



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:09 AM GMT

PDB ID : 2PMU
Title : Crystal structure of the DNA-binding domain of PhoP
Authors : Wang, S.
Deposited on : 2007-04-23
Resolution : 1.78 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

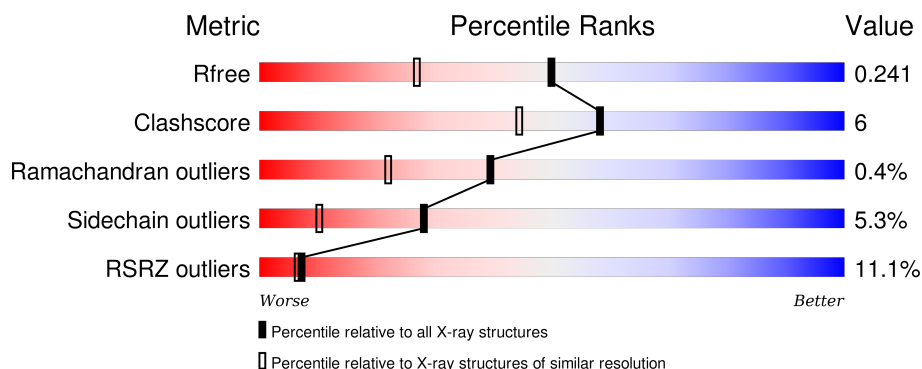
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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}	91344	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	110	<div> <div>5%</div> <div>80% 7% • 11%</div> </div>
1	B	110	<div> <div>15%</div> <div>81% 12% • 6%</div> </div>
1	C	110	<div> <div>10%</div> <div>70% 11% • 16%</div> </div>
1	D	110	<div> <div>4%</div> <div>83% • • 13%</div> </div>
1	E	110	<div> <div>16%</div> <div>81% 11% • 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	110	

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
3	K	A	2002	-	-	-	X
3	K	D	2001	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5358 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 response regulator PHOP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	0	1	0
			805	520	138	147			
1	B	103	Total	C	N	O	0	1	0
			849	546	148	155			
1	C	92	Total	C	N	O	0	1	0
			760	491	133	136			
1	D	96	Total	C	N	O	0	1	0
			793	514	136	143			
1	E	103	Total	C	N	O	0	1	0
			849	546	148	155			
1	F	93	Total	C	N	O	0	1	0
			763	492	131	140			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	GLY	-	EXPRESSION TAG	UNP P71814
A	141	THR	-	EXPRESSION TAG	UNP P71814
A	142	HIS	-	EXPRESSION TAG	UNP P71814
A	143	MET	-	EXPRESSION TAG	UNP P71814
A	248	LYS	-	EXPRESSION TAG	UNP P71814
A	249	LEU	-	EXPRESSION TAG	UNP P71814
B	140	GLY	-	EXPRESSION TAG	UNP P71814
B	141	THR	-	EXPRESSION TAG	UNP P71814
B	142	HIS	-	EXPRESSION TAG	UNP P71814
B	143	MET	-	EXPRESSION TAG	UNP P71814
B	248	LYS	-	EXPRESSION TAG	UNP P71814
B	249	LEU	-	EXPRESSION TAG	UNP P71814
C	140	GLY	-	EXPRESSION TAG	UNP P71814
C	141	THR	-	EXPRESSION TAG	UNP P71814
C	142	HIS	-	EXPRESSION TAG	UNP P71814
C	143	MET	-	EXPRESSION TAG	UNP P71814
C	248	LYS	-	EXPRESSION TAG	UNP P71814

