



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:40 AM UTC

PDB ID : 8FZ3 / pdb_00008fz3
Title : Sterile Alpha Motif of Human Translocation ETS Leukemia, Non-Polymer
Crystal Form
Authors : Averett, J.C.; Nawarathnage, S.D.; Moody, J.D.
Deposited on : 2023-01-27
Resolution : 2.78 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

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

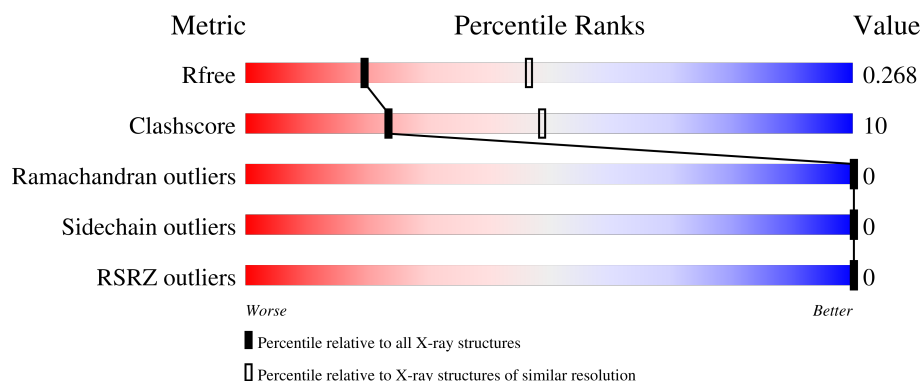
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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 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 $\leq 5\%$. 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	170	 37% 9% 54%
1	B	170	 35% 11% 55%
1	C	170	 30% 16% 54%
1	D	170	 41% 6% 54%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4731 atoms, of which 2247 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 Transcription factor ETV6, Activated CDC42 kinase 1 fusion.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	78	Total	C	H	N	O	S	0	1	0
			1257	417	612	112	115	1			
1	B	77	Total	C	H	N	O	S	0	0	0
			1188	401	576	105	105	1			
1	C	78	Total	C	H	N	O	S	0	0	0
			1126	388	533	103	101	1			
1	D	79	Total	C	H	N	O	S	0	0	0
			1122	388	526	100	107	1			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P41212
A	2	HIS	-	expression tag	UNP P41212
A	3	HIS	-	expression tag	UNP P41212
A	4	HIS	-	expression tag	UNP P41212
A	5	HIS	-	expression tag	UNP P41212
A	6	HIS	-	expression tag	UNP P41212
A	7	HIS	-	expression tag	UNP P41212
A	8	HIS	-	expression tag	UNP P41212
A	9	HIS	-	expression tag	UNP P41212
A	10	HIS	-	expression tag	UNP P41212
A	11	HIS	-	expression tag	UNP P41212
A	45	SER	ARG	engineered mutation	UNP P41212
A	77	GLU	VAL	engineered mutation	UNP P41212
A	89	GLY	-	linker	UNP P41212
B	1	GLY	-	expression tag	UNP P41212
B	2	HIS	-	expression tag	UNP P41212
B	3	HIS	-	expression tag	UNP P41212
B	4	HIS	-	expression tag	UNP P41212
B	5	HIS	-	expression tag	UNP P41212
B	6	HIS	-	expression tag	UNP P41212
B	7	HIS	-	expression tag	UNP P41212

Continued on next page...

