



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4NUF  
Title : Crystal Structure of SHP/EID1  
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Deposited on : 2013-12-03  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

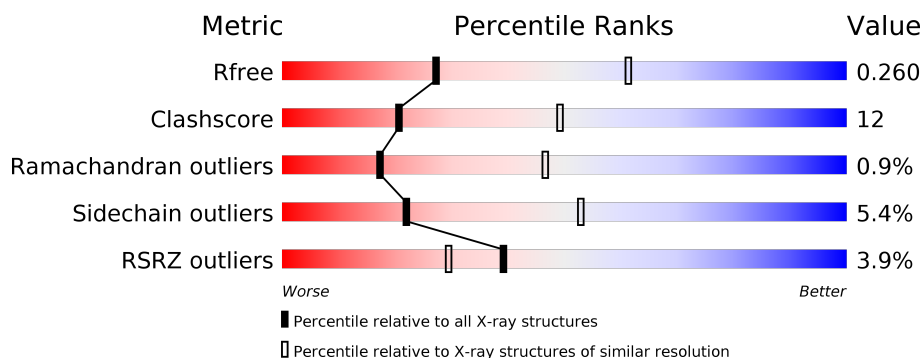
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	580	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 5%</div> </div> </div>
2	P	16	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>38%</div> </div> </div>
3	B	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4493 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 Maltose ABC transporter periplasmic protein, Nuclear receptor subfamily 0 group B member 2 chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4295	2769	712	798	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP K0BGG6
A	369	ASN	-	linker	UNP K0BGG6
A	370	ALA	-	linker	UNP K0BGG6
A	371	ALA	-	linker	UNP K0BGG6
A	372	ALA	-	linker	UNP K0BGG6
A	1053	GLU	-	linker	UNP K0BGG6
A	1054	PHE	-	linker	UNP K0BGG6
A	1085	ASP	GLU	engineered mutation	UNP Q62227
A	1126	THR	LEU	engineered mutation	UNP Q62227
A	1127	THR	GLU	engineered mutation	UNP Q62227
A	1128	ARG	GLU	engineered mutation	UNP Q62227
A	1228	ARG	LYS	engineered mutation	UNP Q62227

- Molecule 2 is a protein called EID1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	16	Total	C	N	O	S	0	0	0
			126	80	23	22	1			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	B	2	Total	C	O	0	0	0
			23	12	11			

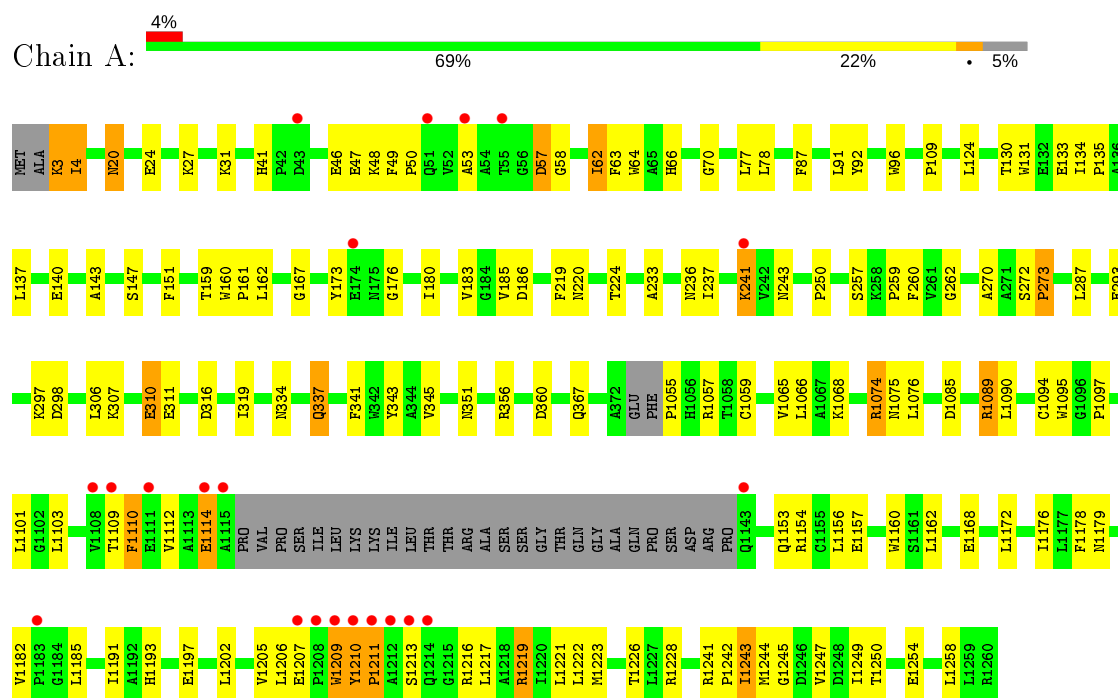
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	P	1	Total	O	0	0
			1	1		

