Full wwPDB X-ray Structure Validation Report (i)

Aug 10, 2021 – 10:28 AM EDT

PDB ID	:	5W3U
Title	:	Crystal structure of SsoPox AsB5 mutant (V27A-I76T-Y97W-Y99F-L130P-L 226V)
Authors	:	Hiblot, J.; Gotthard, G.; Jacquet, P.; Daude, D.; Bergonzi, C.; Chabriere, E.; Elias, M.
Deposited on	:	2017-06-08
Resolution	:	2.50 Å(reported)

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

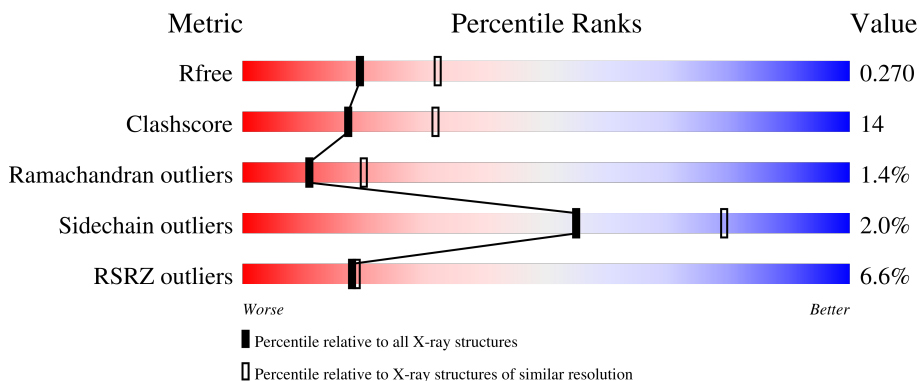|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		14
Ramachandran outliers		1.4%
Sidechain outliers		2.0%
RSRZ outliers		6.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	4% 75% 18% 7%
1	B	314	2% 72% 21% • 5%
1	C	314	3% 61% 29% • 8%
1	D	314	16% 54% 36% • 6%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9481 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aryldialkylphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2343	1501	399	439	4			
1	B	297	Total	C	N	O	S	0	0	0
			2375	1520	406	443	6			
1	C	289	Total	C	N	O	S	0	0	0
			2301	1468	394	433	6			
1	D	294	Total	C	N	O	S	0	1	0
			2349	1502	399	442	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	VAL	engineered mutation	UNP Q97VT7
A	76	THR	ILE	engineered mutation	UNP Q97VT7
A	97	TRP	TYR	engineered mutation	UNP Q97VT7
A	99	PHE	TYR	engineered mutation	UNP Q97VT7
A	130	PRO	LEU	engineered mutation	UNP Q97VT7
A	226	VAL	LEU	engineered mutation	UNP Q97VT7
B	27	ALA	VAL	engineered mutation	UNP Q97VT7
B	76	THR	ILE	engineered mutation	UNP Q97VT7
B	97	TRP	TYR	engineered mutation	UNP Q97VT7
B	99	PHE	TYR	engineered mutation	UNP Q97VT7
B	130	PRO	LEU	engineered mutation	UNP Q97VT7
B	226	VAL	LEU	engineered mutation	UNP Q97VT7
C	27	ALA	VAL	engineered mutation	UNP Q97VT7
C	76	THR	ILE	engineered mutation	UNP Q97VT7
C	97	TRP	TYR	engineered mutation	UNP Q97VT7
C	99	PHE	TYR	engineered mutation	UNP Q97VT7
C	130	PRO	LEU	engineered mutation	UNP Q97VT7
C	226	VAL	LEU	engineered mutation	UNP Q97VT7
D	27	ALA	VAL	engineered mutation	UNP Q97VT7
D	76	THR	ILE	engineered mutation	UNP Q97VT7
D	97	TRP	TYR	engineered mutation	UNP Q97VT7

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W O R L D W I D E
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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
D	99	PHE	TYR	engineered mutation	UNP Q97VT7
D	130	PRO	LEU	engineered mutation	UNP Q97VT7
D	226	VAL	LEU	engineered mutation	UNP Q97VT7

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

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

- Molecule 6 is water.

