wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 06:43 AM EDT

PDB ID	:	6NL7
Title	:	Crystal structure of B1 immunoglobulin-binding domain of Streptococcal Protein G (T16F, T18A, V21H, T25H, K28Y, V29I, K31R, Q32A, Y33L, N35K, D36A, N37Q)
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Deposited on	:	2019-01-08
Resolution	:	1.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

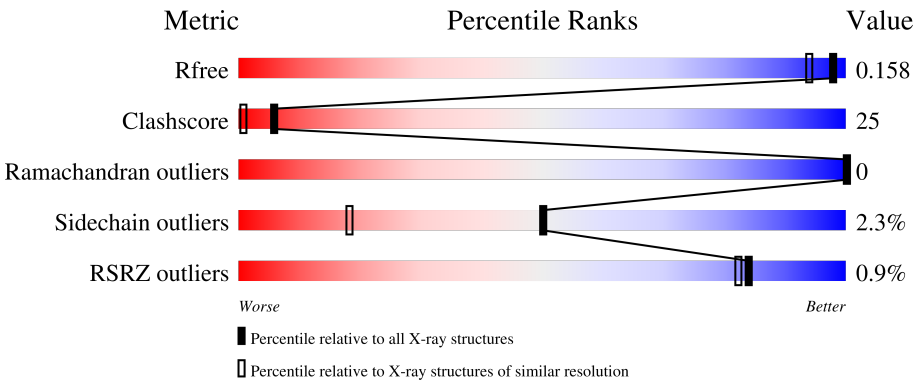
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	56	73% 27%
1	B	56	2% 70% 29% •
1	C	56	2% 77% 20% •
1	D	56	77% 23%

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	ACT	A	103	-	X	-	-
3	ACT	C	101	-	-	X	-
4	NA	A	106	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2325 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 Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	56	491	318	73	98	2	0	9	0
1	B	56	484	316	72	94	2	0	8	0
1	C	56	482	313	73	94	2	0	8	0
1	D	56	473	306	72	93	2	0	6	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P19909
A	16	PHE	THR	engineered mutation	UNP P19909
A	18	ALA	THR	engineered mutation	UNP P19909
A	21	HIS	VAL	engineered mutation	UNP P19909
A	25	HIS	THR	engineered mutation	UNP P19909
A	28	TYR	LYS	engineered mutation	UNP P19909
A	29	ILE	VAL	engineered mutation	UNP P19909
A	31	ARG	LYS	engineered mutation	UNP P19909
A	32	ALA	GLN	engineered mutation	UNP P19909
A	33	LEU	TYR	engineered mutation	UNP P19909
A	35	LYS	ASN	engineered mutation	UNP P19909
A	36	ALA	ASP	engineered mutation	UNP P19909
A	37	GLN	ASN	engineered mutation	UNP P19909
B	1	MET	-	initiating methionine	UNP P19909
B	16	PHE	THR	engineered mutation	UNP P19909
B	18	ALA	THR	engineered mutation	UNP P19909
B	21	HIS	VAL	engineered mutation	UNP P19909
B	25	HIS	THR	engineered mutation	UNP P19909
B	28	TYR	LYS	engineered mutation	UNP P19909
B	29	ILE	VAL	engineered mutation	UNP P19909
B	31	ARG	LYS	engineered mutation	UNP P19909