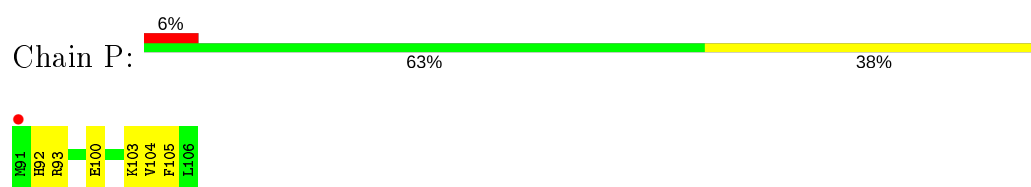
### 3 Residue-property plots [i](#)

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: Maltose ABC transporter periplasmic protein, Nuclear receptor subfamily 0 group B member 2 chimeric construct



- Molecule 2: EID1 peptide



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.39Å 105.15Å 136.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.3 (30.00-2.80) 94.3 (29.77-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.196 , 0.245 0.213 , 0.260	Depositor DCC
$R_{free}$ test set	1410 reflections (6.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

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	0.45	0/4401	0.55	0/5982
2	P	0.48	0/127	0.53	0/169
All	All	0.45	0/4528	0.55	0/6151

There are no bond length outliers.

There are no bond angle outliers.

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	4295	0	4268	106	0
2	P	126	0	128	5	0
3	B	23	0	21	0	0
4	A	48	0	0	4	0
4	P	1	0	0	0	0
All	All	4493	0	4417	109	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 12.

