



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 10:54 PM EST

PDB ID : 4I99  
Title : Crystal structure of the SmcHead bound to the C-winged helix domain of ScpA  
Authors : Shin, H.C.; Soh, Y.M.; Oh, B.H.  
Deposited on : 2012-12-05  
Resolution : 2.30 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.

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 ⓘ](#)) 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 : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

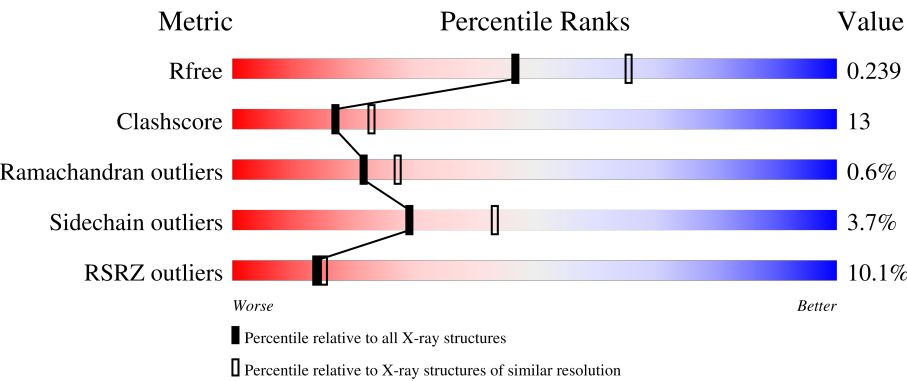
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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  $\geq 3$ , 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	354	<div><div>6%</div><div><div></div><div>72%</div><div>17%</div><div>•</div><div>9%</div></div></div>
1	B	354	<div><div>7%</div><div><div></div><div>69%</div><div>21%</div><div>•</div><div>8%</div></div></div>
2	C	87	<div><div>7%</div><div><div></div><div>56%</div><div>21%</div><div>•</div><div>20%</div></div></div>
2	D	87	<div><div>29%</div><div><div></div><div>52%</div><div>26%</div><div>•</div><div>21%</div></div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6236 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.

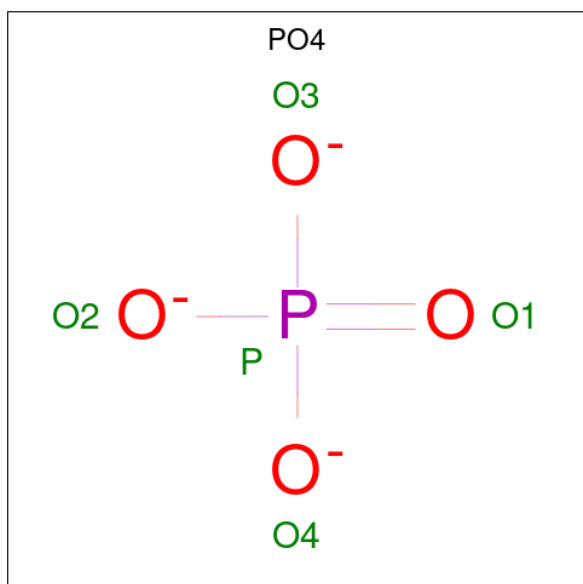
- Molecule 1 is a protein called Chromosome partition protein Smc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	Se	0	0	0
			2498	1598	426	465	9			
1	B	326	Total	C	N	O	Se	0	0	0
			2520	1613	430	468	9			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	70	Total	C	N	O	S	0	0	0
			578	388	82	106	2			
2	D	69	Total	C	N	O	S	0	0	0
			534	358	77	97	2			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

