
5	A	405	GOL	O1-C1-C2-C3
5	A	408	GOL	C1-C2-C3-O3
5	A	410	GOL	C1-C2-C3-O3
5	B	406	GOL	O1-C1-C2-C3
5	B	409	GOL	O1-C1-C2-C3
5	D	405	GOL	C1-C2-C3-O3
5	B	409	GOL	O1-C1-C2-O2
6	A	406	EDO	O1-C1-C2-O2
6	C	404	EDO	O1-C1-C2-O2
6	D	407	EDO	O1-C1-C2-O2
4	B	408	PEG	O1-C1-C2-O2
5	A	405	GOL	O1-C1-C2-O2
5	B	407	GOL	O2-C2-C3-O3
5	D	405	GOL	O1-C1-C2-O2
5	D	405	GOL	O2-C2-C3-O3
5	A	404	GOL	O2-C2-C3-O3
5	B	406	GOL	O1-C1-C2-O2
5	D	406	GOL	O2-C2-C3-O3
4	A	403	PEG	C4-C3-O2-C2
6	A	411	EDO	O1-C1-C2-O2
5	A	408	GOL	O2-C2-C3-O3
5	A	410	GOL	O2-C2-C3-O3
4	A	403	PEG	C1-C2-O2-C3
6	A	407	EDO	O1-C1-C2-O2
6	B	401	EDO	O1-C1-C2-O2
6	C	405	EDO	O1-C1-C2-O2

There are no ring outliers.

17 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	406	GOL	7	0
6	D	407	EDO	6	0
5	A	409	GOL	7	0
6	B	401	EDO	1	0
4	B	408	PEG	1	0
5	A	410	GOL	1	0
5	B	404	GOL	1	0
6	A	407	EDO	1	0
6	A	411	EDO	2	0
5	B	406	GOL	2	0
5	A	408	GOL	2	0
6	C	404	EDO	3	0
6	A	406	EDO	2	0
5	A	404	GOL	1	0
6	B	410	EDO	2	0
5	C	403	GOL	3	0
6	D	408	EDO	13	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%)	-0.32	5 (1%)	72	75	19, 32, 52, 80	0
1	B	313/314 (99%)	-0.36	4 (1%)	77	80	19, 30, 54, 86	0
1	C	313/314 (99%)	-0.17	8 (2%)	56	61	22, 39, 61, 93	0
1	D	313/314 (99%)	-0.06	5 (1%)	72	75	24, 43, 66, 107	0
All	All	1252/1256 (99%)	-0.23	22 (1%)	68	72	19, 36, 61, 107	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	8.7
1	C	1	MET	7.2
1	C	268	PRO	4.7
1	D	268	PRO	4.4
1	C	266	ALA	4.0
1	D	270	TYR	3.8
1	A	1[A]	MET	3.8
1	D	274	LEU	3.4
1	B	1[A]	MET	3.2
1	B	266	ALA	3.2
1	C	265	THR	3.1
1	A	266	ALA	2.9
1	D	272	PRO	2.9
1	C	277	ARG	2.7
1	A	272	PRO	2.6
1	B	273	LYS	2.6
1	A	268	PRO	2.6
1	B	270	TYR	2.3
1	C	274	LEU	2.2
1	A	206	ILE	2.1
1	C	269	GLU	2.0
1	C	229	PHE	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	A	137	12/13	0.98	0.11	17,18,21,23	0
1	KCX	B	137	12/13	0.98	0.09	18,19,21,21	0
1	KCX	C	137	12/13	0.98	0.09	24,27,29,31	0
1	KCX	D	137	12/13	0.98	0.08	25,30,34,35	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
4	PEG	B	408	7/7	0.76	0.18	55,65,69,75	0
5	GOL	A	408	6/6	0.79	0.16	51,60,67,69	0
5	GOL	B	407	6/6	0.81	0.19	43,55,63,73	0
6	EDO	B	410	4/4	0.83	0.17	48,53,55,64	0
6	EDO	B	401	4/4	0.84	0.15	53,54,56,60	0
5	GOL	D	405	6/6	0.84	0.13	64,66,72,73	0
6	EDO	A	406	4/4	0.85	0.16	43,51,52,56	0
5	GOL	D	406	6/6	0.87	0.17	55,62,65,66	0
5	GOL	A	409	6/6	0.89	0.39	50,61,62,66	0
6	EDO	A	407	4/4	0.89	0.18	58,58,66,68	0
6	EDO	D	408	4/4	0.89	0.82	89,94,97,102	0
6	EDO	D	407	4/4	0.90	0.69	54,61,63,69	0
5	GOL	B	409	6/6	0.91	0.17	50,57,64,67	0
6	EDO	C	404	4/4	0.91	0.12	52,53,53,55	0
5	GOL	A	410	6/6	0.91	0.13	30,35,52,57	0
4	PEG	A	403	7/7	0.91	0.15	56,57,69,71	0
6	EDO	A	411	4/4	0.92	0.16	40,59,65,65	0
6	EDO	D	403	4/4	0.93	0.08	44,47,55,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	C	403	6/6	0.94	0.13	46,58,61,64	0
6	EDO	C	405	4/4	0.94	0.15	41,45,47,50	0
5	GOL	B	404	6/6	0.94	0.10	43,48,50,51	0
5	GOL	A	405	6/6	0.94	0.17	33,35,44,48	0
5	GOL	A	404	6/6	0.94	0.11	36,40,47,49	0
5	GOL	B	406	6/6	0.95	0.11	30,40,46,53	0
5	GOL	B	405	6/6	0.97	0.14	33,34,42,58	0
5	GOL	D	404	6/6	0.97	0.15	26,36,44,51	0
2	FE2	C	401	1/1	0.98	0.10	24,24,24,24	0
2	FE2	D	401	1/1	0.99	0.09	23,23,23,23	0
3	CO	B	403	1/1	0.99	0.11	22,22,22,22	0
3	CO	C	402	1/1	0.99	0.07	30,30,30,30	0
3	CO	D	402	1/1	0.99	0.11	25,25,25,25	0
2	FE2	B	402	1/1	0.99	0.10	18,18,18,18	0
2	FE2	A	401	1/1	0.99	0.10	19,19,19,19	0
3	CO	A	402	1/1	1.00	0.11	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.