All (109) 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:A:1101:LEU:HD22	1:A:1176:ILE:HD12	1.65	0.77
1:A:1210:TYR:HB2	1:A:1211:PRO:HD3	1.68	0.75
1:A:124:LEU:HD11	1:A:137:LEU:HD21	1.70	0.73
1:A:337:GLN:H	1:A:337:GLN:NE2	1.88	0.70
1:A:186:ASP:OD1	1:A:367:GLN:HG3	1.92	0.70
1:A:337:GLN:H	1:A:337:GLN:HE21	1.38	0.69
1:A:1244:MET:HE2	1:A:1247:VAL:HG21	1.75	0.68
1:A:1244:MET:HG3	1:A:1247:VAL:HG21	1.76	0.68
1:A:1065:VAL:HG21	1:A:1103:LEU:HD23	1.77	0.67
1:A:241:LYS:HA	4:A:1430:HOH:O	1.95	0.66
1:A:173:TYR:OH	1:A:176:GLY:HA2	1.96	0.65
1:A:1210:TYR:CB	1:A:1211:PRO:HD3	2.27	0.64
1:A:70:GLY:HA3	1:A:334:ASN:O	1.97	0.64
1:A:62:ILE:HD13	1:A:63:PHE:N	2.13	0.63
1:A:186:ASP:CG	1:A:367:GLN:HG3	2.20	0.62
1:A:3:LYS:O	1:A:4:ILE:HB	2.00	0.62
1:A:1202:LEU:O	1:A:1205:VAL:HG12	2.00	0.61
1:A:1059:CYS:HB2	1:A:1243:ILE:HD12	1.83	0.61
1:A:91:LEU:HD13	1:A:109:PRO:HG2	1.84	0.59
1:A:1162:LEU:HD22	1:A:1223:MET:SD	2.43	0.58
1:A:1068:LYS:HB3	2:P:105:PHE:CZ	2.39	0.58
1:A:173:TYR:CZ	1:A:176:GLY:HA2	2.39	0.57
1:A:1241:ARG:HB3	1:A:1242:PRO:HD3	1.86	0.57
1:A:151:PHE:HE2	1:A:159:THR:HG22	1.70	0.57
1:A:220:ASN:HD21	1:A:237:ILE:HG12	1.70	0.56
1:A:1110:PHE:CE2	1:A:1153:GLN:HB3	2.40	0.56
1:A:307:LYS:O	1:A:311:GLU:HG3	2.06	0.56
1:A:46:GLU:HG3	1:A:47:GLU:HG3	1.86	0.56
1:A:161:PRO:HG3	1:A:259:PRO:HA	1.88	0.55
1:A:92:TYR:OH	1:A:310:GLU:HG2	2.07	0.55
1:A:4:ILE:HG13	1:A:57:ASP:HA	1.88	0.55
1:A:46:GLU:HB3	1:A:64:TRP:CZ2	2.42	0.55
1:A:1210:TYR:H	1:A:1211:PRO:CD	2.19	0.54
1:A:4:ILE:HG22	1:A:273:PRO:HD3	1.89	0.54
1:A:219:PHE:HA	1:A:224:THR:HG22	1.88	0.54
1:A:1250:THR:O	1:A:1254:GLU:HG3	2.07	0.53
1:A:1075:ASN:O	1:A:1076:LEU:HB3	2.07	0.52
1:A:337:GLN:N	1:A:337:GLN:NE2	2.55	0.52
1:A:48:LYS:HZ2	1:A:48:LYS:HB2	1.74	0.51
1:A:91:LEU:HD12	1:A:96:TRP:CZ2	2.45	0.51
1:A:1153:GLN:O	1:A:1157:GLU:HG3	2.11	0.51
1:A:1209:TRP:HB3	1:A:1213:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HG21	1:A:272:SER:HA	1.92	0.50
1:A:1097:PRO:HG3	1:A:1228:ARG:HA	1.93	0.50
1:A:48:LYS:NZ	1:A:48:LYS:HB2	2.27	0.50
1:A:1182:VAL:HB	1:A:1185:LEU:HD22	1.93	0.50
1:A:53:ALA:HB3	1:A:77:LEU:HD13	1.93	0.49
1:A:130:THR:O	1:A:133:GLU:HG2	2.12	0.49
1:A:1110:PHE:CZ	1:A:1153:GLN:HB3	2.46	0.49
1:A:1207:GLU:O	1:A:1209:TRP:N	2.46	0.49
1:A:180:ILE:HG22	1:A:337:GLN:HG3	1.94	0.48
2:P:100:GLU:HA	2:P:103:LYS:NZ	2.28	0.48
1:A:236:ASN:HB2	4:A:1420:HOH:O	2.13	0.48
1:A:131:TRP:CE2	1:A:162:LEU:HD13	2.48	0.48
1:A:316:ASP:HB3	1:A:319:ILE:HG12	1.95	0.48
1:A:1097:PRO:HB2	1:A:1176:ILE:HG21	1.95	0.47
1:A:134:ILE:HB	1:A:135:PRO:HD3	1.95	0.47
1:A:20:ASN:HB2	1:A:298:ASP:OD2	2.15	0.47
