



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2017 – 05:46 PM EDT

PDB ID : 5UVF
Title : Crystal Structure of the Human vaccinia-related kinase bound to BI-D1870
Authors : Counago, R.M.; Bountra, C.; Arruda, P.; Edwards, A.M.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on : 2017-02-20
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

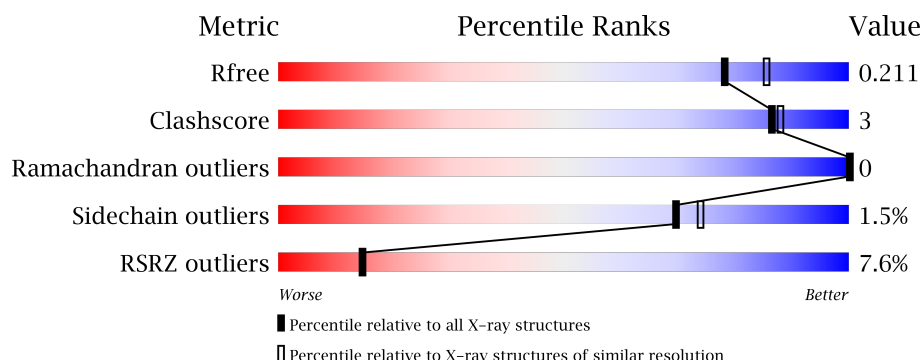
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	364	<div> <div>7%</div> <div>83%</div> <div>13%</div> </div>
1	B	364	<div> <div>6%</div> <div>83%</div> <div>13%</div> </div>
1	C	364	<div> <div>5%</div> <div>78%</div> <div>17%</div> </div>
1	D	364	<div> <div>8%</div> <div>76%</div> <div>5%</div> <div>19%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	7DZ	B	402	-	-	-	X
3	PO4	A	402	-	-	-	X
4	PEG	C	406	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10449 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 Serine/threonine-protein kinase VRK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2468	1581	416	459	12			
1	B	316	Total	C	N	O	S	0	0	0
			2474	1584	419	459	12			
1	C	301	Total	C	N	O	S	0	0	0
			2344	1501	401	430	12			
1	D	296	Total	C	N	O	S	0	0	0
			2310	1481	400	417	12			

There are 52 discrepancies between the modelled and reference sequences:

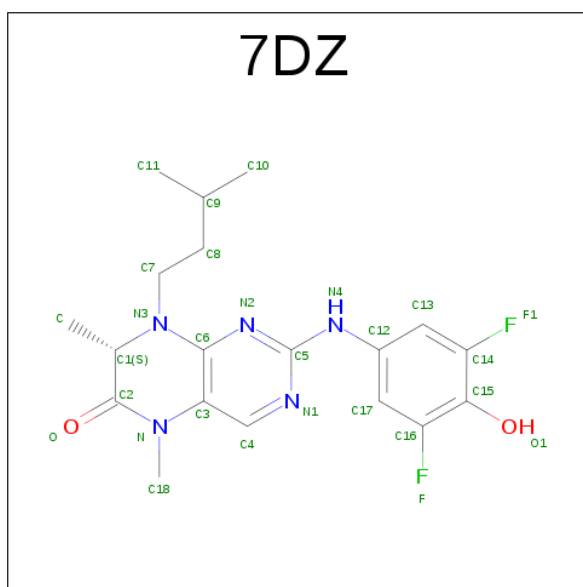
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q99986
A	2	MET	-	expression tag	UNP Q99986
A	34	ALA	LYS	engineered mutation	UNP Q99986
A	35	ALA	LYS	engineered mutation	UNP Q99986
A	36	ALA	GLU	engineered mutation	UNP Q99986
A	212	ALA	GLU	engineered mutation	UNP Q99986
A	214	ALA	LYS	engineered mutation	UNP Q99986
A	215	ALA	GLU	engineered mutation	UNP Q99986
A	292	ALA	GLU	engineered mutation	UNP Q99986
A	293	ALA	LYS	engineered mutation	UNP Q99986
A	295	ALA	LYS	engineered mutation	UNP Q99986
A	359	ALA	LYS	engineered mutation	UNP Q99986
A	360	ALA	LYS	engineered mutation	UNP Q99986
B	1	SER	-	expression tag	UNP Q99986
B	2	MET	-	expression tag	UNP Q99986
B	34	ALA	LYS	engineered mutation	UNP Q99986
B	35	ALA	LYS	engineered mutation	UNP Q99986
B	36	ALA	GLU	engineered mutation	UNP Q99986
B	212	ALA	GLU	engineered mutation	UNP Q99986
B	214	ALA	LYS	engineered mutation	UNP Q99986
B	215	ALA	GLU	engineered mutation	UNP Q99986