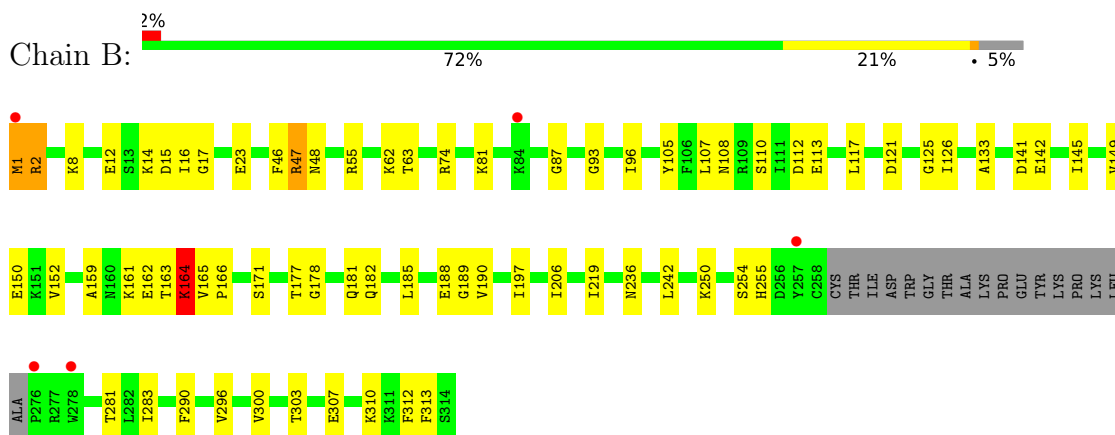| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total 29	O 29	0	0
6	B	28	Total 28	O 28	0	0
6	C	12	Total 12	O 12	0	0
6	D	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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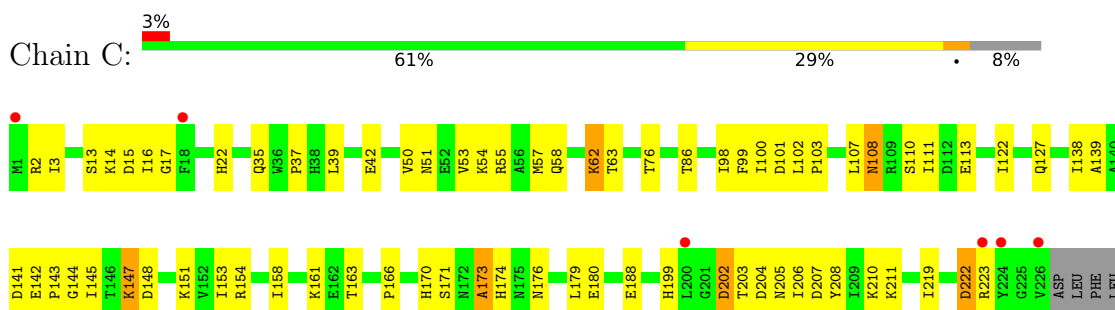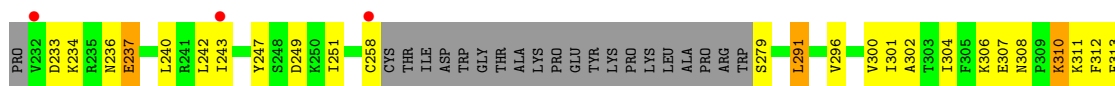
- Molecule 1: Aryldialkylphosphatase

Chain A:
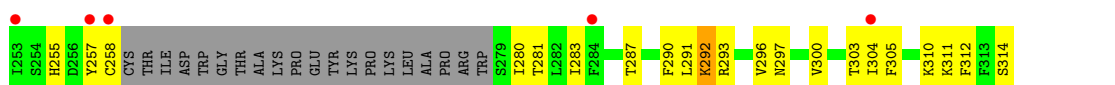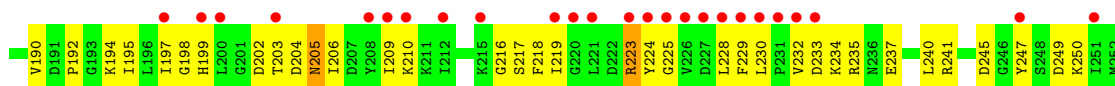
- Molecule 1: Aryldialkylphosphatase

Chain B:

- Molecule 1: Aryldialkylphosphatase

Chain C:

PRO V232 D233 K234 R235 N236 E237 L240 R241 L242 I243 Y247 S248 D249 K250 I251 C258 CYS THR ILE ASP TRP GLY THR ALA LYS PRO GLU TYR LYS PRO LYS LEU ALA PRO ARG TRP S279 L291 V296 V300 I301 A302 T303 I304 F305 K306 E307 N308 P309 K310 K311 F312 F313

S314

• Molecule 1: Aryldialkylphosphatase

Chain D:

16%

54%   36%   •   6%

M1 R2 L5 S10 I11 E12 S13 K14 D15 I21 H24 Q35 N41 E45 F46 V50 N51 E52 V53 K54 R55 D66 P67 M70 R74 R77 K81 V82 L90 G95 I96 W97 I98 D101 L102 P103 F104 Y105 F106 L107 N108 R109 S110 I111

D112 E113 I114 A115 D116 L117 F118 I119 H120 D121 E124 G125 I126 Q127 G128 T129 K137 A140 D141 E142 P143 G144 I145 T146 K147 D148 V149 V152 I153 R154 A157 N160 K161 P166 I167 I168 T169 H170 S171 N172 A173 H174 N175 N176 L179 E180 R183 I184 L185 T186 E187

V190 D191 P192 G193 K194 I195 L196 I197 G198 H199 I200 G201 D202 T203 D204 N205 I206 D207 Y208 I209 K210 K211 I212 K215 G216 S217 F218 I219 G220 L221 D222 R223 Y224 G225 V226 D227 L228 F229 L230 P231 V232 D233 K234 R235 N236 E237 L240 R241 D245 G246 Y247 S248 D249 K250 I251 M252

I253 S254 H255 D256 Y257 C258 CYS THR ILE ASP TRP GLY THR ALA LYS PRO GLU TYR LYS PRO LYS LEU ALA PRO ARG TRP S279 I280 T281 L282 I283 F284 T287 F290 L291 K292 R293 V296 N297 V300 T303 I304 F305 K310 K311 F312 F313 S314

