Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2017 – 01:45 AM EST

PDB ID	:	5UGE
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	:	2017-01-08
Resolution	:	1.80 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:

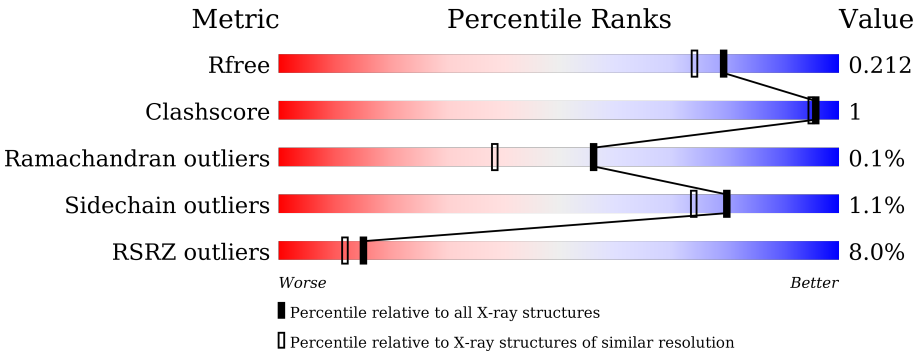
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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	7% 84% · 13%
1	B	364	5% 82% · 13%
1	C	364	5% 79% · 19%
1	D	364	9% 79% · 19%

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	584	B	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10418 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
			2462	1577	416	457	12			
1	B	315	Total	C	N	O	S	0	1	0
			2477	1586	420	458	13			
1	C	294	Total	C	N	O	S	0	0	0
			2304	1478	391	423	12			
1	D	296	Total	C	N	O	S	0	0	0
			2304	1478	397	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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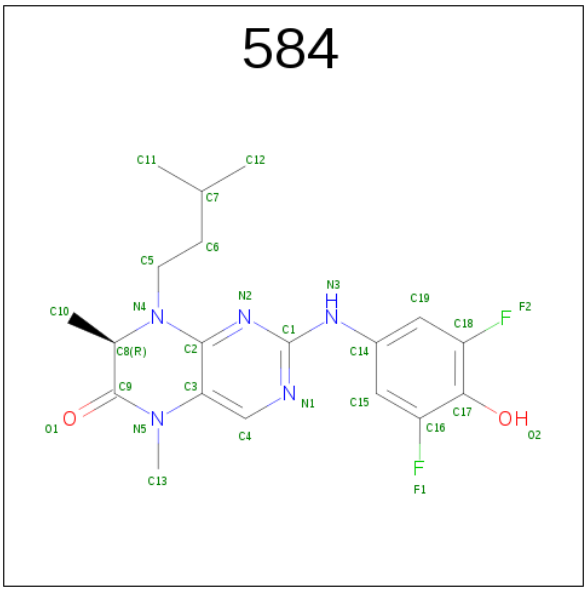
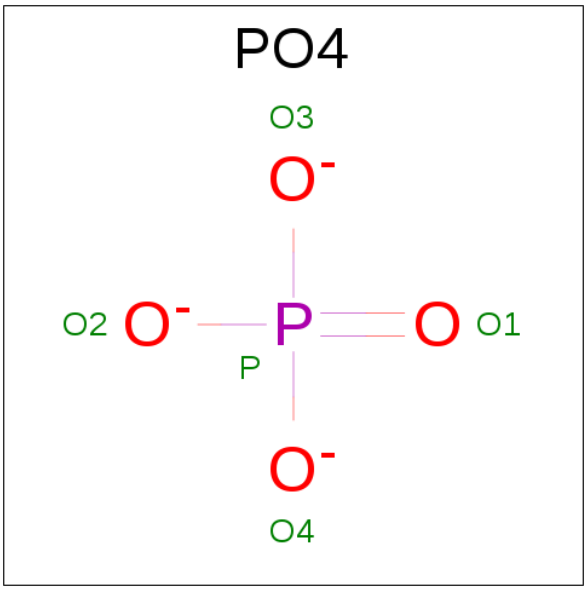
Chain	Residue	Modelled	Actual	Comment	Reference
B	292	ALA	GLU	engineered mutation	UNP Q99986
B	293	ALA	LYS	engineered mutation	UNP Q99986
B	295	ALA	LYS	engineered mutation	UNP Q99986
B	359	ALA	LYS	engineered mutation	UNP Q99986
B	360	ALA	LYS	engineered mutation	UNP Q99986
C	1	SER	-	expression tag	UNP 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 (7R)-2-[(3,5-difluoro-4-hydroxyphenyl)amino]-5,7-dimethyl-8-(3-methylbutyl)-7,8-dihydropteridin-6(5H)-one (three-letter code: 584) (formula: $C_{19}H_{23}F_2N_5O_2$).