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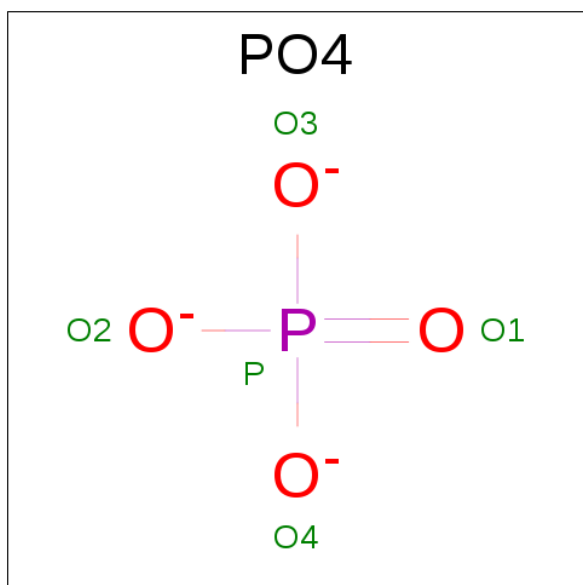
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	ALA	GLU	engineered mutation	UNP Q99986
B	293	ALA	LYS	engineered mutation	UNP Q99986
B	295	ALA	LYS	engineered mutation	UNP Q99986
B	359	ALA	LYS	engineered mutation	UNP Q99986
B	360	ALA	LYS	engineered mutation	UNP Q99986
C	1	SER	-	expression tag	UNP Q99986
C	2	MET	-	expression tag	UNP Q99986
C	34	ALA	LYS	engineered mutation	UNP Q99986
C	35	ALA	LYS	engineered mutation	UNP Q99986
C	36	ALA	GLU	engineered mutation	UNP Q99986
C	212	ALA	GLU	engineered mutation	UNP Q99986
C	214	ALA	LYS	engineered mutation	UNP Q99986
C	215	ALA	GLU	engineered mutation	UNP Q99986
C	292	ALA	GLU	engineered mutation	UNP Q99986
C	293	ALA	LYS	engineered mutation	UNP Q99986
C	295	ALA	LYS	engineered mutation	UNP Q99986
C	359	ALA	LYS	engineered mutation	UNP Q99986
C	360	ALA	LYS	engineered mutation	UNP Q99986
D	1	SER	-	expression tag	UNP Q99986
D	2	MET	-	expression tag	UNP Q99986
D	34	ALA	LYS	engineered mutation	UNP Q99986
D	35	ALA	LYS	engineered mutation	UNP Q99986
D	36	ALA	GLU	engineered mutation	UNP Q99986
D	212	ALA	GLU	engineered mutation	UNP Q99986
D	214	ALA	LYS	engineered mutation	UNP Q99986
D	215	ALA	GLU	engineered mutation	UNP Q99986
D	292	ALA	GLU	engineered mutation	UNP Q99986
D	293	ALA	LYS	engineered mutation	UNP Q99986
D	295	ALA	LYS	engineered mutation	UNP Q99986
D	359	ALA	LYS	engineered mutation	UNP Q99986
D	360	ALA	LYS	engineered mutation	UNP Q99986

- Molecule 2 is (7S)-2-[(3,5-difluoro-4-hydroxyphenyl)amino]-5,7-dimethyl-8-(3-methylbutyl)-7,8-dihydropteridin-6(5H)-one (three-letter code: 7DZ) (formula: C₁₉H₂₃F₂N₅O₂).



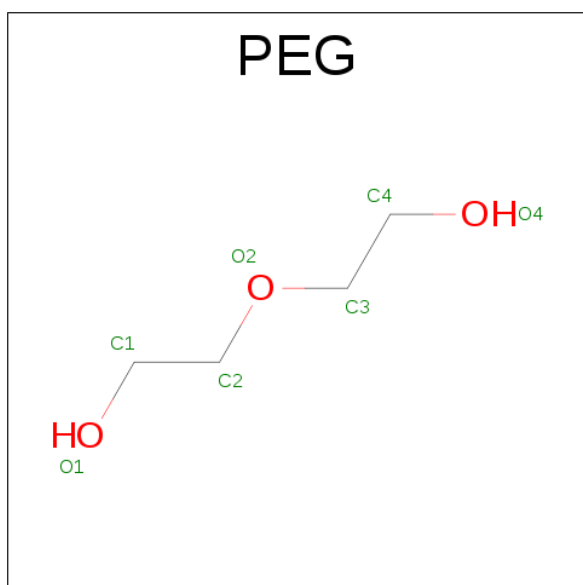
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	19	2	5	2		
2	B	1	Total	C	F	N	O	0	0
			28	19	2	5	2		
2	C	1	Total	C	F	N	O	0	0
			28	19	2	5	2		
2	D	1	Total	C	F	N	O	0	0
			28	19	2	5	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0