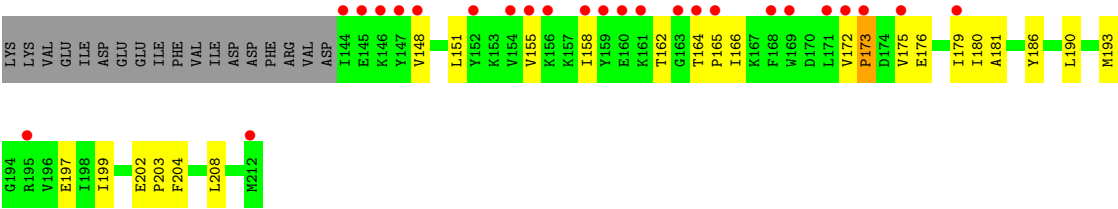


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	43	Total	O	0	0
			43	43		
4	C	5	Total	O	0	0
			5	5		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.86Å 117.86Å 94.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.46 – 2.30 29.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.46-2.30) 99.8 (29.46-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.221 , 0.236 0.226 , 0.239	Depositor DCC
$R_{free}$ test set	2800 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.38	0/2531	0.60	0/3386
1	B	0.38	0/2553	0.59	0/3415
2	C	0.37	0/592	0.51	0/803
2	D	0.34	0/547	0.50	0/748
All	All	0.37	0/6223	0.58	0/8352

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 [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	2498	0	2557	49	0
1	B	2520	0	2586	73	0
2	C	578	0	587	16	0
2	D	534	0	510	25	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	43	0	0	1	0
4	B	43	0	0	3	0
4	C	5	0	0	0	0
All	All	6236	0	6240	155	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 13.