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: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	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

- Molecule 4 is water.

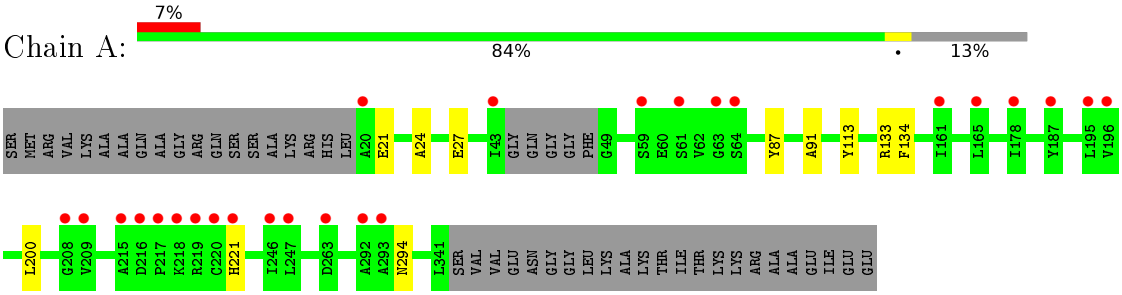
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	175	Total O 175 175	0	0
4	B	196	Total O 196 196	0	0
4	C	192	Total O 192 192	0	0
4	D	176	Total O 176 176	0	0

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.

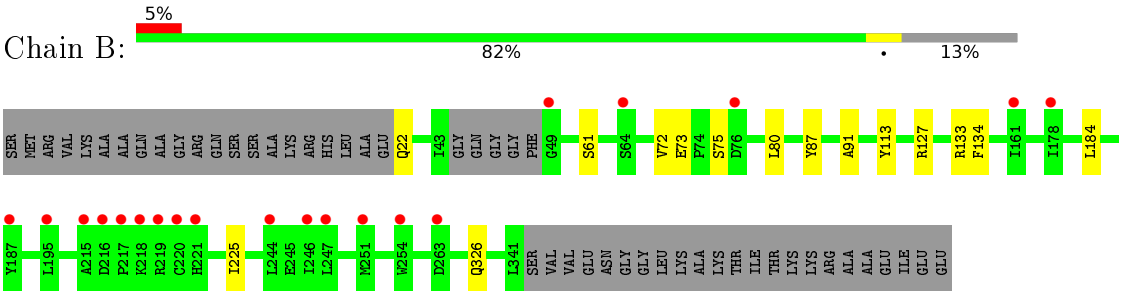
- Molecule 1: Serine/threonine-protein kinase VRK1

Chain A:



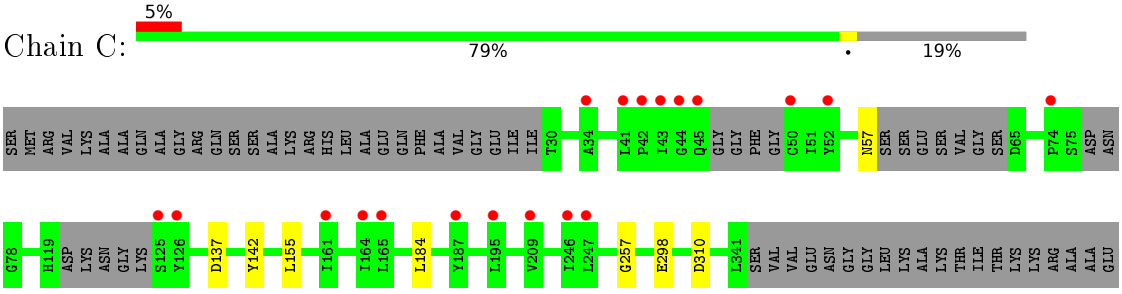
- Molecule 1: Serine/threonine-protein kinase VRK1