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

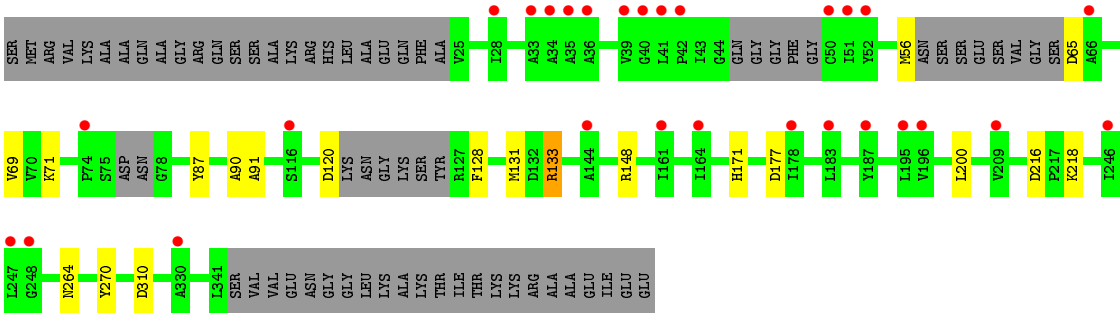
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	161	Total	O	0	0
			161	161		
6	B	193	Total	O	0	0
			193	193		
6	C	165	Total	O	0	0
			165	165		
6	D	164	Total	O	0	0
			164	164		

- Molecule 1: Serine/threonine-protein kinase VRK1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.14Å 95.24Å 192.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 2.00 29.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.66-2.00) 96.8 (29.66-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.173 , 0.204 0.179 , 0.211	Depositor DCC
R_{free} test set	5538 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10449	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, PEG, 7DZ, 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	0/2527	0.63	0/3432
1	B	0.51	0/2532	0.61	0/3436
1	C	0.49	0/2399	0.60	0/3253
1	D	0.51	0/2364	0.60	0/3201
All	All	0.50	0/9822	0.61	0/13322

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	2468	0	2371	6	0
1	B	2474	0	2390	11	0
1	C	2344	0	2227	12	0
1	D	2310	0	2213	12	0
2	A	28	0	0	2	0
2	B	28	0	0	2	0
2	C	28	0	0	2	0
2	D	28	0	0	1	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	20	0	0	0	0
3	D	15	0	0	0	0
4	C	7	0	10	0	0
5	C	1	0	0	0	0
6	A	161	0	0	1	0
6	B	193	0	0	1	0
6	C	165	0	0	1	0
6	D	164	0	0	0	0
All	All	10449	0	9211	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 3.