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.93Å 105.95Å 152.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.50 49.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.64-2.50) 99.5 (49.64-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.212 , 0.272 0.211 , 0.270	Depositor DCC
R_{free} test set	2355 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9481	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, EDO, CO, GOL, KCX

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	0.31	0/2376	0.52	0/3207
1	B	0.29	0/2409	0.51	0/3250
1	C	0.28	0/2329	0.55	1/3138 (0.0%)
1	D	0.32	0/2383	0.55	0/3214
All	All	0.30	0/9497	0.53	1/12809 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	291	LEU	CA-CB-CG	8.52	134.90	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2343	0	2354	42	0
1	B	2375	0	2392	50	0
1	C	2301	0	2318	84	0
1	D	2349	0	2367	90	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	16	1	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	B	4	0	6	0	0
6	A	29	0	0	0	0
6	B	28	0	0	0	0
6	C	12	0	0	3	0
6	D	2	0	0	0	0
All	All	9481	0	9477	260	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 14.

All (260) 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:163:THR:O	1:B:164:LYS:HD2	1.37	1.20
1:C:100:ILE:HD11	6:C:510:HOH:O	1.51	1.09
1:C:291:LEU:HD13	1:C:296:VAL:HG21	1.30	1.09
1:B:163:THR:O	1:B:164:LYS:CD	2.16	0.93
1:C:2:ARG:NH1	1:C:13:SER:OG	2.02	0.92
1:C:179:LEU:HD11	1:C:211:LYS:HE3	1.50	0.90
1:D:292:LYS:H	1:D:296:VAL:HB	1.38	0.87
1:C:219:ILE:O	1:C:219:ILE:HD12	1.76	0.85
1:C:291:LEU:CD1	1:C:296:VAL:HG21	2.07	0.83
1:B:178:GLY:HA2	1:B:181:GLN:HE21	1.46	0.80
1:C:100:ILE:CD1	6:C:510:HOH:O	2.17	0.79
1:A:2:ARG:HH12	1:A:13:SER:HB3	1.46	0.79
1:D:2:ARG:HB2	1:D:12:GLU:HA	1.63	0.79
1:D:223:ARG:O	1:D:235:ARG:NH2	2.16	0.78
1:C:17:GLY:HA3	1:C:62:LYS:HE3	1.67	0.76
1:C:207:ASP:HA	1:C:210:LYS:HD3	1.67	0.76
1:C:145:ILE:HG13	1:C:180:GLU:HG2	1.66	0.76
1:A:51:ASN:OD1	1:A:52:GLU:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:HB2	1:B:197:ILE:HD11	1.68	0.74
1:B:107:LEU:O	1:B:108:ASN:OD1	2.07	0.73
1:C:15:ASP:O	1:C:62:LYS:NZ	2.17	0.73
1:A:180:GLU:OE1	1:A:183:ARG:NH1	2.22	0.73
1:C:139:ALA:HA	1:C:170:HIS:HB3	1.71	0.72
1:D:24:HIS:HB2	1:D:258:CYS:HA	1.72	0.72
1:B:303:THR:HA	1:B:307:GLU:HB2	1.72	0.72
1:D:2:ARG:HH22	1:D:314:SER:HA	1.56	0.70
1:C:222:ASP:OD1	1:C:223:ARG:NE	2.24	0.70
1:D:232:VAL:HA	1:D:235:ARG:HD2	1.74	0.69
1:A:164:LYS:HG2	4:A:404:GOL:H12	1.75	0.69
1:B:17:GLY:HA3	1:B:62:LYS:HE2	1.75	0.69
1:D:74:ARG:HD2	1:D:127:GLN:HE22	1.59	0.67
1:D:255:HIS:CE1	1:D:283:ILE:HG12	2.29	0.67
1:B:96:ILE:HB	1:B:152:VAL:HG21	1.75	0.67
1:C:296:VAL:HB	1:C:300:VAL:HG11	1.77	0.67
1:C:233:ASP:HB2	1:C:236:ASN:HB2	1.76	0.67
1:D:224:TYR:HB2	1:D:255:HIS:HA	1.76	0.66
1:C:251:ILE:HG23	1:C:304:ILE:HG12	1.77	0.66
1:C:291:LEU:HD13	1:C:296:VAL:CG2	2.18	0.64
1:D:169:THR:HG22	1:D:197:ILE:HA	1.79	0.64
1:D:209:ILE:HG23	1:D:219:ILE:HD13	1.80	0.63
1:D:14:LYS:HA	1:D:310:LYS:HD2	1.78	0.63
1:D:224:TYR:N	1:D:255:HIS:O	2.20	0.63
1:C:161:LYS:HE3	1:C:188:GLU:O	1.99	0.63
1:B:15:ASP:O	1:B:62:LYS:NZ	2.28	0.62
1:D:41:ASN:O	1:D:45:GLU:HG3	2.00	0.62
1:D:202:ASP:HB3	1:D:230:LEU:HB2	1.80	0.62
1:B:110:SER:HB3	1:B:113:GLU:HG3	1.82	0.62
1:C:240:LEU:HD13	1:C:291:LEU:HD22	1.83	0.61