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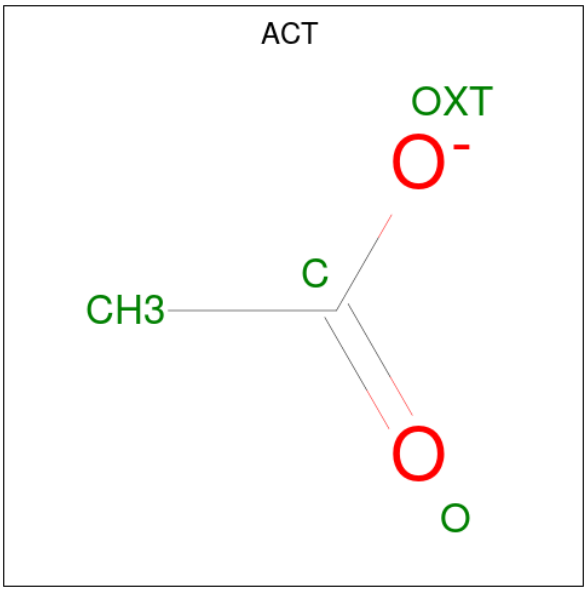
Chain	Residue	Modelled	Actual	Comment	Reference
B	32	ALA	GLN	engineered mutation	UNP P19909
B	33	LEU	TYR	engineered mutation	UNP P19909
B	35	LYS	ASN	engineered mutation	UNP P19909
B	36	ALA	ASP	engineered mutation	UNP P19909
B	37	GLN	ASN	engineered mutation	UNP P19909
C	1	MET	-	initiating methionine	UNP P19909
C	16	PHE	THR	engineered mutation	UNP P19909
C	18	ALA	THR	engineered mutation	UNP P19909
C	21	HIS	VAL	engineered mutation	UNP P19909
C	25	HIS	THR	engineered mutation	UNP P19909
C	28	TYR	LYS	engineered mutation	UNP P19909
C	29	ILE	VAL	engineered mutation	UNP P19909
C	31	ARG	LYS	engineered mutation	UNP P19909
C	32	ALA	GLN	engineered mutation	UNP P19909
C	33	LEU	TYR	engineered mutation	UNP P19909
C	35	LYS	ASN	engineered mutation	UNP P19909
C	36	ALA	ASP	engineered mutation	UNP P19909
C	37	GLN	ASN	engineered mutation	UNP P19909
D	1	MET	-	initiating methionine	UNP P19909
D	16	PHE	THR	engineered mutation	UNP P19909
D	18	ALA	THR	engineered mutation	UNP P19909
D	21	HIS	VAL	engineered mutation	UNP P19909
D	25	HIS	THR	engineered mutation	UNP P19909
D	28	TYR	LYS	engineered mutation	UNP P19909
D	29	ILE	VAL	engineered mutation	UNP P19909
D	31	ARG	LYS	engineered mutation	UNP P19909
D	32	ALA	GLN	engineered mutation	UNP P19909
D	33	LEU	TYR	engineered mutation	UNP P19909
D	35	LYS	ASN	engineered mutation	UNP P19909
D	36	ALA	ASP	engineered mutation	UNP P19909
D	37	GLN	ASN	engineered mutation	UNP P19909

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0
			Total	Zn		
2	B	2	2	2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

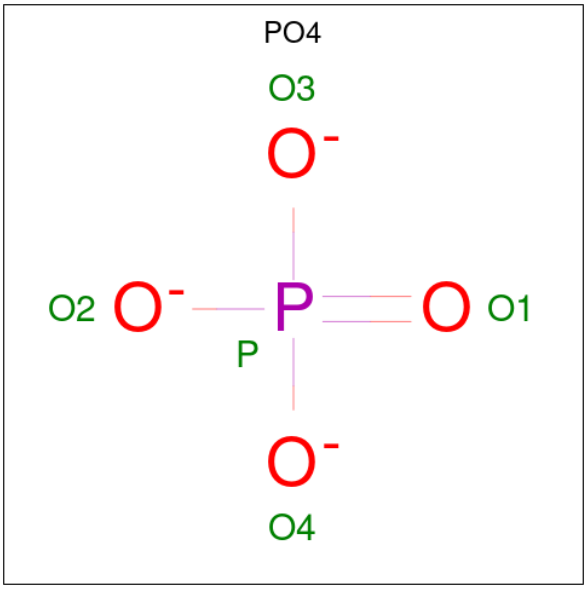
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0
			Total	Na		
4	B	1	1	1	0	0
			Total	Na		
4	C	1	1	1	0	0

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

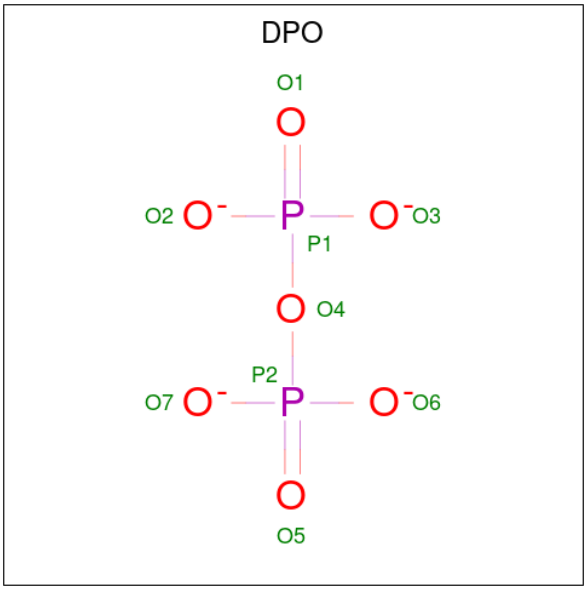
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	B	1	9	7	2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	105	105	105	0	0
			Total	O		
8	B	73	73	73	0	0
			Total	O		
8	C	83	83	83	0	0
			Total	O		
8	D	74	74	74	0	0