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:C:114:TRP:HB2	1:C:130:ILE:HG22	1.72	0.71
2:C:402:7DZ:O1	6:C:501:HOH:O	2.12	0.67
1:B:22:GLN:HG2	1:B:72:VAL:HG11	1.79	0.65
1:D:264:ASN:HB3	1:D:270:TYR:CD2	2.32	0.64
1:D:65:ASP:HA	1:D:133:ARG:HH21	1.64	0.63
1:C:87:TYR:HA	1:C:91:ALA:HB3	1.80	0.62
1:D:87:TYR:HA	1:D:91:ALA:HB3	1.82	0.61
1:B:73:GLU:HB2	1:B:80:LEU:HD22	1.83	0.59
1:D:90:ALA:HB1	1:D:171:HIS:HB3	1.87	0.56
1:B:22:GLN:NE2	1:B:119:HIS:ND1	2.50	0.56
2:B:402:7DZ:C11	2:B:402:7DZ:C	2.85	0.54
1:A:200:LEU:HD13	1:A:221:HIS:CG	2.43	0.53
1:C:114:TRP:HB2	1:C:130:ILE:CG2	2.39	0.52
1:B:148:ARG:HH11	1:B:148:ARG:HG2	1.75	0.51
2:B:402:7DZ:N2	2:B:402:7DZ:C13	2.73	0.51
1:C:90:ALA:HB1	1:C:171:HIS:HB3	1.92	0.50
2:A:401:7DZ:N2	2:A:401:7DZ:C13	2.75	0.50
1:C:87:TYR:HD2	1:C:129:MET:HE1	1.77	0.49
1:B:22:GLN:HE21	1:B:119:HIS:CE1	2.31	0.48
2:D:403:7DZ:C13	2:D:403:7DZ:N2	2.76	0.48
1:A:43:ILE:HG23	1:A:53:LEU:HG	1.95	0.48
1:B:52:TYR:HB2	1:B:70:VAL:CG1	2.44	0.48
2:C:402:7DZ:N2	2:C:402:7DZ:C13	2.77	0.48
1:D:90:ALA:CB	1:D:171:HIS:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:VAL:HG13	1:D:133:ARG:HG2	1.96	0.47
1:C:87:TYR:CD2	1:C:129:MET:HE1	2.49	0.47
1:D:216:ASP:OD1	1:D:218:LYS:HG2	2.14	0.47
1:D:65:ASP:HA	1:D:133:ARG:NH2	2.29	0.47
1:D:148:ARG:HH11	1:D:148:ARG:HG2	1.80	0.47
1:C:87:TYR:CD2	1:C:129:MET:CE	2.98	0.46
1:C:186:ASN:HB3	1:C:189:ASN:O	2.15	0.46
1:A:184:LEU:HD22	1:A:196:VAL:HG11	1.98	0.46
1:A:87:TYR:HD1	1:A:91:ALA:HB3	1.81	0.45
1:B:133:ARG:C	1:B:133:ARG:HD3	2.36	0.45
1:B:73:GLU:HB2	1:B:80:LEU:CD2	2.45	0.45
1:B:148:ARG:NH1	1:B:148:ARG:HG2	2.33	0.43
1:C:87:TYR:CD1	1:C:91:ALA:HB3	2.53	0.43
1:C:169:HIS:CG	1:C:240:ARG:HG2	2.54	0.42
1:C:204:TYR:CE2	1:C:205:CYS:HB2	2.54	0.42
2:A:401:7DZ:O1	6:A:501:HOH:O	2.22	0.42
1:D:177:ASP:HB2	1:D:200:LEU:HD11	2.01	0.42
1:A:99:TRP:CD2	1:A:167:TYR:HD2	2.38	0.41
1:B:184:LEU:HD22	1:B:196:VAL:HG11	2.02	0.41
1:A:301:LYS:HE3	1:A:323:ILE:HG12	2.02	0.41
1:C:90:ALA:CB	1:C:171:HIS:HB3	2.50	0.41
1:D:131:MET:HB3	1:D:131:MET:HE3	1.90	0.40
1:D:71:LYS:O	1:D:128:PHE:HA	2.21	0.40
1:B:127:ARG:HG3	6:B:613:HOH:O	2.21	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	313/364 (86%)	307 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	312/364 (86%)	308 (99%)	4 (1%)	0	100	100
1	C	291/364 (80%)	284 (98%)	7 (2%)	0	100	100
1	D	286/364 (79%)	281 (98%)	5 (2%)	0	100	100
All	All	1202/1456 (83%)	1180 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	251/304 (83%)	247 (98%)	4 (2%)	68	72
1	B	253/304 (83%)	250 (99%)	3 (1%)	75	80
1	C	232/304 (76%)	229 (99%)	3 (1%)	73	78
1	D	228/304 (75%)	224 (98%)	4 (2%)	64	68
All	All	964/1216 (79%)	950 (98%)	14 (2%)	70	74

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	50	CYS
1	A	103	ARG
1	A	133	ARG
1	B	61	SER
1	B	75	SER
1	B	133	ARG
1	C	82	THR
1	C	133	ARG
1	C	310	ASP
1	D	56	MET
1	D	120	ASP
1	D	133	ARG

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Mol	Chain	Res	Type
1	D	310	ASP