1:D:203:THR:HG22	1:D:205:ASN:HB3	1.83	0.61
1:B:177:THR:O	1:B:181:GLN:HG3	2.01	0.61
1:B:161:LYS:NZ	1:B:188:GLU:O	2.26	0.60
1:C:100:ILE:HG13	1:C:101:ASP:H	1.66	0.60
1:D:126:ILE:O	1:D:129:THR:OG1	2.17	0.60
1:D:297:ASN:O	1:D:300:VAL:HG12	2.02	0.60
1:C:2:ARG:HH22	1:C:13:SER:CB	2.15	0.60
1:C:291:LEU:HD12	1:C:301:ILE:HD11	1.83	0.60
1:C:98:ILE:HD12	1:C:102:LEU:HD23	1.84	0.59
1:C:35:GLN:HG3	1:D:70:MET:HB2	1.85	0.59
1:A:307:GLU:OE1	1:A:310:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASP:OD1	1:B:142:GLU:N	2.35	0.59
1:B:16:ILE:HD11	1:B:63:THR:HG21	1.83	0.59
1:B:206:ILE:HD11	1:B:242:LEU:HG	1.84	0.58
1:D:290:PHE:HD1	1:D:293:ARG:HH11	1.51	0.58
1:A:291:LEU:HB3	1:A:296:VAL:HG21	1.86	0.58
1:C:111:ILE:HG22	1:C:151:LYS:HG2	1.86	0.57
1:D:46:PHE:CE1	1:D:81:LYS:HD2	2.40	0.57
1:C:2:ARG:HH22	1:C:13:SER:HB2	1.68	0.57
1:A:39:LEU:HD22	1:B:105:TYR:OH	2.05	0.56
1:D:172:ASN:OD1	1:D:173:ALA:N	2.38	0.56
1:A:206:ILE:HD11	1:A:242:LEU:HG	1.88	0.56
1:C:171:SER:O	1:C:199:HIS:HB2	2.06	0.56
1:C:166:PRO:HB2	1:C:312:PHE:CZ	2.40	0.56
1:C:251:ILE:O	1:C:308:ASN:ND2	2.38	0.56
1:B:296:VAL:HG13	1:B:300:VAL:CG1	2.36	0.56
1:C:51:ASN:HA	1:C:54:LYS:HE2	1.88	0.56
1:A:2:ARG:HH12	1:A:13:SER:CB	2.18	0.55
1:D:67:PRO:HB2	1:D:137:KCX:HG2	1.89	0.55
1:D:202:ASP:H	1:D:223:ARG:HH21	1.55	0.55
1:A:241:ARG:NH1	1:A:245:ASP:OD2	2.40	0.55
1:C:219:ILE:HD12	1:C:251:ILE:HA	1.88	0.55
1:D:77:ARG:NH2	1:D:127:GLN:O	2.41	0.54
1:A:33:ARG:HD2	1:A:40:TYR:CD2	2.43	0.54
1:C:219:ILE:CD1	1:C:251:ILE:HA	2.38	0.54
1:B:1:MET:SD	1:B:1:MET:N	2.81	0.54
1:D:108:ASN:OD1	1:D:109:ARG:N	2.40	0.53
1:A:2:ARG:NH1	1:A:13:SER:H	2.06	0.53
1:D:304:ILE:HD11	1:D:305:PHE:CE2	2.44	0.53
1:B:178:GLY:HA2	1:B:181:GLN:NE2	2.21	0.53
1:B:159:ALA:O	1:B:163:THR:OG1	2.20	0.53
1:D:210:LYS:HB2	1:D:247:TYR:CZ	2.44	0.53
1:D:157:ALA:O	1:D:161:LYS:HD3	2.09	0.52
1:A:240:LEU:HD11	1:A:244:LYS:HE3	1.91	0.52
1:B:126:ILE:HD11	1:B:133:ALA:HB2	1.90	0.52
1:D:233:ASP:OD1	1:D:234:LYS:N	2.42	0.52
1:D:287:THR:O	1:D:291:LEU:HD12	2.09	0.52
1:A:150:GLU:O	1:A:154:ARG:HG3	2.09	0.52
1:C:243:ILE:HD12	1:C:291:LEU:HD21	1.91	0.52
1:A:46:PHE:HE1	1:A:81:LYS:HB3	1.74	0.52
1:B:74:ARG:NH1	1:B:93:GLY:O	2.37	0.51
1:B:8:LYS:NZ	1:B:87:GLY:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:VAL:HG13	1:B:300:VAL:HG11	1.93	0.51
1:B:1:MET:SD	1:B:12:GLU:HG3	2.51	0.51
1:C:110:SER:OG	1:C:113:GLU:HG3	2.11	0.51
1:A:173:ALA:HB1	1:A:203:THR:HB	1.91	0.51
1:A:2:ARG:HH22	1:A:314:SER:HA	1.74	0.51
1:D:297:ASN:OD1	1:D:297:ASN:N	2.43	0.51
1:A:52:GLU:OE2	1:A:280:ILE:HG22	2.10	0.51
1:A:77:ARG:NH1	1:A:127:GLN:O	2.38	0.51
1:D:105:TYR:O	1:D:109:ARG:NH1	2.44	0.50
1:A:55:ARG:O	1:A:58:GLN:HB2	2.12	0.50
1:B:236:ASN:HB3	1:B:290:PHE:CE2	2.47	0.50
1:C:2:ARG:CZ	1:C:13:SER:OG	2.60	0.50
1:A:150:GLU:OE1	1:A:154:ARG:NH1	2.45	0.50
1:D:291:LEU:C	1:D:293:ARG:H	2.15	0.50
1:C:3:ILE:HD11	1:C:313:PHE:HB3	1.94	0.49
1:D:202:ASP:H	1:D:223:ARG:NH2	2.10	0.49
1:C:142:GLU:O	1:C:144:GLY:N	2.44	0.49
1:C:199:HIS:H	1:C:223:ARG:HH11	1.59	0.49
1:C:99:PHE:CE1	1:C:141:ASP:HB2	2.47	0.49
1:A:33:ARG:NH2	1:A:42:GLU:HG3	2.28	0.49
1:D:160:ASN:OD1	1:D:190:VAL:HG13	2.13	0.49
1:D:120:HIS:O	1:D:124:GLU:HB2	2.13	0.49
1:B:171:SER:HB3	1:B:181:GLN:NE2	2.27	0.48
1:C:127:GLN:HE21	1:D:35:GLN:HA	1.77	0.48
1:C:291:LEU:O	1:C:296:VAL:HG22	2.13	0.48