Chain B:



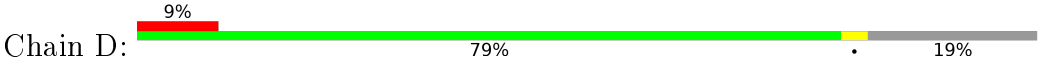
- Molecule 1: Serine/threonine-protein kinase VRK1

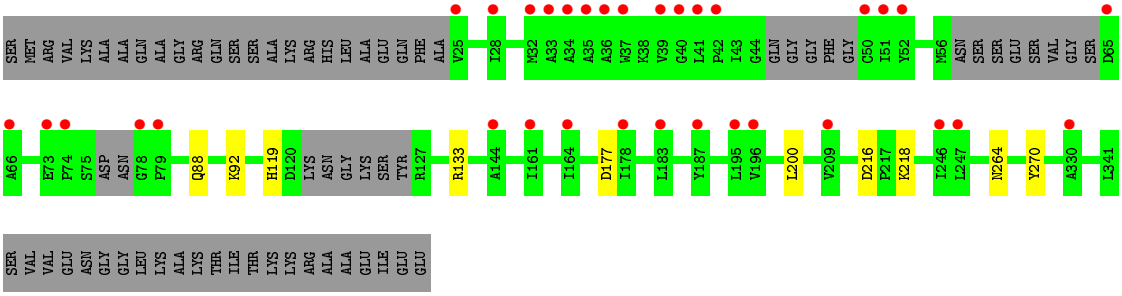
Chain C:



- Molecule 1: Serine/threonine-protein kinase VRK1

Chain D:




SER MET ARG VAL LYS ALA ALA GLN ALA GLY ARG GLN SER SER ALA LYS ARG HIS LEU ALA GLU GLN PHE ALA V25 I28 MQ2 A33 A34 A35 A36 M37 K38 V39 G40 L41 P42 I43 G44 GLN GLY GLY PHE GLY C50 I51 Y52 M56 ASN SER SER GLU SER VAL GLY SER D65
A66 E73 P74 S75 ASP ASN G78 P79 Q88 N92 H119 D120 LYS ASN GLY LYS SER TYR R127 R133 A144 I161 I164 D177 I178 L183 Y187 L195 V196 L200 V209 D216 P217 K218 I246 I247 M264 Y270 A330 L341
SER VAL VAL GLU ASN GLY GLY LEU LYS ALA LYS THR ILE THR LYS LYS ARG ALA ALA GLU ILE GLU GLU

4 Data and refinement statistics (i)

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)	26.35 – 1.80 29.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.35-1.80) 99.7 (29.66-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.80Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.183 , 0.208 0.190 , 0.212	Depositor DCC
R_{free} test set	7872 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10418	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 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 584, 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	0.51	0/2521	0.64	0/3424
1	B	0.51	0/2539	0.61	0/3444
1	C	0.50	0/2359	0.60	0/3199
1	D	0.52	0/2358	0.61	0/3194
All	All	0.51	0/9777	0.62	0/13261

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

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	2462	0	2360	6	0
1	B	2477	0	2395	9	0
1	C	2304	0	2198	3	0
1	D	2304	0	2202	4	0
2	A	28	0	22	3	0
2	B	28	0	22	2	0
2	C	28	0	22	1	0
2	D	28	0	22	1	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	175	0	0	0	0
4	B	196	0	0	1	0
4	C	192	0	0	0	0
4	D	176	0	0	0	0
All	All	10418	0	9243	28	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 1.