All (155) 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:170:ALA:HB3	1:B:1009:LYS:HD2	1.49	0.92
1:B:25:SER:HB2	1:B:1139:LYS:HD2	1.56	0.86
2:D:190:LEU:HA	2:D:193:MET:HE3	1.60	0.83
1:B:1134:MSE:HE2	2:D:181:ALA:HB1	1.62	0.82
1:B:150:LYS:HE3	1:B:151:PHE:CZ	2.20	0.76
1:A:1014:MSE:O	1:A:1018:GLU:HG2	1.89	0.72
1:B:122:THR:HG22	1:B:124:SER:H	1.53	0.72
1:A:1063:VAL:HG12	1:A:1064:LYS:N	2.05	0.72
1:B:1014:MSE:O	1:B:1018:GLU:HG3	1.91	0.71
1:A:1017:PHE:HE2	1:A:1052:LEU:HD21	1.56	0.70
2:D:164:THR:HB	2:D:165:PRO:HD2	1.72	0.69
1:B:1162:LYS:C	1:B:1163:ILE:HD12	2.13	0.68
1:B:1066:ILE:HB	1:B:1069:MSE:HE2	1.76	0.68
1:B:48:PHE:CE2	1:B:104:ARG:HG2	2.28	0.68
1:A:1064:LYS:HE2	1:A:1069:MSE:HA	1.75	0.67
1:B:1139:LYS:HD3	2:D:204:PHE:CZ	2.29	0.67
2:D:190:LEU:HD23	2:D:193:MET:HE1	1.78	0.66
2:D:148:VAL:HG22	2:D:186:TYR:CD1	2.31	0.66
1:B:45:ALA:O	1:B:49:VAL:HG22	1.97	0.65
1:A:1063:VAL:HG12	1:A:1064:LYS:H	1.60	0.65
1:B:126:ILE:O	1:B:129:ILE:HG22	1.97	0.65
1:B:147:ASP:O	1:B:150:LYS:HG2	1.97	0.65
2:D:173:PRO:HG2	2:D:179:ILE:HG21	1.79	0.65
1:A:1035:GLY:HA3	1:A:1058:PRO:O	1.98	0.64
1:B:149:THR:O	1:B:152:ILE:HB	1.98	0.64
1:A:91:ARG:HE	1:A:96:ASP:HA	1.62	0.64
1:B:48:PHE:CZ	1:B:104:ARG:HG2	2.34	0.63
1:B:155:SER:OG	1:B:158:GLU:HG3	1.98	0.63
1:B:63:ILE:HG22	1:B:106:VAL:HG21	1.80	0.61
1:B:104:ARG:HG3	1:B:105:ARG:N	2.15	0.61
1:A:126:ILE:O	1:A:129:ILE:HG22	1.99	0.61
1:B:1066:ILE:CB	1:B:1069:MSE:HE2	2.32	0.59
1:B:148:ILE:HB	4:B:1333:HOH:O	2.02	0.59
1:B:1063:VAL:HG12	1:B:1064:LYS:N	2.16	0.59
1:B:1041:LEU:HD23	1:B:1052:LEU:HD13	1.83	0.59
1:B:1057:LYS:HG2	1:B:1063:VAL:HA	1.84	0.59
1:A:166:ILE:HD13	1:A:1085:ILE:CG2	2.33	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:LYS:HE2	4:B:1335:HOH:O	2.03	0.58
1:A:1161:MSE:HE1	2:C:177:PRO:HD3	1.85	0.58
1:B:1066:ILE:CA	1:B:1069:MSE:HE2	2.33	0.58
1:B:148:ILE:HG23	1:B:149:THR:N	2.19	0.57
1:B:1146:ARG:NH1	2:D:197:GLU:HG3	2.18	0.57
1:B:1015:ARG:HH11	1:B:1015:ARG:HG3	1.71	0.56
1:B:1017:PHE:HE1	1:B:1052:LEU:HD11	1.70	0.56
1:B:1018:GLU:O	1:B:1022:ARG:HG3	2.06	0.56
1:A:1017:PHE:CE2	1:A:1052:LEU:HD21	2.39	0.55
1:A:1113:ASP:HA	1:A:1116:LYS:HE3	1.89	0.55
2:C:152:TYR:OH	2:C:156:LYS:HE3	2.06	0.54
2:D:148:VAL:HG22	2:D:186:TYR:HD1	1.70	0.54
2:D:151:LEU:O	2:D:155:VAL:HG23	2.07	0.54
1:B:1119:SER:HA	1:B:1122:SER:O	2.08	0.53
1:A:115:TRP:HA	1:A:120:ARG:HA	1.91	0.53
1:B:1146:ARG:O	1:B:1147:ASP:HB2	2.09	0.53
2:D:155:VAL:HG13	2:D:166:ILE:HD12	1.89	0.53
1:A:168:GLY:O	1:A:169:ILE:HB	2.09	0.52
1:A:1107:ASN:OD1	1:A:1110:ARG:NH1	2.42	0.52