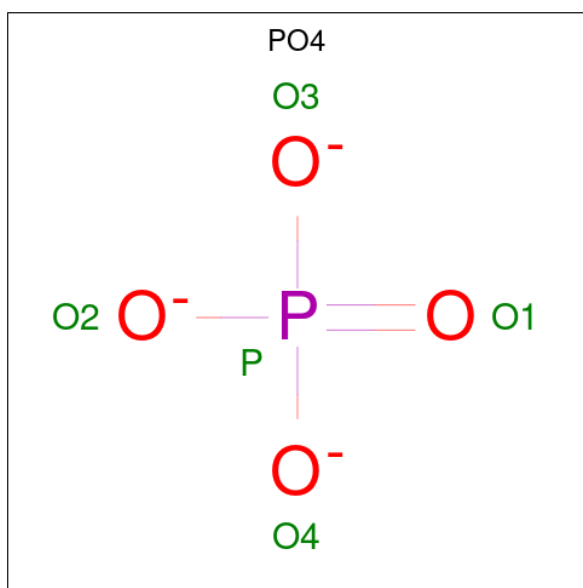
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	HIS	-	expression tag	UNP P41212
B	9	HIS	-	expression tag	UNP P41212
B	10	HIS	-	expression tag	UNP P41212
B	11	HIS	-	expression tag	UNP P41212
B	45	SER	ARG	engineered mutation	UNP P41212
B	77	GLU	VAL	engineered mutation	UNP P41212
B	89	GLY	-	linker	UNP P41212
C	1	GLY	-	expression tag	UNP P41212
C	2	HIS	-	expression tag	UNP P41212
C	3	HIS	-	expression tag	UNP P41212
C	4	HIS	-	expression tag	UNP P41212
C	5	HIS	-	expression tag	UNP P41212
C	6	HIS	-	expression tag	UNP P41212
C	7	HIS	-	expression tag	UNP P41212
C	8	HIS	-	expression tag	UNP P41212
C	9	HIS	-	expression tag	UNP P41212
C	10	HIS	-	expression tag	UNP P41212
C	11	HIS	-	expression tag	UNP P41212
C	45	SER	ARG	engineered mutation	UNP P41212
C	77	GLU	VAL	engineered mutation	UNP P41212
C	89	GLY	-	linker	UNP P41212
D	1	GLY	-	expression tag	UNP P41212
D	2	HIS	-	expression tag	UNP P41212
D	3	HIS	-	expression tag	UNP P41212
D	4	HIS	-	expression tag	UNP P41212
D	5	HIS	-	expression tag	UNP P41212
D	6	HIS	-	expression tag	UNP P41212
D	7	HIS	-	expression tag	UNP P41212
D	8	HIS	-	expression tag	UNP P41212
D	9	HIS	-	expression tag	UNP P41212
D	10	HIS	-	expression tag	UNP P41212
D	11	HIS	-	expression tag	UNP P41212
D	45	SER	ARG	engineered mutation	UNP P41212
D	77	GLU	VAL	engineered mutation	UNP P41212
D	89	GLY	-	linker	UNP P41212

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

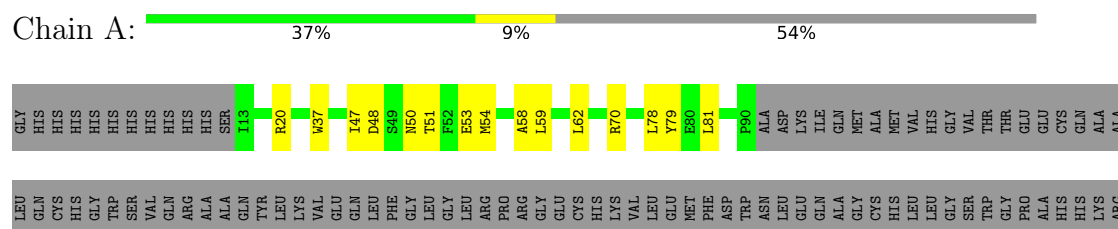
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	9	Total	O	0	0
			9	9		
4	C	7	Total	O	0	0
			7	7		
4	D	5	Total	O	0	0
			5	5		

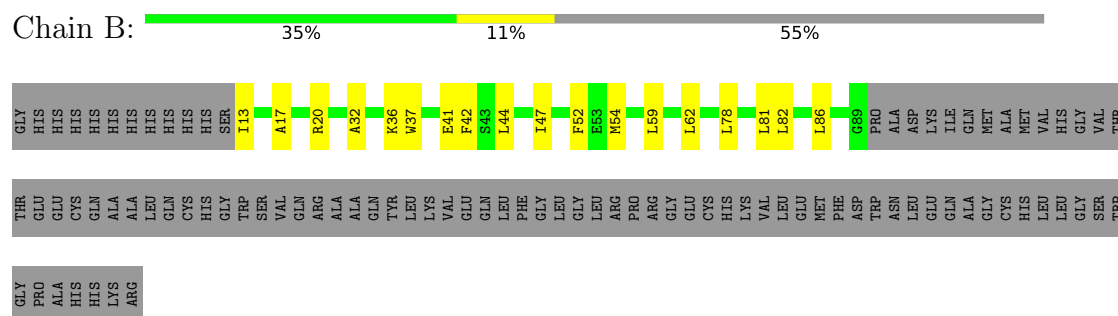
3 Residue-property plots

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.