1:A:1055:PRO:C	1:A:1057:ARG:H	2.17	0.47
1:A:1209:TRP:O	1:A:1209:TRP:HD1	1.98	0.47
1:A:183:VAL:HG12	1:A:185:VAL:HG22	1.97	0.47
1:A:24:GLU:HA	1:A:27:LYS:HE3	1.97	0.47
1:A:1074:ARG:NH2	1:A:1258:LEU:HD13	2.31	0.46
1:A:1244:MET:CE	1:A:1247:VAL:HG21	2.46	0.46
1:A:20:ASN:HA	1:A:20:ASN:HD22	1.61	0.46
1:A:92:TYR:CE2	1:A:310:GLU:HG2	2.50	0.46
1:A:1210:TYR:HB2	1:A:1211:PRO:CD	2.40	0.45
1:A:1222:LEU:O	1:A:1222:LEU:HD23	2.16	0.45
1:A:1197:GLU:OE2	2:P:92:HIS:HA	2.16	0.45
1:A:1222:LEU:O	1:A:1226:THR:HG23	2.16	0.45
1:A:1206:LEU:HD22	1:A:1216:ARG:HD3	1.99	0.45
1:A:233:ALA:O	1:A:237:ILE:HG13	2.17	0.45
1:A:66:HIS:HE1	1:A:262:GLY:HA2	1.82	0.45
1:A:1210:TYR:N	1:A:1211:PRO:CD	2.79	0.45
1:A:1156:LEU:HD12	1:A:1156:LEU:HA	1.86	0.44
1:A:337:GLN:HE21	1:A:337:GLN:N	2.12	0.44
1:A:1219:ARG:HG3	4:A:1441:HOH:O	2.16	0.44
1:A:131:TRP:CD1	1:A:250:PRO:HB2	2.52	0.44
1:A:31:LYS:NZ	1:A:31:LYS:HB2	2.32	0.44
1:A:343:TYR:CE2	1:A:1114:GLU:HG3	2.53	0.44
1:A:257:SER:O	1:A:259:PRO:HD3	2.18	0.44
1:A:310:GLU:HG3	1:A:311:GLU:N	2.32	0.44
1:A:87:PHE:HZ	1:A:287:LEU:HD13	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:LEU:O	1:A:1094:CYS:HB2	2.18	0.43
1:A:351:ASN:OD1	1:A:356:ARG:NH1	2.51	0.43
1:A:1245:GLY:O	1:A:1247:VAL:HG23	2.18	0.43
1:A:1178:PHE:HB3	1:A:1191:ILE:HG23	2.01	0.42
1:A:1244:MET:CE	1:A:1247:VAL:HG11	2.49	0.42
1:A:91:LEU:HD23	1:A:306:LEU:HA	2.01	0.42
1:A:1241:ARG:HG3	1:A:1241:ARG:HH11	1.84	0.42
1:A:1244:MET:HE3	1:A:1247:VAL:HG11	2.02	0.42
1:A:78:LEU:C	1:A:270:ALA:HB2	2.40	0.42
1:A:1209:TRP:CD1	1:A:1209:TRP:C	2.93	0.42
2:P:104:VAL:HG23	2:P:105:PHE:CD1	2.54	0.42
1:A:341:PHE:O	1:A:345:VAL:HG23	2.20	0.42
1:A:160:TRP:N	1:A:161:PRO:CD	2.82	0.42
1:A:140:GLU:O	1:A:143:ALA:HB3	2.20	0.41
1:A:1101:LEU:HD22	1:A:1176:ILE:CD1	2.43	0.41
1:A:293:GLU:O	1:A:297:LYS:HB2	2.20	0.41
1:A:49:PHE:N	1:A:50:PRO:HD2	2.35	0.41
2:P:92:HIS:O	2:P:93:ARG:HG2	2.20	0.41
1:A:1193:HIS:HB3	4:A:1434:HOH:O	2.21	0.41
1:A:1109:THR:HA	1:A:1160:TRP:CH2	2.56	0.41
1:A:1095:TRP:CE3	1:A:1249:ILE:HG21	2.56	0.41
1:A:1168:GLU:OE1	1:A:1206:LEU:HD21	2.21	0.41
1:A:24:GLU:HA	1:A:27:LYS:CE	2.51	0.40
1:A:4:ILE:HG12	1:A:58:GLY:O	2.20	0.40
1:A:1085:ASP:O	1:A:1089:ARG:HB2	2.22	0.40
1:A:41:HIS:ND1	1:A:41:HIS:O	2.54	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	543/580 (94%)	505 (93%)	33 (6%)	5 (1%)	17	46
2	P	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
All	All	557/596 (94%)	518 (93%)	34 (6%)	5 (1%)	17	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1210	TYR
1	A	1211	PRO
1	A	167	GLY
1	A	4	ILE
1	A	1112	VAL