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	249	LEU	-	EXPRESSION TAG	UNP P71814
D	140	GLY	-	EXPRESSION TAG	UNP P71814
D	141	THR	-	EXPRESSION TAG	UNP P71814
D	142	HIS	-	EXPRESSION TAG	UNP P71814
D	143	MET	-	EXPRESSION TAG	UNP P71814
D	248	LYS	-	EXPRESSION TAG	UNP P71814
D	249	LEU	-	EXPRESSION TAG	UNP P71814
E	140	GLY	-	EXPRESSION TAG	UNP P71814
E	141	THR	-	EXPRESSION TAG	UNP P71814
E	142	HIS	-	EXPRESSION TAG	UNP P71814
E	143	MET	-	EXPRESSION TAG	UNP P71814
E	248	LYS	-	EXPRESSION TAG	UNP P71814
E	249	LEU	-	EXPRESSION TAG	UNP P71814
F	140	GLY	-	EXPRESSION TAG	UNP P71814
F	141	THR	-	EXPRESSION TAG	UNP P71814
F	142	HIS	-	EXPRESSION TAG	UNP P71814
F	143	MET	-	EXPRESSION TAG	UNP P71814
F	248	LYS	-	EXPRESSION TAG	UNP P71814
F	249	LEU	-	EXPRESSION TAG	UNP P71814

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	D	1	Total O P 9 7 2	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		

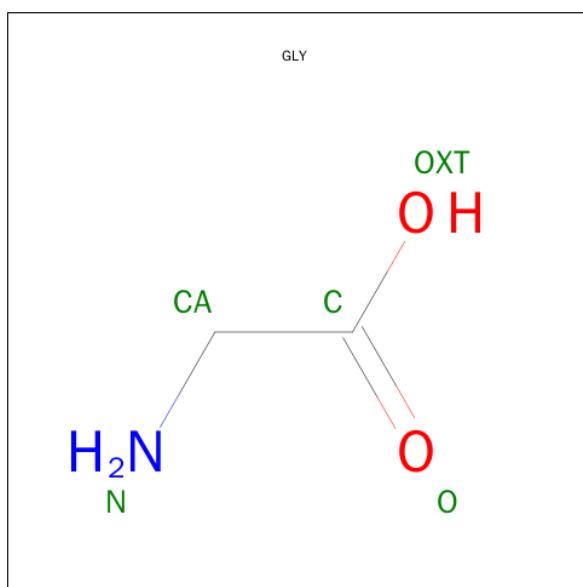
- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	X	0	0
			1	1		
4	A	1	Total	X	0	0
			1	1		
4	D	1	Total	X	0	0
			1	1		
4	E	1	Total	X	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	E	2	Total	Cl	0	0
			2	2		

- Molecule 6 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			15	6	3	6		

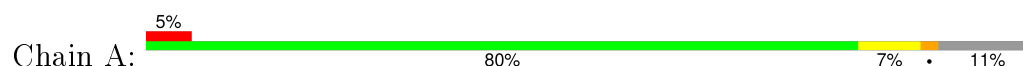
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	108	Total	O	0	0
			108	108		
7	B	72	Total	O	0	0
			72	72		
7	C	65	Total	O	0	0
			65	65		
7	D	107	Total	O	0	0
			107	107		
7	E	70	Total	O	0	0
			70	70		
7	F	67	Total	O	0	0
			67	67		

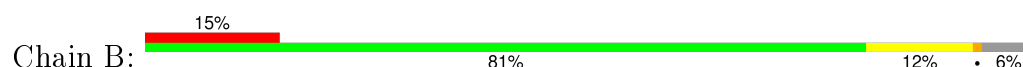
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: response regulator PHOP



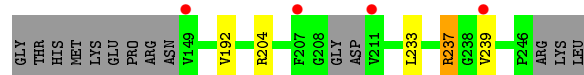
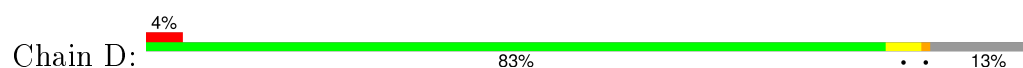
- Molecule 1: response regulator PHOP