1:D:52:GLU:OE1	1:D:55:ARG:NH2	2.45	0.48
1:D:249:ASP:OD1	1:D:249:ASP:N	2.45	0.48
1:D:102:LEU:HD22	1:D:148:ASP:OD2	2.13	0.48
1:C:173:ALA:HB2	1:C:202:ASP:HB2	1.95	0.48
1:D:225:GLY:HA3	1:D:257:TYR:HA	1.94	0.48
1:A:46:PHE:CE1	1:A:81:LYS:HB3	2.48	0.48
1:B:166:PRO:HB2	1:B:312:PHE:CZ	2.49	0.48
1:D:290:PHE:HD1	1:D:293:ARG:NH1	2.11	0.47
1:B:46:PHE:CE1	1:B:81:LYS:HG2	2.49	0.47
1:C:138:ILE:HD12	1:C:153:ILE:HG12	1.95	0.47
1:C:55:ARG:O	1:C:58:GLN:HB2	2.14	0.47
1:C:176:ASN:HA	1:C:208:TYR:OH	2.14	0.47
1:B:23:GLU:OE1	1:B:254:SER:OG	2.32	0.47
1:C:204:ASP:O	1:C:206:ILE:N	2.47	0.47
1:D:96:ILE:CD1	1:D:98:ILE:HG12	2.44	0.47
1:D:111:ILE:HG13	1:D:112:ASP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:THR:HG22	1:D:198:GLY:H	1.80	0.47
1:A:255:HIS:CE1	1:A:283:ILE:HG12	2.49	0.47
1:D:52:GLU:OE2	1:D:280:ILE:HG22	2.15	0.47
1:C:39:LEU:HD21	1:D:105:TYR:OH	2.14	0.47
1:D:255:HIS:NE2	1:D:283:ILE:HG12	2.30	0.47
1:A:291:LEU:HB3	1:A:296:VAL:CG2	2.44	0.47
1:C:242:LEU:O	1:C:247:TYR:HB2	2.15	0.47
1:D:74:ARG:HH11	1:D:126:ILE:HG23	1.80	0.47
1:D:141:ASP:H	1:D:143:PRO:HD2	1.80	0.47
1:D:197:ILE:O	1:D:197:ILE:HD12	2.15	0.46
1:B:161:LYS:NZ	1:B:189:GLY:O	2.47	0.46
1:C:310:LYS:O	1:C:314:SER:OG	2.27	0.46
1:B:149:VAL:O	1:B:152:VAL:HG12	2.15	0.46
1:D:10:SER:O	1:D:11:ILE:HD12	2.16	0.46
1:C:35:GLN:OE1	1:D:74:ARG:HB3	2.15	0.46
1:D:55:ARG:HD2	1:D:281:THR:HG21	1.98	0.46
1:A:297:ASN:ND2	1:A:299:GLU:HB2	2.32	0.45
1:A:166:PRO:HB2	1:A:312:PHE:CZ	2.51	0.45
1:A:224:TYR:HE2	1:A:236:ASN:OD1	1.99	0.45
1:B:181:GLN:O	1:B:185:LEU:HD12	2.16	0.45
1:B:219:ILE:HG12	1:B:250:LYS:O	2.17	0.45
1:C:202:ASP:OD1	1:C:202:ASP:N	2.49	0.45
1:C:258:CYS:SG	6:C:512:HOH:O	2.61	0.45
1:D:140:ALA:HB2	1:D:149:VAL:HG21	1.98	0.45
1:D:96:ILE:HG13	1:D:152:VAL:HG21	1.97	0.45
1:D:194:LYS:HE2	1:D:194:LYS:HA	1.99	0.45
1:A:236:ASN:HB3	1:A:290:PHE:CD2	2.51	0.45
1:D:192:PRO:HB2	1:D:216:GLY:HA3	1.98	0.45
1:D:218:PHE:HA	1:D:250:LYS:HB3	1.99	0.45
1:C:14:LYS:HA	1:C:310:LYS:HD2	1.98	0.45
1:D:5:LEU:HD22	1:D:11:ILE:HD13	1.99	0.45
1:A:255:HIS:NE2	1:A:283:ILE:HG23	2.32	0.44
1:C:234:LYS:HE2	1:C:234:LYS:HB2	1.86	0.44
1:B:145:ILE:HD11	1:B:150:GLU:HB2	1.99	0.44
1:B:162:GLU:N	1:B:162:GLU:OE1	2.50	0.44
1:D:95:GLY:HA2	1:D:118:PHE:CE1	2.52	0.44
1:D:169:THR:CG2	1:D:197:ILE:HA	2.45	0.44
1:B:121:ASP:HA	1:B:125:GLY:O	2.18	0.44
1:C:173:ALA:HB1	1:C:203:THR:OG1	2.17	0.44
1:D:237:GLU:HA	1:D:240:LEU:HB3	1.99	0.44
1:A:297:ASN:OD1	1:A:297:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:VAL:HB	1:C:86:THR:HG21	1.98	0.44
1:C:98:ILE:HD11	1:C:103:PRO:HD3	2.00	0.44
1:B:47:ARG:HG3	1:B:48:ASN:N	2.33	0.44
1:C:100:ILE:CG1	1:C:101:ASP:H	2.29	0.44
1:C:37:PRO:C	1:C:39:LEU:H	2.21	0.44
1:D:66:ASP:HB2	1:D:90:LEU:HD11	1.99	0.44
1:D:179:LEU:O	1:D:183:ARG:HB2	2.18	0.44
1:C:16:ILE:HD11	1:C:63:THR:HG21	1.98	0.43
1:C:107:LEU:O	1:C:108:ASN:HB2	2.18	0.43
1:D:14:LYS:HG3	1:D:15:ASP:OD1	2.17	0.43
1:D:14:LYS:O	1:D:310:LYS:NZ	2.50	0.43
1:C:154:ARG:O	1:C:158:ILE:HG13	2.18	0.43
1:A:53:VAL:O	1:A:57:MET:HG3	2.18	0.43
1:B:185:LEU:HB3	1:B:190:VAL:HG21	1.99	0.43
1:D:50:VAL:O	1:D:54:LYS:HG2	2.18	0.43
1:D:184:ILE:O	1:D:187:GLU:HG3	2.17	0.43
1:A:166:PRO:HB3	1:A:194:LYS:HD2	2.00	0.43
1:A:200:LEU:O	1:A:203:THR:HG22	2.18	0.43
1:D:167:ILE:HB	1:D:195:ILE:HD12	2.00	0.43
1:D:14:LYS:HA	1:D:310:LYS:CD	2.47	0.43