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

Mol	Chain	Res	Type
1	B	22	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	7DZ	A	401	-	29,30,30	0.46	0	31,44,44	1.90	5 (16%)
3	PO4	A	402	-	4,4,4	0.98	0	6,6,6	0.47	0
3	PO4	A	403	-	4,4,4	0.94	0	6,6,6	0.39	0
3	PO4	B	401	-	4,4,4	1.28	0	6,6,6	0.51	0
2	7DZ	B	402	-	29,30,30	0.50	0	31,44,44	1.70	5 (16%)
3	PO4	C	401	-	4,4,4	1.07	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7DZ	C	402	-	29,30,30	0.50	0	31,44,44	1.52	5 (16%)
3	PO4	C	403	-	4,4,4	0.95	0	6,6,6	0.50	0
3	PO4	C	404	-	4,4,4	0.94	0	6,6,6	0.32	0
3	PO4	C	405	-	4,4,4	0.88	0	6,6,6	0.48	0
4	PEG	C	406	-	6,6,6	0.46	0	5,5,5	0.38	0
3	PO4	D	401	-	4,4,4	1.04	0	6,6,6	0.44	0
3	PO4	D	402	-	4,4,4	1.03	0	6,6,6	0.34	0
2	7DZ	D	403	-	29,30,30	0.50	0	31,44,44	1.49	5 (16%)
3	PO4	D	404	-	4,4,4	0.95	0	6,6,6	0.43	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	7DZ	A	401	-	-	0/9/29/29	0/3/3/3
3	PO4	A	402	-	-	0/0/0/0	0/0/0/0
3	PO4	A	403	-	-	0/0/0/0	0/0/0/0
3	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	7DZ	B	402	-	-	0/9/29/29	0/3/3/3
3	PO4	C	401	-	-	0/0/0/0	0/0/0/0
2	7DZ	C	402	-	-	0/9/29/29	0/3/3/3
3	PO4	C	403	-	-	0/0/0/0	0/0/0/0
3	PO4	C	404	-	-	0/0/0/0	0/0/0/0
3	PO4	C	405	-	-	0/0/0/0	0/0/0/0
4	PEG	C	406	-	-	0/4/4/4	0/0/0/0
3	PO4	D	401	-	-	0/0/0/0	0/0/0/0
3	PO4	D	402	-	-	0/0/0/0	0/0/0/0
2	7DZ	D	403	-	-	0/9/29/29	0/3/3/3
3	PO4	D	404	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	7DZ	C17-C16-C15	-2.71	121.71	123.78
2	B	402	7DZ	C17-C16-C15	-2.65	121.76	123.78
2	C	402	7DZ	C13-C14-C15	-2.61	121.79	123.78
2	D	403	7DZ	C13-C14-C15	-2.55	121.83	123.78
2	B	402	7DZ	C13-C14-C15	-2.48	121.89	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	7DZ	C17-C16-C15	-2.48	121.89	123.78
2	C	402	7DZ	C17-C16-C15	-2.46	121.91	123.78
2	A	401	7DZ	C13-C14-C15	-2.28	122.04	123.78
2	D	403	7DZ	F1-C14-C15	2.20	118.71	116.94
2	B	402	7DZ	F-C16-C15	2.21	118.71	116.94
2	A	401	7DZ	F1-C14-C15	2.24	118.74	116.94
2	C	402	7DZ	F1-C14-C15	2.28	118.76	116.94
2	B	402	7DZ	F1-C14-C15	2.37	118.84	116.94
2	D	403	7DZ	F-C16-C15	2.48	118.92	116.94
2	C	402	7DZ	F-C16-C15	2.54	118.97	116.94
2	A	401	7DZ	F-C16-C15	2.86	119.23	116.94
2	D	403	7DZ	C8-C7-N3	6.11	117.37	112.61
2	C	402	7DZ	C8-C7-N3	6.40	117.59	112.61
2	B	402	7DZ	C8-C7-N3	7.59	118.51	112.61
2	A	401	7DZ	C8-C7-N3	8.99	119.61	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	7DZ	2	0
2	B	402	7DZ	2	0
2	C	402	7DZ	2	0
2	D	403	7DZ	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 ⓘ