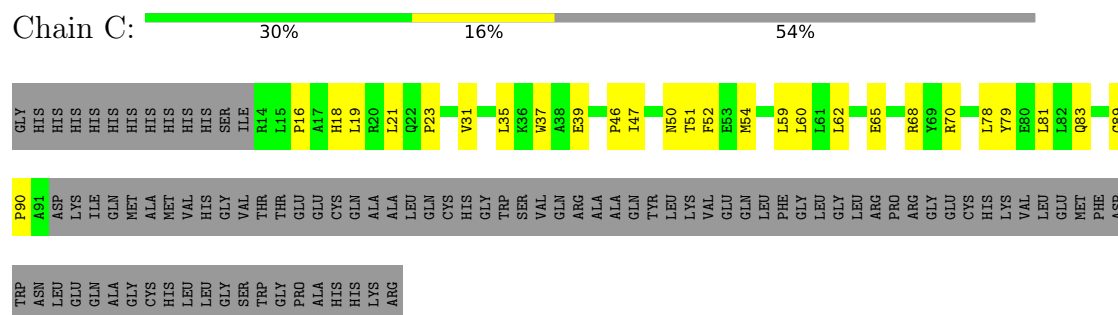
- Molecule 1: Transcription factor ETV6, Activated CDC42 kinase 1 fusion



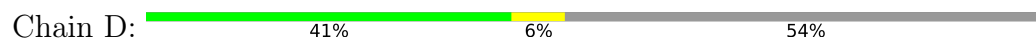
- Molecule 1: Transcription factor ETV6, Activated CDC42 kinase 1 fusion



- Molecule 1: Transcription factor ETV6, Activated CDC42 kinase 1 fusion



- Molecule 1: Transcription factor ETV6, Activated CDC42 kinase 1 fusion



GLN	ARG	ALA	ALA	GLN	TYR	LEU	LYS	VAL	GLU	GLN	LEU	PHE	GLY	LEU	LEU	ARG	PRO	ARG	GLY	GLU	CYS	HIS	LYS	VAL	LEU	GLU	MET	PHE	ASP	TRP	ASN	LEU	GLU	GLN	ALA	GLY	CYS	HIS	LEU	LEU	GLY	SER	TRP	GLY	PRO	ALA	HIS	HIS	LYS	ARG	
HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	ILE	R14	L21	L35	D48	T51	F52	K64	S74	G75	Y79	Q83	D92	LYS	ILE	GLN	MET	ALA	MET	VAL	HIS	GLY	VAL	THR	THR	GLU	GLU	CYS	GLN	ALA	ALA	LEU	GLN	CYS	HIS	GLY	TRP	SER	VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	61.51Å 61.51Å 166.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.84 – 2.78 44.84 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.84-2.78) 94.0 (44.84-2.78)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.229 , 0.267 0.229 , 0.268	Depositor DCC
R_{free} test set	467 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 84.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4731	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% 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, 0.333 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, 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	0.50	0/668	0.52	0/909
1	B	0.76	0/630	0.60	0/857
1	C	0.51	0/611	0.61	0/833
1	D	0.34	0/614	0.46	0/842
All	All	0.55	0/2523	0.55	0/3441

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	645	612	612	12	0
1	B	612	576	576	14	0
1	C	593	533	530	17	0
1	D	596	526	526	6	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	B	5	0	0	0	0
4	A	10	0	0	0	0
4	B	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	7	0	0	0	0
4	D	5	0	0	0	0
All	All	2484	2247	2244	48	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 10.