1:A:1063:VAL:CG1	1:A:1064:LYS:N	2.71	0.52
2:C:167:LYS:HA	2:C:208:LEU:HD23	1.91	0.52
1:A:123:ARG:NH1	1:A:127:LEU:HD11	2.24	0.52
2:D:179:ILE:HD12	2:D:179:ILE:N	2.24	0.52
1:A:166:ILE:HD13	1:A:1085:ILE:HG21	1.91	0.52
1:A:1063:VAL:CG1	1:A:1064:LYS:H	2.21	0.52
2:D:176:GLU:HB2	2:D:179:ILE:HD13	1.91	0.52
2:C:166:ILE:HG21	2:C:171:LEU:HD13	1.92	0.51
1:B:10:LYS:HB2	1:B:10:LYS:NZ	2.26	0.51
2:C:179:ILE:HD12	2:C:179:ILE:N	2.26	0.51
2:D:190:LEU:HD23	2:D:193:MET:CE	2.39	0.51
1:A:1031:LEU:HG	1:A:1076:LEU:HD22	1.93	0.51
1:A:1116:LYS:O	1:A:1119:SER:HB2	2.10	0.50
1:B:1063:VAL:CG1	1:B:1064:LYS:N	2.74	0.50
1:A:45:ALA:O	1:A:49:VAL:HG22	2.11	0.50
1:B:1036:SER:HA	4:B:1307:HOH:O	2.12	0.50
1:B:1038:ARG:NH1	1:B:1040:ILE:HD11	2.27	0.49
1:B:1043:ASN:C	1:B:1043:ASN:HD22	2.16	0.49
1:B:1109:LYS:HE3	1:B:1113:ASP:OD2	2.11	0.49
1:B:1162:LYS:HG3	1:B:1163:ILE:HD12	1.95	0.49
2:D:158:ILE:HG22	2:D:158:ILE:O	2.12	0.49
1:A:1069:MSE:HB3	1:A:1073:GLU:HB2	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:VAL:HG21	2:C:180:ILE:HG12	1.94	0.48
1:A:167:SER:CB	1:A:1016:THR:HG21	2.43	0.48
1:A:1154:SER:HB2	2:C:204:PHE:CE1	2.49	0.48
1:B:25:SER:HB2	1:B:1139:LYS:CD	2.36	0.48
1:B:104:ARG:HD3	1:B:114:TYR:CZ	2.49	0.47
1:A:167:SER:HB2	1:A:1016:THR:HG21	1.95	0.47
1:A:1139:LYS:HD3	2:C:204:PHE:CZ	2.50	0.47
1:B:170:ALA:CB	1:B:1009:LYS:HD2	2.33	0.47
2:C:173:PRO:HG2	2:C:179:ILE:HG21	1.96	0.47
2:D:202:GLU:HB3	2:D:203:PRO:HD2	1.96	0.47
1:B:10:LYS:HB2	1:B:10:LYS:HZ2	1.78	0.47
2:C:175:VAL:HG13	2:C:175:VAL:O	2.15	0.47
1:A:127:LEU:O	1:A:131:THR:HG23	2.14	0.46
1:B:2:PRO:HD3	1:B:92:GLY:HA3	1.97	0.46
1:A:1161:MSE:CE	2:C:177:PRO:HD3	2.45	0.46
1:B:148:ILE:CG2	1:B:149:THR:N	2.78	0.46
2:D:176:GLU:O	2:D:180:ILE:HG22	2.16	0.46
1:B:1083:PHE:CD1	1:B:1114:LEU:HD12	2.50	0.46
1:B:160:ARG:NH1	1:B:164:ASP:OD1	2.48	0.46
1:A:160:ARG:NH1	1:A:164:ASP:OD1	2.49	0.46
1:B:61:SER:HB2	1:B:65:ASP:OD2	2.15	0.45
1:B:152:ILE:HG22	1:B:153:LYS:N	2.29	0.45
1:A:59:ARG:HH11	1:A:59:ARG:HG2	1.81	0.45
2:D:162:THR:O	2:D:164:THR:HG23	2.15	0.45
2:C:179:ILE:HD12	2:C:179:ILE:H	1.81	0.45
1:B:1086:GLN:OE1	1:B:1118:SER:HB3	2.16	0.45
1:B:1019:ALA:HA	1:B:1022:ARG:NH1	2.31	0.45
1:A:1104:ASP:O	1:A:1108:VAL:HG23	2.17	0.45
1:B:154:MSE:HE2	1:B:158:GLU:C	2.36	0.45
1:B:1057:LYS:HE2	1:B:1063:VAL:CG2	2.47	0.45
1:B:150:LYS:C	1:B:152:ILE:H	2.20	0.44
2:C:176:GLU:HB2	2:C:179:ILE:HD13	1.99	0.44
1:A:149:THR:HG22	1:A:149:THR:O	2.17	0.44
1:B:2:PRO:O	1:B:1092:PRO:HB3	2.18	0.44
1:B:1057:LYS:HE2	1:B:1063:VAL:HG23	1.99	0.44