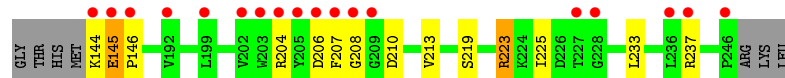
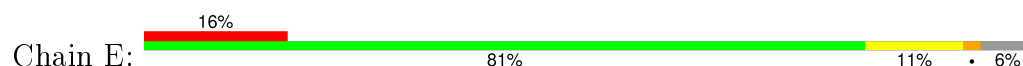
- Molecule 1: response regulator PHOP



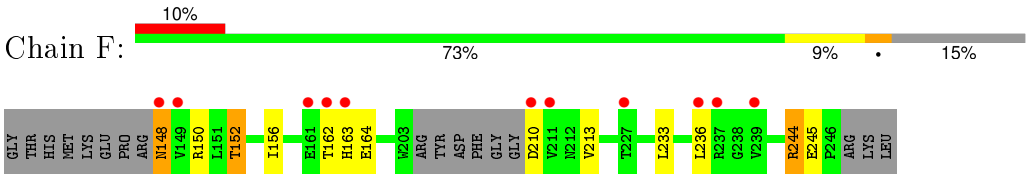
- Molecule 1: response regulator PHOP



- Molecule 1: response regulator PHOP



- Molecule 1: response regulator PHOP



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.88Å 101.13Å 86.93Å 90.00° 126.72° 90.00°	Depositor
Resolution (Å)	20.00 – 1.78 19.56 – 1.78	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-1.78) 94.5 (19.56-1.78)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.196 , 0.238 0.199 , 0.241	Depositor DCC
R_{free} test set	3310 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.2	EDS
Estimated twinning fraction	0.025 for -k,-h,-1/2*h+1/2*k-l 0.027 for k,h,-1/2*h-1/2*k-l 0.480 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 65214 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5358	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UNX, K, PO4, CL

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	0.82	0/827	0.81	0/1123
1	B	0.72	0/872	0.84	2/1183 (0.2%)
1	C	0.66	0/779	0.71	0/1057
1	D	0.81	0/814	0.78	0/1104
1	E	0.75	0/872	0.86	2/1183 (0.2%)
1	F	0.68	0/782	0.69	0/1062
All	All	0.74	0/4946	0.79	4/6712 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	223	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	B	223	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	B	223	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	E	223	ARG	NE-CZ-NH1	-7.15	116.72	120.30

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	805	0	809	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	849	0	854	12	0
1	C	760	0	777	13	0
1	D	793	0	801	4	0
1	E	849	0	854	10	0
1	F	763	0	773	8	0
2	A	5	0	0	0	0
2	D	14	0	0	0	0
2	E	5	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	B	1	0	0	1	0
5	D	1	0	0	1	0
5	E	2	0	0	1	0
6	B	15	0	6	0	0
7	A	108	0	0	0	0
7	B	72	0	0	0	0
7	C	65	0	0	4	0
7	D	107	0	0	0	0
7	E	70	0	0	0	0
7	F	67	0	0	1	0
All	All	5358	0	4874	57	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 6.