### 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	448/474 (94%)	423 (94%)	25 (6%)	21	51
2	P	13/13 (100%)	13 (100%)	0	100	100
All	All	461/487 (95%)	436 (95%)	25 (5%)	22	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	20	ASN
1	A	57	ASP
1	A	62	ILE
1	A	147	SER
1	A	241	LYS
1	A	243	ASN
1	A	260	PHE
1	A	273	PRO
1	A	310	GLU
1	A	337	GLN

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Mol	Chain	Res	Type
1	A	360	ASP
1	A	1066	LEU
1	A	1074	ARG
1	A	1089	ARG
1	A	1110	PHE
1	A	1114	GLU
1	A	1154	ARG
1	A	1172	LEU
1	A	1179	ASN
1	A	1209	TRP
1	A	1217	LEU
1	A	1219	ARG
1	A	1221	LEU
1	A	1243	ILE

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

Mol	Chain	Res	Type
1	A	20	ASN
1	A	51	GLN
1	A	74	GLN
1	A	102	ASN
1	A	203	ASN
1	A	220	ASN
1	A	243	ASN
1	A	327	GLN
1	A	337	GLN
1	A	357	GLN
1	A	369	ASN
1	A	1143	GLN
1	A	1179	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

2 monosaccharides 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	$\# Z  > 2$
3	GLC	B	1	3	12,12,12	0.86	0	17,17,17	0.50	0
3	GLC	B	2	3	11,11,12	1.17	1 (9%)	15,15,17	0.92	1 (6%)

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
3	GLC	B	1	3	-	0/2/22/22	0/1/1/1
3	GLC	B	2	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	GLC	C2-C3	3.01	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	GLC	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	549/580 (94%)	-0.15	21 (3%) 40 30	15, 30, 57, 107	0
2	P	16/16 (100%)	-0.16	1 (6%) 20 12	19, 28, 57, 67	0
All	All	565/596 (94%)	-0.15	22 (3%) 39 29	15, 30, 57, 107	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1210	TYR	6.7
1	A	1209	TRP	5.3
1	A	1115	ALA	4.7
1	A	1211	PRO	4.5
1	A	241	LYS	3.8
1	A	1213	SER	3.6
1	A	1208	PRO	3.3
1	A	1212	ALA	3.3
1	A	1207	GLU	3.1
1	A	55	THR	3.1
1	A	1114	GLU	2.7
1	A	1108	VAL	2.7
1	A	1109	THR	2.5
1	A	1214	GLN	2.5
2	P	91	MET	2.4
1	A	43	ASP	2.4
1	A	1143	GLN	2.2
1	A	1183	PRO	2.2
1	A	1111	GLU	2.2
1	A	51	GLN	2.1
1	A	174	GLU	2.1
1	A	53	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	B	2	11/12	0.96	0.19	12,18,20,20	0
3	GLC	B	1	12/12	0.96	0.21	22,23,28,29	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.