3 Residue-property plots (i)

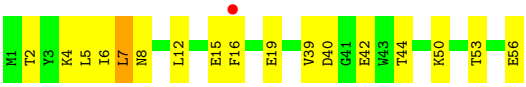
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Immunoglobulin G-binding protein G

Chain A:

• Molecule 1: Immunoglobulin G-binding protein G

Chain B:



• Molecule 1: Immunoglobulin G-binding protein G

Chain C:

• Molecule 1: Immunoglobulin G-binding protein G

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.90Å 63.06Å 53.23Å 90.00° 103.31° 90.00°	Depositor
Resolution (Å)	40.06 – 1.40 40.02 – 1.40	Depositor EDS
% Data completeness (in resolution range)	90.0 (40.06-1.40) 90.1 (40.02-1.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.113 , 0.158 0.114 , 0.158	Depositor DCC
R_{free} test set	2317 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	11.3	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2325	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7386e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DPO, ZN, PO4, ACT, 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	0.87	1/526 (0.2%)	0.95	4/705 (0.6%)
1	B	0.83	1/516 (0.2%)	0.88	0/692
1	C	0.83	0/515	0.92	0/694
1	D	0.82	1/500 (0.2%)	0.87	0/674
All	All	0.84	3/2057 (0.1%)	0.90	4/2765 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	27	GLU	CD-OE2	-6.01	1.19	1.25
1	B	42	GLU	CD-OE2	-5.63	1.19	1.25
1	A	42	GLU	CD-OE1	-5.07	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40[A]	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	40[B]	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	40[A]	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	40[B]	ASP	CB-CG-OD2	-6.01	112.89	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	491	0	498	13	0
1	B	484	0	498	37	0
1	C	482	0	493	41	2
1	D	473	0	475	17	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	8	0	6	0	1
3	B	12	0	9	0	1
3	C	8	0	6	4	0
3	D	4	0	3	1	0
4	A	2	0	0	2	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	1	0
7	B	9	0	0	1	0
8	A	105	0	0	8	2
8	B	73	0	0	18	1
8	C	83	0	0	8	1
8	D	74	0	0	10	0
All	All	2325	0	1988	100	5

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 25.

The worst 5 of 100 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:16:PHE:CE1	1:C:12:LEU:HD21	1.55	1.41
1:D:50:LYS:HG3	8:D:253:HOH:O	1.18	1.34
1:B:44:THR:OG1	1:B:53[B]:THR:HG22	1.31	1.28
8:B:255:HOH:O	1:C:16:PHE:HB3	1.48	1.10
1:B:16:PHE:CE1	1:C:12:LEU:CD2	2.36	1.08

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:247:HOH:O	8:C:281:HOH:O[2_446]	1.49	0.71
1:D:25:HIS:NE2	3:A:104:ACT:O[1_556]	1.94	0.26
1:C:21:HIS:CE1	8:A:201:HOH:O[1_455]	2.08	0.12
1:C:25:HIS:NE2	3:B:106:ACT:OXT[1_455]	2.10	0.10
1:D:22:ASP:OD2	8:A:297:HOH:O[1_556]	2.18	0.02

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	61/56 (109%)	59 (97%)	2 (3%)	0	100	100
1	B	60/56 (107%)	59 (98%)	1 (2%)	0	100	100
1	C	61/56 (109%)	59 (97%)	2 (3%)	0	100	100
1	D	59/56 (105%)	57 (97%)	2 (3%)	0	100	100
All	All	241/224 (108%)	234 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	52/43 (121%)	52 (100%)	0	100	100
1	B	51/43 (119%)	48 (94%)	3 (6%)	19	2
1	C	51/43 (119%)	48 (94%)	3 (6%)	19	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	49/43 (114%)	49 (100%)	0	100	100
All	All	203/172 (118%)	197 (97%)	6 (3%)	50	10