All (57) 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:F:210:ASP:O	1:F:213:VAL:HG12	1.76	0.84
1:D:237:ARG:NE	1:D:237:ARG:H	1.80	0.79
1:A:150:ARG:CG	1:A:150:ARG:HH11	1.94	0.79
1:B:204:ARG:HD3	7:C:306:HOH:O	1.83	0.78
1:C:149:VAL:HG13	1:C:150:ARG:H	1.52	0.74
1:A:237:ARG:CD	1:A:237:ARG:H	2.00	0.74
1:A:237:ARG:H	1:A:237:ARG:NE	1.86	0.72
1:B:145:GLU:H	1:B:146:PRO:CD	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:HG2	1:A:150:ARG:HH11	1.61	0.65
1:B:145:GLU:N	1:B:146:PRO:CD	2.62	0.62
1:B:207:PHE:CG	1:B:208:GLY:N	2.67	0.61
1:D:237:ARG:CD	1:D:237:ARG:H	2.15	0.60
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.65	0.59
1:B:210:ASP:O	1:B:213:VAL:HG12	2.03	0.58
1:E:207:PHE:CG	1:E:208:GLY:N	2.70	0.58
1:B:145:GLU:N	1:B:146:PRO:HD2	2.19	0.57
1:F:152:THR:HG23	1:F:156:ILE:O	2.09	0.53
1:C:152:THR:CG2	1:C:156:ILE:O	2.58	0.52
1:C:152:THR:HG23	1:C:156:ILE:O	2.10	0.50
1:E:210:ASP:O	1:E:213:VAL:HG12	2.10	0.50
1:B:204:ARG:HG3	5:B:3003:CL:CL	2.49	0.49
1:C:162:THR:CG2	1:C:164:GLU:HG3	2.42	0.49
1:C:192:VAL:HG11	1:C:236:LEU:HD11	1.95	0.49
1:B:207:PHE:CE1	1:C:152:THR:HB	2.47	0.49
1:F:152:THR:CG2	1:F:156:ILE:O	2.60	0.49
1:C:236:LEU:HD12	1:C:239:VAL:HB	1.93	0.49
1:D:192:VAL:HG11	1:D:239:VAL:HG12	1.94	0.49
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.26	0.49
1:D:204:ARG:NH1	5:D:3004:CL:CL	2.83	0.48
1:A:192:VAL:HG11	1:A:239:VAL:HG12	1.96	0.48
1:B:145:GLU:H	1:B:146:PRO:HD3	1.79	0.47
1:E:145:GLU:N	1:E:146:PRO:CD	2.79	0.46
1:C:192:VAL:CG1	1:C:236:LEU:HD11	2.46	0.46
1:A:150:ARG:CG	1:A:150:ARG:NH1	2.62	0.46
1:B:222:ARG:NE	1:B:231:ARG:HH12	2.15	0.45
1:C:162:THR:HG22	1:C:164:GLU:HG3	1.97	0.45
1:C:149:VAL:HG12	7:C:305:HOH:O	2.16	0.45
1:E:204:ARG:HH12	1:E:206:ASP:HB3	1.82	0.44
1:A:237:ARG:N	1:A:237:ARG:CD	2.76	0.44
1:B:222:ARG:HE	1:B:231:ARG:HH12	1.66	0.44
1:E:204:ARG:HG3	5:E:3002:CL:CL	2.54	0.44
1:E:219:SER:O	1:E:223:ARG:HG3	2.18	0.44
1:E:204:ARG:NH1	1:E:206:ASP:HB3	2.31	0.44
1:C:150:ARG:HB2	7:C:287:HOH:O	2.16	0.43
1:A:237:ARG:H	1:A:237:ARG:HD3	1.81	0.43
1:E:145:GLU:H	1:E:146:PRO:CD	2.30	0.43
1:F:244:ARG:NH2	7:F:280:HOH:O	2.51	0.43
1:A:184:TYR:OH	1:A:197:LYS:HG2	2.19	0.42
1:F:162:THR:HG22	1:F:164:GLU:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:PHE:CE2	1:F:152:THR:HB	2.55	0.41
1:B:204:ARG:NH1	1:B:206:ASP:HB3	2.34	0.41
1:C:162:THR:HG22	1:C:162:THR:O	2.18	0.41
1:A:204:ARG:CD	1:A:206:ASP:OD1	2.69	0.41
1:F:162:THR:CG2	1:F:164:GLU:HG3	2.51	0.41
1:C:148:ASN:ND2	7:C:306:HOH:O	2.53	0.41
1:E:145:GLU:N	1:E:146:PRO:HD2	2.36	0.41
1:F:148:ASN:ND2	1:F:150:ARG:O	2.55	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	97/110 (88%)	93 (96%)	4 (4%)	0	100	100
1	B	102/110 (93%)	93 (91%)	8 (8%)	1 (1%)	19	5
1	C	89/110 (81%)	86 (97%)	3 (3%)	0	100	100
1	D	93/110 (84%)	90 (97%)	3 (3%)	0	100	100
1	E	102/110 (93%)	95 (93%)	6 (6%)	1 (1%)	19	5
1	F	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
All	All	573/660 (87%)	546 (95%)	25 (4%)	2 (0%)	39	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	GLU
1	E	145	GLU