All (28) 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:22:GLN:HG2	1:B:72:VAL:HG11	1.75	0.68
1:A:24:ALA:O	1:A:27:GLU:HB2	1.94	0.67
1:A:87:TYR:HD1	1:A:91:ALA:HB3	1.60	0.67
1:B:80:LEU:HG	1:B:127:ARG:HD2	1.87	0.56
1:D:177:ASP:HB2	1:D:200:LEU:HD11	1.89	0.55
2:B:401:584:N2	2:B:401:584:H11	2.22	0.55
1:A:200:LEU:HD13	1:A:221:HIS:CG	2.46	0.51
1:B:73:GLU:HB2	1:B:80:LEU:HD22	1.92	0.51
2:C:401:584:N2	2:C:401:584:H11	2.26	0.50
2:A:401:584:N2	2:A:401:584:H12	2.28	0.48
1:B:87:TYR:HD1	1:B:91:ALA:CB	2.25	0.48
1:B:87:TYR:HD1	1:B:91:ALA:HB3	1.79	0.48
2:D:401:584:N2	2:D:401:584:H12	2.29	0.48
1:C:155:LEU:HD21	1:C:298:GLU:HG3	1.96	0.47
1:D:216:ASP:OD1	1:D:218:LYS:HG2	2.14	0.47
1:D:88:GLN:O	1:D:92:LYS:HE2	2.15	0.47
1:D:264:ASN:HB3	1:D:270:TYR:CD2	2.51	0.46
1:A:87:TYR:HB3	1:A:113:TYR:HB2	1.98	0.46
1:B:73:GLU:HB2	1:B:80:LEU:CD2	2.45	0.46
1:A:87:TYR:HD1	1:A:91:ALA:CB	2.27	0.45
1:B:134:PHE:HB2	1:B:184:LEU:HD23	1.99	0.44
1:C:137:ASP:HB3	1:C:184:LEU:HD22	1.99	0.43
1:B:87:TYR:HB3	1:B:113:TYR:HB2	2.01	0.43
1:B:127:ARG:HG3	4:B:571:HOH:O	2.19	0.42
1:A:134:PHE:O	2:A:401:584:H13	2.20	0.41
1:C:142:TYR:OH	1:C:257:GLY:HA2	2.21	0.41
2:B:401:584:N2	2:B:401:584:C15	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:584:N2	2:A:401:584:C19	2.84	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	313/364 (86%)	304 (97%)	8 (3%)	1 (0%)	46 29
1	B	312/364 (86%)	302 (97%)	10 (3%)	0	100 100
1	C	284/364 (78%)	277 (98%)	7 (2%)	0	100 100
1	D	286/364 (79%)	276 (96%)	10 (4%)	0	100 100
All	All	1195/1456 (82%)	1159 (97%)	35 (3%)	1 (0%)	56 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASN

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	249/304 (82%)	247 (99%)	2 (1%)	86 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	254/304 (84%)	249 (98%)	5 (2%)	63 49
1	C	231/304 (76%)	229 (99%)	2 (1%)	84 80
1	D	227/304 (75%)	225 (99%)	2 (1%)	84 80
All	All	961/1216 (79%)	950 (99%)	11 (1%)	80 74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	133	ARG
1	B	61	SER
1	B	75	SER
1	B	133	ARG
1	B	225	ILE
1	B	326	GLN
1	C	57	ASN
1	C	310	ASP
1	D	119	HIS
1	D	133	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

8 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	$\#\|Z\| > 2$
2	584	A	401	-	28,30,30	0.45	0	32,44,44	0.66	0
2	584	B	401	-	28,30,30	0.45	0	32,44,44	0.54	0
3	PO4	B	402	-	4,4,4	1.81	3 (75%)	6,6,6	0.26	0
2	584	C	401	-	28,30,30	0.48	0	32,44,44	0.59	0
3	PO4	C	402	-	4,4,4	1.79	2 (50%)	6,6,6	0.26	0
2	584	D	401	-	28,30,30	0.44	0	32,44,44	0.61	0
3	PO4	D	402	-	4,4,4	1.88	3 (75%)	6,6,6	0.23	0
3	PO4	D	403	-	4,4,4	1.80	2 (50%)	6,6,6	0.22	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	584	A	401	-	-	0/9/29/29	0/3/3/3
2	584	B	401	-	-	0/9/29/29	0/3/3/3
3	PO4	B	402	-	-	0/0/0/0	0/0/0/0
2	584	C	401	-	-	0/9/29/29	0/3/3/3
3	PO4	C	402	-	-	0/0/0/0	0/0/0/0
2	584	D	401	-	-	0/9/29/29	0/3/3/3
3	PO4	D	402	-	-	0/0/0/0	0/0/0/0
3	PO4	D	403	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	PO4	P-O2	2.07	1.60	1.53
3	B	402	PO4	P-O3	2.08	1.60	1.53
3	C	402	PO4	P-O3	2.08	1.60	1.53
3	B	402	PO4	P-O4	2.08	1.60	1.53
3	D	402	PO4	P-O3	2.09	1.60	1.53
3	D	403	PO4	P-O3	2.11	1.60	1.53
3	D	402	PO4	P-O4	2.13	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	PO4	P-O4	2.16	1.60	1.53
3	D	403	PO4	P-O4	2.17	1.60	1.53
3	D	402	PO4	P-O2	2.23	1.60	1.53