1:D:74:ARG:HD2	1:D:127:GLN:NE2	2.31	0.43
1:D:137:KCX:OQ2	1:D:170:HIS:HB2	2.18	0.43
1:A:255:HIS:NE2	1:A:283:ILE:HG12	2.33	0.43
1:B:312:PHE:HD2	1:B:313:PHE:CE1	2.36	0.43
1:C:39:LEU:HD23	1:C:39:LEU:O	2.19	0.43
1:D:143:PRO:HB2	1:D:144:GLY:H	1.67	0.43
1:D:161:LYS:HE3	1:D:190:VAL:HG22	2.01	0.43
1:A:110:SER:OG	1:A:113:GLU:HG3	2.19	0.43
1:B:55:ARG:HD2	1:B:281:THR:HG21	1.99	0.43
1:C:147:LYS:HD3	1:C:148:ASP:N	2.34	0.43
1:C:308:ASN:HA	1:C:311:LYS:HE3	2.01	0.42
1:B:178:GLY:O	1:B:197:ILE:HD13	2.19	0.42
1:C:16:ILE:HG22	1:C:310:LYS:HE2	2.02	0.42
1:C:237:GLU:N	1:C:237:GLU:OE1	2.52	0.42
1:D:166:PRO:HB2	1:D:312:PHE:CZ	2.54	0.42
1:B:164:LYS:HD3	1:B:165:VAL:N	2.35	0.42
1:C:307:GLU:O	1:C:311:LYS:HG3	2.19	0.42
1:A:76:THR:HG21	1:A:131:ASN:HB2	2.01	0.42
1:B:16:ILE:HG22	1:B:310:LYS:HG2	2.01	0.42
1:C:302:ALA:O	1:C:306:LYS:HB2	2.20	0.42
1:C:50:VAL:O	1:C:54:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:HIS:NE2	1:C:203:THR:HA	2.35	0.42
1:D:300:VAL:O	1:D:303:THR:HB	2.19	0.42
1:B:296:VAL:HG13	1:B:300:VAL:HG13	2.02	0.42
1:C:249:ASP:OD1	1:C:249:ASP:N	2.52	0.42
1:C:53:VAL:O	1:C:57:MET:HG3	2.20	0.42
1:D:173:ALA:HB1	1:D:203:THR:OG1	2.20	0.42
1:A:234:LYS:HD3	1:A:234:LYS:N	2.35	0.42
1:C:307:GLU:O	1:C:310:LYS:HB3	2.20	0.42
1:A:2:ARG:HH12	1:A:13:SER:H	1.67	0.42
1:B:14:LYS:HA	1:B:310:LYS:HD3	2.02	0.42
1:C:2:ARG:NH2	1:C:13:SER:OG	2.52	0.42
1:B:171:SER:HB3	1:B:181:GLN:HE22	1.86	0.41
1:A:36:TRP:CE3	1:B:117:LEU:HD21	2.54	0.41
1:B:185:LEU:O	1:B:190:VAL:HG22	2.20	0.41
1:C:142:GLU:C	1:C:144:GLY:H	2.23	0.41
1:B:255:HIS:CE1	1:B:283:ILE:HG12	2.56	0.41
1:C:13:SER:O	1:C:310:LYS:HE2	2.20	0.41
1:C:76:THR:HG22	1:C:127:GLN:OE1	2.20	0.41
1:D:115:ALA:O	1:D:119:ILE:HD12	2.20	0.41
1:C:2:ARG:HB3	1:C:2:ARG:HH11	1.85	0.41
1:D:204:ASP:O	1:D:206:ILE:N	2.54	0.41
1:D:203:THR:CG2	1:D:205:ASN:HB3	2.50	0.41
1:A:102:LEU:HG	1:A:148:ASP:HB3	2.02	0.41
1:C:179:LEU:HB2	1:C:208:TYR:HE1	1.86	0.41
1:C:22:HIS:CE1	1:C:223:ARG:HH22	2.37	0.41
1:D:291:LEU:C	1:D:293:ARG:N	2.73	0.41
1:A:3:ILE:CD1	1:A:13:SER:HA	2.51	0.40
1:C:222:ASP:HB2	1:C:223:ARG:H	1.71	0.40
1:D:183:ARG:HD2	1:D:183:ARG:C	2.42	0.40
1:D:249:ASP:HB2	1:D:311:LYS:NZ	2.35	0.40
1:C:122:ILE:HG21	1:C:163:THR:HB	2.03	0.40
1:D:121:ASP:HA	1:D:125:GLY:O	2.21	0.40
1:D:210:LYS:HB2	1:D:247:TYR:CE1	2.57	0.40
1:C:55:ARG:NH2	1:C:279:SER:OG	2.52	0.40
1:D:170:HIS:HA	1:D:199:HIS:HD2	1.87	0.40
1:D:184:ILE:HD12	1:D:184:ILE:H	1.86	0.40
1:D:192:PRO:O	1:D:217:SER:HA	2.22	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	288/314 (92%)	270 (94%)	17 (6%)	1 (0%)	41	61
1	B	292/314 (93%)	273 (94%)	17 (6%)	2 (1%)	22	39
1	C	282/314 (90%)	252 (89%)	24 (8%)	6 (2%)	7	11
1	D	290/314 (92%)	248 (86%)	35 (12%)	7 (2%)	6	9
All	All	1152/1256 (92%)	1043 (90%)	93 (8%)	16 (1%)	11	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	108	ASN
1	C	173	ALA
1	C	205	ASN
1	D	143	PRO
1	D	205	ASN
1	D	223	ARG
1	D	292	LYS
1	D	229	PHE
1	A	205	ASN
1	B	2	ARG
1	B	164	LYS
1	C	237	GLU
1	D	146	THR
1	C	222	ASP
1	C	143	PRO
1	D	67	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	253/271 (93%)	253 (100%)	0	100	100
1	B	257/271 (95%)	252 (98%)	5 (2%)	57	80
1	C	249/271 (92%)	244 (98%)	5 (2%)	55	79
1	D	255/271 (94%)	245 (96%)	10 (4%)	32	57
All	All	1014/1084 (94%)	994 (98%)	20 (2%)	55	79