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	89/99 (90%)	85 (96%)	4 (4%)	34	14
1	B	94/99 (95%)	91 (97%)	3 (3%)	46	26
1	C	85/99 (86%)	77 (91%)	8 (9%)	11	2
1	D	88/99 (89%)	86 (98%)	2 (2%)	58	40
1	E	94/99 (95%)	90 (96%)	4 (4%)	35	16
1	F	86/99 (87%)	79 (92%)	7 (8%)	15	3
All	All	536/594 (90%)	508 (95%)	28 (5%)	28	11

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	A	211	VAL
1	A	233	LEU
1	A	237	ARG
1	B	229	GLU
1	B	230	LYS
1	B	233	LEU
1	C	148	ASN
1	C	152	THR
1	C	163	HIS
1	C	211	VAL
1	C	230	LYS
1	C	233	LEU
1	C	236	LEU
1	C	245	GLU
1	D	233	LEU
1	D	237	ARG
1	E	144	LYS
1	E	225	ILE
1	E	233	LEU
1	E	237	ARG
1	F	148	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	152	THR
1	F	163	HIS
1	F	233	LEU
1	F	236	LEU
1	F	244	ARG
1	F	245	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	148	ASN
1	F	148	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are unknown and 7 are monoatomic - leaving 8 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
2	PO4	A	1004	-	4,4,4	0.34	0	6,6,6	0.35	0
6	GLY	B	4001	-	1,4,4	0.95	0	0,4,4	0.00	-
6	GLY	B	4002	-	1,4,4	0.96	0	0,4,4	0.00	-
6	GLY	B	4003	-	1,4,4	1.07	0	0,4,4	0.00	-
2	PO4	D	1001[A]	-	4,4,4	0.67	0	6,6,6	0.27	0
2	PO4	D	1001[B]	-	4,4,4	0.53	0	6,6,6	0.28	0
2	PO4	D	1002	-	4,4,4	0.48	0	6,6,6	0.29	0
2	PO4	E	1003	-	4,4,4	0.42	0	6,6,6	0.28	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
2	PO4	A	1004	-	-	0/0/0/0	0/0/0/0
6	GLY	B	4001	-	-	0/0/2/2	0/0/0/0
6	GLY	B	4002	-	-	0/0/2/2	0/0/0/0
6	GLY	B	4003	-	-	0/0/2/2	0/0/0/0
2	PO4	D	1001[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1001[B]	-	-	0/0/0/0	0/0/0/0
2	PO4	D	1002	-	-	0/0/0/0	0/0/0/0
2	PO4	E	1003	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