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	317/364 (87%)	0.23	25 (7%)	13 13	35, 49, 79, 101	0
1	B	316/364 (86%)	0.13	22 (6%)	17 17	33, 49, 76, 90	0
1	C	301/364 (82%)	0.26	19 (6%)	21 21	30, 50, 88, 128	0
1	D	296/364 (81%)	0.32	28 (9%)	9 9	31, 48, 100, 130	0
All	All	1230/1456 (84%)	0.23	94 (7%)	15 15	30, 49, 87, 130	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	25	VAL	10.0
1	A	217	PRO	6.6
1	C	24	ALA	6.5
1	B	220	CYS	5.4
1	D	50	CYS	5.0
1	D	41	LEU	5.0
1	B	217	PRO	4.7
1	C	41	LEU	4.5
1	B	215	ALA	4.3
1	C	42	PRO	4.1
1	C	50	CYS	3.9
1	D	34	ALA	3.7
1	C	126	TYR	3.7
1	A	247	LEU	3.7
1	D	35	ALA	3.7
1	C	23	PHE	3.7
1	D	33	ALA	3.6
1	D	247	LEU	3.6
1	B	161	ILE	3.5
1	D	161	ILE	3.5
1	C	161	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	51	ILE	3.4
1	A	187	TYR	3.3
1	B	187	TYR	3.3
1	D	39	VAL	3.3
1	A	161	ILE	3.3
1	A	215	ALA	3.3
1	A	61	SER	3.2
1	B	219	ARG	3.2
1	D	40	GLY	3.2
1	D	52	TYR	3.1
1	B	247	LEU	3.0
1	D	195	LEU	3.0
1	C	44	GLY	3.0
1	A	293	ALA	3.0
1	D	246	ILE	2.9
1	D	36	ALA	2.9
1	D	66	ALA	2.9
1	C	28	ILE	2.8
1	C	43	ILE	2.8
1	A	178	ILE	2.8
1	A	263	ASP	2.8
1	C	247	LEU	2.7
1	D	74	PRO	2.7
1	A	64	SER	2.7
1	B	218	LYS	2.7
1	B	216	ASP	2.7
1	D	178	ILE	2.7
1	A	165	LEU	2.7
1	A	20	ALA	2.6
1	A	59	SER	2.6
1	D	209	VAL	2.6
1	A	196	VAL	2.6
1	D	187	TYR	2.6
1	A	208	GLY	2.5
1	A	246	ILE	2.5
1	D	28	ILE	2.5
1	B	122	ASN	2.5
1	B	248	GLY	2.4
1	A	195	LEU	2.4
1	D	330	ALA	2.4
1	C	165	LEU	2.3
1	A	221	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	101	ARG	2.3
1	B	59	SER	2.3
1	B	124	LYS	2.3
1	B	76	ASP	2.3
1	B	49	GLY	2.3
1	D	183	LEU	2.2
1	D	144	ALA	2.2
1	D	164	ILE	2.2
1	D	42	PRO	2.2
1	A	209	VAL	2.2
1	C	187	TYR	2.2
1	B	164	ILE	2.2
1	A	244	LEU	2.2
1	D	196	VAL	2.2
1	B	195	LEU	2.1
1	C	209	VAL	2.1
1	C	178	ILE	2.1
1	C	195	LEU	2.1
1	D	248	GLY	2.1
1	D	116	SER	2.1
1	A	292	ALA	2.1
1	B	251	MET	2.1
1	A	218	LYS	2.1
1	C	74	PRO	2.0
1	A	164	ILE	2.0
1	A	62	VAL	2.0
1	C	26	GLY	2.0
1	B	334	LYS	2.0
1	B	244	LEU	2.0
1	A	216	ASP	2.0
1	B	25	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
2	7DZ	B	402	28/28	0.74	0.28	5.00	67,78,87,89	0
3	PO4	A	402	5/5	0.97	0.21	3.79	76,77,80,80	0
4	PEG	C	406	7/7	0.80	0.24	2.93	45,56,64,66	0
2	7DZ	A	401	28/28	0.89	0.17	0.94	55,66,72,73	0
3	PO4	B	401	5/5	0.97	0.12	0.55	65,66,71,72	0
3	PO4	D	401	5/5	0.91	0.13	0.06	74,74,76,79	0
2	7DZ	C	402	28/28	0.92	0.14	-0.09	46,65,75,77	0
3	PO4	C	403	5/5	0.96	0.14	-0.12	72,73,75,75	0
2	7DZ	D	403	28/28	0.92	0.13	-0.26	50,63,73,75	0
3	PO4	D	404	5/5	0.96	0.17	-	93,95,96,96	0
3	PO4	C	405	5/5	0.92	0.19	-	96,97,98,98	0
3	PO4	C	404	5/5	0.94	0.09	-	94,94,95,97	0
3	PO4	A	403	5/5	0.95	0.10	-	87,87,89,89	0
5	CL	C	407	1/1	0.90	0.21	-	85,85,85,85	0
3	PO4	D	402	5/5	0.95	0.15	-	69,70,71,73	0
3	PO4	C	401	5/5	0.96	0.15	-	61,65,69,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.