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	2	ARG
1	B	47	ARG
1	B	112	ASP
1	B	164	LYS
1	C	42	GLU
1	C	62	LYS
1	C	147	LYS
1	C	202	ASP
1	C	310	LYS
1	D	77	ARG
1	D	82	VAL
1	D	102	LEU
1	D	109	ARG
1	D	154	ARG
1	D	176	ASN
1	D	179	LEU
1	D	228	LEU
1	D	241	ARG
1	D	245	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	B	58	GLN
1	B	108	ASN
1	B	181	GLN
1	C	38	HIS

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Mol	Chain	Res	Type
1	D	22	HIS
1	D	127	GLN
1	D	131	ASN
1	D	176	ASN
1	D	199	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	KCX	C	137	1,2,3	7,11,12	0.79	0	4,12,14	0.92	0
1	KCX	B	137	1,2,3	7,11,12	0.78	0	4,12,14	0.91	0
1	KCX	D	137	1,2,3	7,11,12	0.82	0	4,12,14	0.61	0
1	KCX	A	137	1,2,3	7,11,12	0.63	0	4,12,14	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	137	1,2,3	-	2/7/10/12	-
1	KCX	B	137	1,2,3	-	0/7/10/12	-
1	KCX	D	137	1,2,3	-	2/7/10/12	-
1	KCX	A	137	1,2,3	-	0/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	137	KCX	N-CA-CB-CG
1	D	137	KCX	C-CA-CB-CG
1	C	137	KCX	N-CA-CB-CG
1	C	137	KCX	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	GOL	C	403	-	5,5,5	0.38	0	5,5,5	0.36	0
5	EDO	B	403	-	3,3,3	0.44	0	2,2,2	0.35	0
4	GOL	A	403	-	5,5,5	0.37	0	5,5,5	0.33	0
4	GOL	A	404	-	5,5,5	0.40	0	5,5,5	0.31	0
4	GOL	B	404	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	D	403	-	5,5,5	0.36	0	5,5,5	0.39	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	GOL	C	403	-	-	2/4/4/4	-
5	EDO	B	403	-	-	0/1/1/1	-
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	A	404	-	-	2/4/4/4	-
4	GOL	B	404	-	-	3/4/4/4	-
4	GOL	D	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	GOL	1	0