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 [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, 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	98/110 (89%)	0.86	5 (5%) 32 30	32, 38, 57, 78	0
1	B	103/110 (93%)	1.15	16 (15%) 3 3	30, 39, 56, 63	0
1	C	92/110 (83%)	0.85	11 (11%) 6 5	31, 39, 51, 57	0
1	D	96/110 (87%)	0.84	4 (4%) 40 38	32, 38, 53, 62	0
1	E	103/110 (93%)	1.12	18 (17%) 2 2	30, 39, 56, 65	0
1	F	93/110 (84%)	1.02	11 (11%) 6 5	33, 39, 51, 69	0
All	All	585/660 (88%)	0.98	65 (11%) 7 6	30, 39, 56, 78	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	149	VAL	7.5
1	A	209	GLY	7.0
1	E	207	PHE	6.6
1	B	204	ARG	6.3
1	F	211	VAL	5.5
1	D	149	VAL	5.3
1	B	205	TYR	5.0
1	B	239	VAL	5.0
1	E	205	TYR	4.9
1	B	208	GLY	4.8
1	C	211	VAL	4.7
1	E	204	ARG	4.7
1	A	149	VAL	4.5
1	B	203	TRP	4.3
1	F	161	GLU	4.1
1	B	237	ARG	4.1
1	B	246	PRO	4.1
1	E	209	GLY	3.7
1	F	239	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	146	PRO	3.6
1	B	207	PHE	3.6
1	E	228	GLY	3.5
1	A	211	VAL	3.5
1	E	227	THR	3.4
1	B	228	GLY	3.4
1	F	237	ARG	3.4
1	E	236	LEU	3.3
1	B	209	GLY	3.1
1	D	239	VAL	3.1
1	C	161	GLU	3.1
1	E	203	TRP	3.1
1	F	236	LEU	3.1
1	E	246	PRO	3.0
1	F	148	ASN	3.0
1	E	237	ARG	3.0
1	C	239	VAL	3.0
1	D	211	VAL	2.9
1	D	207	PHE	2.8
1	C	237	ARG	2.8
1	A	210	ASP	2.8
1	C	212	ASN	2.8
1	B	206	ASP	2.8
1	B	199	LEU	2.7
1	C	235	THR	2.6
1	E	206	ASP	2.6
1	E	199	LEU	2.6
1	F	163	HIS	2.6
1	E	202	VAL	2.6
1	F	162	THR	2.6
1	C	246	PRO	2.5
1	E	208	GLY	2.5
1	F	210	ASP	2.4
1	E	145	GLU	2.4
1	B	202	VAL	2.4
1	B	144	LYS	2.3
1	C	163	HIS	2.2
1	E	144	LYS	2.2
1	B	200	ASP	2.1
1	B	236	LEU	2.1
1	C	162	THR	2.1
1	F	227	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	149	VAL	2.0
1	E	192	VAL	2.0
1	A	161	GLU	2.0
1	C	159	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	K	A	2002	1/1	0.97	0.20	5.29	36,36,36,36	0
3	K	D	2001	1/1	0.99	0.21	5.02	35,35,35,35	0
6	GLY	B	4001	5/5	0.85	0.15	1.65	58,61,62,62	0
2	PO4	A	1004	5/5	0.93	0.19	1.44	42,47,50,51	0
2	PO4	D	1002	5/5	0.93	0.16	0.38	40,46,49,50	0
5	CL	D	3004	1/1	0.95	0.14	-0.54	34,34,34,34	0
3	K	E	2003	1/1	0.99	0.12	-0.94	32,32,32,32	0
6	GLY	B	4002	5/5	0.79	0.12	-1.22	51,54,57,58	0
6	GLY	B	4003	5/5	0.88	0.13	-1.55	45,49,54,55	0
2	PO4	D	1001[B]	5/5	0.98	0.10	-2.12	23,23,28,34	4
2	PO4	D	1001[A]	5/5	0.98	0.10	-2.12	22,25,27,34	4
5	CL	E	3001	1/1	0.98	0.08	-3.35	33,33,33,33	0
4	UNX	A	6002	1/1	0.93	0.57	-	29,29,29,29	0
4	UNX	B	5002	1/1	0.96	0.24	-	38,38,38,38	0
4	UNX	E	5001	1/1	0.96	0.33	-	36,36,36,36	0
2	PO4	E	1003	5/5	0.89	0.19	-	55,59,61,63	0
5	CL	B	3003	1/1	0.99	0.17	-	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	UNX	D	6001	1/1	0.90	0.15	-	24,24,24,24	0
5	CL	E	3002	1/1	0.99	0.18	-	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.