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8[A]	ASN
1	C	8[B]	ASN
1	C	12	LEU
1	B	7[B]	LEU
1	B	7[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	B	8	ASN
1	D	21	HIS
1	D	37	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	ACT	D	101	-	3,3,3	0.58	0	3,3,3	0.50	0
3	ACT	B	106	2	3,3,3	1.25	1 (33%)	3,3,3	0.82	0
3	ACT	C	102	-	3,3,3	0.83	0	3,3,3	2.16	2 (66%)
6	PO4	A	108	4	4,4,4	1.84	1 (25%)	6,6,6	0.98	0
3	ACT	A	103	2	3,3,3	1.55	1 (33%)	3,3,3	2.56	2 (66%)
3	ACT	B	104	2	3,3,3	2.24	1 (33%)	3,3,3	0.97	0
3	ACT	C	101	-	3,3,3	1.04	0	3,3,3	0.97	0
3	ACT	B	105	2	3,3,3	1.11	0	3,3,3	0.30	0
3	ACT	A	104	2	3,3,3	1.12	0	3,3,3	1.93	1 (33%)
7	DPO	B	101	-	6,8,8	0.80	0	13,13,13	2.70	5 (38%)
6	PO4	B	108	4	4,4,4	2.98	2 (50%)	6,6,6	1.72	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DPO	B	101	-	-	0/6/6/6	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	108	PO4	P-O1	4.51	1.61	1.50
3	B	104	ACT	OXT-C	-3.82	1.12	1.30
6	B	108	PO4	P-O3	-3.80	1.43	1.54
6	A	108	PO4	P-O1	3.20	1.58	1.50
3	A	103	ACT	O-C	-2.65	1.10	1.22

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	101	DPO	P2-O4-P1	-5.46	114.08	132.83
7	B	101	DPO	O3-P1-O2	4.40	124.45	107.64
7	B	101	DPO	O4-P2-O5	-4.04	88.78	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	101	DPO	O6-P2-O5	4.03	126.45	110.68
6	B	108	PO4	O3-P-O1	-3.44	98.31	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	101	ACT	1	0
3	B	106	ACT	0	1
3	C	101	ACT	4	0
3	A	104	ACT	0	1
7	B	101	DPO	1	0
6	B	108	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	56/56 (100%)	-0.35	0 100 100	7, 12, 26, 41	0
1	B	56/56 (100%)	-0.26	1 (1%) 68 68	9, 16, 33, 42	0
1	C	56/56 (100%)	-0.24	1 (1%) 68 68	9, 16, 42, 59	0
1	D	56/56 (100%)	-0.34	0 100 100	9, 16, 33, 40	0
All	All	224/224 (100%)	-0.30	2 (0%) 84 82	7, 15, 35, 59	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	PHE	2.3
1	C	40[A]	ASP	2.1

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, 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
6	PO4	B	108	5/5	0.73	0.18	34,35,45,51	0
6	PO4	A	108	5/5	0.87	0.23	36,43,45,50	0
7	DPO	B	101	9/9	0.91	0.24	29,32,37,40	0
3	ACT	D	101	4/4	0.94	0.14	21,27,27,29	0
3	ACT	A	104	4/4	0.95	0.15	19,22,30,33	0
3	ACT	B	106	4/4	0.95	0.15	17,21,26,31	0
3	ACT	A	103	4/4	0.96	0.09	16,18,27,30	0
3	ACT	C	101	4/4	0.96	0.21	32,36,37,49	0
3	ACT	B	104	4/4	0.97	0.11	18,20,30,32	0
3	ACT	B	105	4/4	0.97	0.08	15,19,19,23	0
3	ACT	C	102	4/4	0.98	0.07	18,18,20,30	0
4	NA	A	106	1/1	0.99	0.09	20,20,20,20	0
4	NA	B	107	1/1	0.99	0.05	17,17,17,17	0
4	NA	C	103	1/1	0.99	0.07	27,27,27,27	0
2	ZN	A	102	1/1	1.00	0.03	14,14,14,14	0
2	ZN	B	102	1/1	1.00	0.04	14,14,14,14	0
5	CL	A	107	1/1	1.00	0.07	10,10,10,10	0
2	ZN	B	103	1/1	1.00	0.03	16,16,16,16	0
4	NA	A	105	1/1	1.00	0.07	19,19,19,19	0
2	ZN	A	101	1/1	1.00	0.04	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.