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, 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	292/314 (92%)	0.29	11 (3%)	40	43	35, 64, 123, 186	0
1	B	296/314 (94%)	0.19	5 (1%)	70	72	42, 76, 112, 162	0
1	C	288/314 (91%)	0.42	10 (3%)	44	47	41, 87, 136, 179	0
1	D	293/314 (93%)	0.97	51 (17%)	1	1	56, 101, 161, 197	0
All	All	1169/1256 (93%)	0.47	77 (6%)	18	19	35, 81, 142, 197	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	230	LEU	8.6
1	D	228	LEU	8.2
1	D	229	PHE	7.8
1	D	258	CYS	7.5
1	D	145	ILE	7.1
1	C	232	VAL	7.0
1	D	209	ILE	6.9
1	D	224	TYR	6.6
1	D	226	VAL	6.0
1	A	278	TRP	5.9
1	D	225	GLY	5.9
1	B	1	MET	5.6
1	A	229	PHE	5.4
1	D	197	ILE	5.3
1	A	230	LEU	5.2
1	D	173	ALA	5.1
1	B	278	TRP	4.9
1	D	223	ARG	4.9
1	D	144	GLY	4.9
1	D	232	VAL	4.7
1	D	219	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	257	TYR	4.5
1	C	258	CYS	4.3
1	D	174	HIS	4.2
1	C	224	TYR	4.2
1	D	227	ASP	4.0
1	A	232	VAL	3.9
1	C	1	MET	3.8
1	C	226	VAL	3.8
1	D	106	PHE	3.7
1	D	231	PRO	3.5
1	D	200	LEU	3.5
1	B	84	LYS	3.5
1	A	257	TYR	3.4
1	D	215	LYS	3.4
1	A	231	PRO	3.2
1	D	221	LEU	3.2
1	B	276	PRO	3.2
1	A	226	VAL	3.1
1	C	223	ARG	3.0
1	D	233	ASP	2.9
1	D	179	LEU	2.9
1	D	199	HIS	2.9
1	A	233	ASP	2.8
1	D	212	ILE	2.7
1	D	180[A]	GLU	2.7
1	A	227	ASP	2.7
1	D	210	LYS	2.7
1	C	200	LEU	2.6
1	D	185	LEU	2.6
1	A	225	GLY	2.5
1	D	105	TYR	2.5
1	D	114	ILE	2.5
1	D	98	ILE	2.5
1	D	304	ILE	2.4
1	D	247	TYR	2.3
1	D	140	ALA	2.3
1	D	208	TYR	2.3
1	D	253	ILE	2.3
1	C	243	ILE	2.3
1	A	2	ARG	2.2
1	B	257	TYR	2.2
1	C	18	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	220	GLY	2.2
1	D	251	ILE	2.2
1	C	314	SER	2.2
1	D	109	ARG	2.2
1	D	21	ILE	2.2
1	D	101	ASP	2.1
1	D	203	THR	2.1
1	D	104	PHE	2.1
1	D	284	PHE	2.1
1	D	124	GLU	2.1
1	D	184	ILE	2.1
1	D	97	TRP	2.1
1	D	108	ASN	2.0
1	D	117	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	D	137	12/13	0.92	0.23	82,93,121,166	0
1	KCX	B	137	12/13	0.96	0.17	50,57,74,75	0
1	KCX	A	137	12/13	0.96	0.18	32,48,62,74	0
1	KCX	C	137	12/13	0.97	0.17	39,54,93,94	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	GOL	D	403	6/6	0.84	0.32	106,119,127,133	0
4	GOL	A	403	6/6	0.88	0.18	91,94,96,104	0
2	FE2	A	401	1/1	0.89	0.24	65,65,65,65	0
3	CO	D	402	1/1	0.89	0.08	162,162,162,162	0
3	CO	C	402	1/1	0.90	0.20	130,130,130,130	0
5	EDO	B	403	4/4	0.90	0.17	66,67,73,73	0
3	CO	B	402	1/1	0.92	0.14	55,55,55,55	0
4	GOL	A	404	6/6	0.93	0.17	67,69,75,76	0
4	GOL	B	404	6/6	0.93	0.19	83,94,112,116	0
2	FE2	B	401	1/1	0.94	0.17	46,46,46,46	0
3	CO	A	402	1/1	0.95	0.16	92,92,92,92	0
4	GOL	C	403	6/6	0.95	0.23	67,73,93,100	0
2	FE2	C	401	1/1	0.98	0.14	78,78,78,78	0
2	FE2	D	401	1/1	0.98	0.13	112,112,112,112	0

6.5 Other polymers ⓘ

There are no such residues in this entry.