All (48) 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:47:ILE:HD13	1:B:78:LEU:HD11	1.65	0.79
1:A:47:ILE:HD13	1:A:78:LEU:HD11	1.77	0.67
1:A:51:THR:CG2	1:A:70:ARG:HB3	2.27	0.65
1:C:54:MET:HE1	1:C:70:ARG:CZ	2.27	0.64
1:C:35:LEU:HD11	1:C:52:PHE:HB2	1.79	0.64
1:A:20:ARG:HD2	1:C:21:LEU:HD21	1.80	0.64
1:C:79:TYR:O	1:C:83:GLN:HG2	1.97	0.64
1:D:35:LEU:HD11	1:D:52:PHE:HB2	1.83	0.61
1:A:37:TRP:CZ3	1:A:81:LEU:HD21	2.43	0.53
1:B:13:ILE:HG23	1:B:37:TRP:CH2	2.44	0.53
1:A:50:ASN:HA	1:A:53:GLU:HG3	1.92	0.51
1:B:37:TRP:CE2	1:B:41:GLU:HG3	2.45	0.51
1:C:59:LEU:HD12	1:C:62:LEU:HD12	1.93	0.51
1:D:21:LEU:H	1:D:21:LEU:HD23	1.78	0.49
1:D:48:ASP:HB3	1:D:51:THR:HG23	1.94	0.48
1:D:79:TYR:O	1:D:83:GLN:HG2	2.13	0.48
1:C:89:GLY:N	1:C:90:PRO:CD	2.77	0.48
1:B:17:ALA:HA	1:B:20:ARG:NE	2.28	0.47
1:B:54:MET:HE3	1:B:59:LEU:HD13	1.96	0.47
1:C:16:PRO:CG	1:C:19:LEU:HD12	2.45	0.46
1:B:54:MET:HE1	1:B:62:LEU:HD22	1.97	0.46
1:C:51:THR:HG22	1:C:52:PHE:CE1	2.49	0.46
1:B:42:PHE:HB2	1:B:44:LEU:HD21	1.97	0.46
1:C:31:VAL:HG23	1:C:59:LEU:HD22	1.98	0.45
1:D:64:LYS:HD3	1:D:79:TYR:CD2	2.52	0.45
1:B:81:LEU:C	1:B:81:LEU:HD13	2.43	0.44
1:B:52:PHE:HD1	1:B:54:MET:HE2	1.83	0.44
1:B:32:ALA:O	1:B:36:LYS:HG3	2.19	0.43
1:C:23:PRO:HB2	1:C:60:LEU:HD11	2.00	0.43
1:A:79:TYR:CD1	1:A:79:TYR:C	2.96	0.43
1:C:50:ASN:O	1:C:51:THR:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:OE2	1:C:46:PRO:HA	2.19	0.42
1:C:65:GLU:HA	1:C:68:ARG:HD2	1.99	0.42
1:B:82:LEU:HG	1:B:86:LEU:HD11	2.01	0.42
1:B:37:TRP:NE1	1:B:41:GLU:HG3	2.33	0.42
1:C:47:ILE:HD13	1:C:78:LEU:HD11	2.02	0.42
1:A:37:TRP:HZ3	1:A:81:LEU:HD21	1.85	0.42
1:A:48:ASP:O	1:A:51:THR:HB	2.19	0.42
1:A:51:THR:HG23	1:A:70:ARG:HB3	2.00	0.42
1:B:17:ALA:HA	1:B:20:ARG:HG3	2.01	0.41
1:C:89:GLY:N	1:C:90:PRO:HD3	2.35	0.41
1:A:54:MET:HE2	1:A:58:ALA:C	2.45	0.41
1:B:54:MET:HE1	1:B:62:LEU:CD2	2.51	0.41
1:C:37:TRP:HZ3	1:C:81:LEU:HD21	1.85	0.41
1:D:74:SER:O	1:D:75:GLY:C	2.62	0.41
1:A:59:LEU:HD12	1:A:62:LEU:HD12	2.02	0.41
1:A:54:MET:HE1	1:A:62:LEU:HD21	2.04	0.40
1:C:18:HIS:CD2	1:C:19:LEU:HG	2.57	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	77/170 (45%)	76 (99%)	1 (1%)	0	100	100
1	B	75/170 (44%)	73 (97%)	2 (3%)	0	100	100
1	C	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
1	D	77/170 (45%)	76 (99%)	1 (1%)	0	100	100
All	All	305/680 (45%)	300 (98%)	5 (2%)	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	67/146 (46%)	67 (100%)	0	100	100
1	B	59/146 (40%)	59 (100%)	0	100	100
1	C	49/146 (34%)	49 (100%)	0	100	100
1	D	53/146 (36%)	53 (100%)	0	100	100
All	All	228/584 (39%)	228 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	50	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	PO4	B	201	-	4,4,4	0.99	0	6,6,6	0.49	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 [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	78/170 (45%)	-0.97	0 100 100	39, 65, 95, 180	1 (1%)
1	B	77/170 (45%)	-0.95	0 100 100	42, 65, 89, 106	0
1	C	78/170 (45%)	-0.54	0 100 100	57, 82, 111, 153	0
1	D	79/170 (46%)	-0.59	0 100 100	53, 77, 117, 149	0
All	All	312/680 (45%)	-0.76	0 100 100	39, 72, 108, 180	1 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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
2	CL	C	201	1/1	0.95	0.08	47,47,47,47	1
2	CL	A	201	1/1	0.97	0.07	85,85,85,85	0
3	PO4	B	201	5/5	0.98	0.06	93,98,104,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.