1:B:1069:MSE:HB3	1:B:1073:GLU:HB2	1.98	0.44
1:A:166:ILE:HD13	1:A:1085:ILE:HG23	1.99	0.44
2:D:190:LEU:CA	2:D:193:MET:HE3	2.39	0.44
1:B:1146:ARG:HH11	2:D:197:GLU:HG3	1.83	0.44
1:B:115:TRP:NE1	1:B:120:ARG:HD3	2.33	0.43
1:A:53:LEU:HD21	1:A:123:ARG:NE	2.34	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LYS:N	1:B:18:LYS:HD2	2.34	0.43
1:B:1066:ILE:HA	1:B:1069:MSE:HE2	2.00	0.43
1:A:16:GLY:HA2	1:A:68:PHE:CD2	2.54	0.43
1:B:10:LYS:NZ	1:B:10:LYS:CB	2.81	0.43
1:B:23:PRO:O	1:B:1141:ILE:HD11	2.19	0.43
1:A:1086:GLN:HB2	1:A:1094:TYR:OH	2.19	0.42
1:A:67:ILE:HA	1:A:80:ALA:HB2	2.01	0.42
1:B:1031:LEU:HB3	1:B:1076:LEU:HD22	2.01	0.42
1:B:119:ARG:HB2	1:B:119:ARG:NH1	2.34	0.42
2:D:199:ILE:HB	2:D:208:LEU:HB2	2.02	0.42
1:B:25:SER:CB	1:B:1139:LYS:HD2	2.39	0.42
2:C:152:TYR:CE2	2:C:195:ARG:HD2	2.54	0.42
1:B:49:VAL:HG13	1:B:82:VAL:HB	2.02	0.42
1:A:37:SER:HB3	1:A:1143:VAL:HG12	2.01	0.42
2:D:172:VAL:HG23	2:D:172:VAL:O	2.20	0.42
2:C:162:THR:HB	2:C:164:THR:HG22	2.01	0.41
1:A:50:LEU:HB3	1:A:137:PRO:HB3	2.01	0.41
1:B:1015:ARG:HG3	1:B:1015:ARG:NH1	2.35	0.41
1:A:107:TYR:HB3	1:A:108:PRO:HD2	2.03	0.41
1:B:133:ALA:O	1:B:134:MSE:HB2	2.20	0.41
1:A:122:THR:HG23	1:A:125:GLU:OE2	2.19	0.41
1:A:49:VAL:HG13	1:A:82:VAL:HB	2.03	0.41
1:B:115:TRP:CE2	1:B:120:ARG:HD3	2.56	0.41
1:B:154:MSE:HE2	1:B:158:GLU:CB	2.51	0.41
1:B:1139:LYS:HE3	1:B:1158:GLU:OE1	2.21	0.41
2:D:203:PRO:O	2:D:204:PHE:HB2	2.20	0.41
1:A:1081:PHE:CE2	1:A:1085:ILE:HD11	2.56	0.41
1:B:122:THR:HG22	1:B:124:SER:N	2.27	0.41
2:D:148:VAL:HG11	2:D:193:MET:HE1	2.03	0.41
1:A:63:ILE:HG22	1:A:106:VAL:HG21	2.03	0.40
1:A:1057:LYS:HA	1:A:1058:PRO:HD2	1.94	0.40
2:D:179:ILE:HD12	2:D:179:ILE:H	1.86	0.40
1:A:1017:PHE:HE2	1:A:1052:LEU:CD2	2.30	0.40
1:A:156:PRO:HD2	4:A:1307:HOH:O	2.21	0.40
1:A:1022:ARG:HB3	1:A:1022:ARG:NH1	2.37	0.40
2:C:169:TRP:O	2:C:172:VAL:HG12	2.21	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	319/354 (90%)	310 (97%)	8 (2%)	1 (0%)	37	47
1	B	322/354 (91%)	311 (97%)	10 (3%)	1 (0%)	37	47
2	C	68/87 (78%)	63 (93%)	4 (6%)	1 (2%)	8	8
2	D	67/87 (77%)	60 (90%)	5 (8%)	2 (3%)	3	2
All	All	776/882 (88%)	744 (96%)	27 (4%)	5 (1%)	22	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	152	ILE
2	C	173	PRO
2	D	173	PRO
1	A	1058	PRO
2	D	175	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	266/285 (93%)	257 (97%)	9 (3%)	32	47
1	B	268/285 (94%)	258 (96%)	10 (4%)	29	43
2	C	64/83 (77%)	59 (92%)	5 (8%)	10	14
2	D	54/83 (65%)	54 (100%)	0	100	100
All	All	652/736 (89%)	628 (96%)	24 (4%)	29	43

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	59	ARG
1	A	78	LYS
1	A	116	LEU
1	A	162	LEU
1	A	1016	THR
1	A	1031	LEU
1	A	1064	LYS
1	A	1086	GLN
1	B	47	LEU
1	B	49	VAL
1	B	104	ARG
1	B	134	MSE
1	B	162	LEU
1	B	1043	ASN
1	B	1062	ASP
1	B	1064	LYS
1	B	1086	GLN
1	B	1114	LEU
2	C	157	LYS
2	C	160	GLU
2	C	171	LEU
2	C	176	GLU
2	C	212	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1043	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands 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	PO4	A	1202	-	4,4,4	1.64	0	6,6,6	0.46	0
3	PO4	A	1201	-	4,4,4	1.80	2 (50%)	6,6,6	0.46	0
3	PO4	B	1201	-	4,4,4	1.74	1 (25%)	6,6,6	0.47	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	PO4	P-O2	-2.08	1.48	1.54
3	A	1201	PO4	P-O4	-2.07	1.48	1.54
3	A	1201	PO4	P-O2	-2.02	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	314/354 (88%)	0.17	21 (6%)	25 27	23, 38, 64, 86	0
1	B	317/354 (89%)	0.21	26 (8%)	19 21	20, 37, 74, 102	0
2	C	70/87 (80%)	0.51	6 (8%)	18 19	28, 43, 74, 79	0
2	D	69/87 (79%)	1.77	25 (36%)	1 1	46, 75, 86, 91	0
All	All	770/882 (87%)	0.36	78 (10%)	14 15	20, 39, 79, 102	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	144	ILE	8.6
1	B	169	ILE	7.3
1	B	1045	GLU	5.9
1	A	169	ILE	5.6
1	B	1163	ILE	5.2
1	B	1060	GLY	5.1
1	B	1059	ALA	4.8
2	C	144	ILE	4.7
2	D	147	TYR	4.7
1	A	1007	LYS	4.7
1	B	1007	LYS	4.1
1	B	1159	LYS	4.1
1	B	170	ALA	4.1
1	B	1008	GLU	3.8
1	A	1158	GLU	3.8
1	B	1063	VAL	3.6
1	B	1066	ILE	3.5
2	D	145	GLU	3.5
2	C	145	GLU	3.5
1	A	1146	ARG	3.5
1	A	1059	ALA	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	160	GLU	3.3
1	A	1159	LYS	3.3
1	B	1158	GLU	3.3
1	B	1160	ALA	3.3
1	A	1160	ALA	3.2
1	B	1061	LYS	3.2
2	D	158	ILE	3.2
2	D	154	VAL	3.0
2	D	155	VAL	3.0
1	B	1062	ASP	3.0
1	A	1009	LYS	3.0
2	C	147	TYR	3.0
2	C	143	ASP	2.9
1	B	151	PHE	2.9
1	A	1064	LYS	2.9
1	A	1058	PRO	2.9
1	B	1157	LEU	2.8
2	D	168	PHE	2.8
2	D	169	TRP	2.7
2	D	164	THR	2.7
2	D	152	TYR	2.7
2	D	163	GLY	2.6
2	D	159	TYR	2.6
1	B	152	ILE	2.6
2	D	161	LYS	2.6
2	D	175	VAL	2.6
2	C	175	VAL	2.5
1	B	1009	LYS	2.5
2	D	179	ILE	2.4
1	A	168	GLY	2.4
1	A	151	PHE	2.4
1	B	148	ILE	2.4
1	B	168	GLY	2.4
2	D	195	ARG	2.4
2	D	171	LEU	2.4
1	B	1162	LYS	2.3
1	A	1008	GLU	2.3
2	D	165	PRO	2.3
1	B	153	LYS	2.2
1	A	1011	ASN	2.2
2	D	148	VAL	2.2
2	D	212	MET	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1012	VAL	2.2
2	D	146	LYS	2.2
2	D	156	LYS	2.2
1	A	1045	GLU	2.1
1	B	18	LYS	2.1
1	A	1010	LYS	2.1
1	B	1043	ASN	2.1
2	D	173	PRO	2.1
1	A	95	ILE	2.0
2	C	179	ILE	2.0
1	A	1063	VAL	2.0
2	D	172	VAL	2.0
1	A	1062	ASP	2.0
1	A	18	LYS	2.0
1	B	1047	PRO	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](#)

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, 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	PO4	A	1201	5/5	0.98	0.07	45,45,47,47	0
3	PO4	A	1202	5/5	0.99	0.05	26,27,28,29	0
3	PO4	B	1201	5/5	0.99	0.05	27,28,29,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.