There are no bond angle outliers.

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	584	3	0
2	B	401	584	2	0
2	C	401	584	1	0
2	D	401	584	1	0

5.7 Other polymers

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^{th} 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%)	0.28	26 (8%)	14	11	36, 49, 79, 100	0
1	B	315/364 (86%)	0.16	20 (6%)	23	19	33, 49, 76, 94	0
1	C	294/364 (80%)	0.22	19 (6%)	22	18	31, 50, 86, 135	0
1	D	296/364 (81%)	0.31	33 (11%)	7	5	32, 48, 102, 128	0
All	All	1222/1456 (83%)	0.24	98 (8%)	15	12	31, 49, 86, 135	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	PRO	6.7
1	A	217	PRO	6.7
1	D	35	ALA	5.6
1	C	50	CYS	5.3
1	D	50	CYS	4.8
1	D	41	LEU	4.8
1	C	126	TYR	4.7
1	C	34	ALA	4.6
1	B	218	LYS	4.6
1	D	40	GLY	4.3
1	B	161	ILE	4.2
1	C	44	GLY	4.2
1	A	61	SER	4.1
1	A	64	SER	4.1
1	B	221	HIS	4.1
1	B	215	ALA	4.1
1	C	41	LEU	4.1
1	A	20	ALA	4.0
1	B	220	CYS	3.9
1	D	161	ILE	3.9
1	B	187	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	215	ALA	3.7
1	A	247	LEU	3.7
1	C	42	PRO	3.7
1	D	247	LEU	3.7
1	B	247	LEU	3.6
1	D	52	TYR	3.6
1	D	33	ALA	3.5
1	A	187	TYR	3.5
1	A	220	CYS	3.5
1	D	34	ALA	3.5
1	C	161	ILE	3.5
1	A	161	ILE	3.5
1	A	209	VAL	3.4
1	D	246	ILE	3.3
1	D	196	VAL	3.3
1	A	293	ALA	3.3
1	C	45	GLN	3.2
1	D	195	LEU	3.1
1	B	219	ARG	3.1
1	A	178	ILE	3.0
1	C	43	ILE	3.0
1	A	246	ILE	3.0
1	C	187	TYR	3.0
1	A	218	LYS	2.9
1	A	59	SER	2.9
1	D	178	ILE	2.9
1	D	51	ILE	2.9
1	B	216	ASP	2.9
1	C	74	PRO	2.8
1	B	195	LEU	2.8
1	A	195	LEU	2.7
1	D	36	ALA	2.7
1	A	165	LEU	2.7
1	B	178	ILE	2.6
1	B	251	MET	2.6
1	D	209	VAL	2.6
1	D	74	PRO	2.6
1	A	219	ARG	2.6
1	C	164	ILE	2.5
1	A	263	ASP	2.5
1	C	247	LEU	2.5
1	D	164	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	39	VAL	2.5
1	D	78	GLY	2.4
1	B	263	ASP	2.4
1	A	208	GLY	2.4
1	C	165	LEU	2.4
1	D	183	LEU	2.3
1	D	330	ALA	2.3
1	D	187	TYR	2.3
1	C	52	TYR	2.3
1	D	28	ILE	2.3
1	D	42	PRO	2.3
1	A	63	GLY	2.2
1	B	49	GLY	2.2
1	D	66	ALA	2.2
1	D	144	ALA	2.2
1	D	73	GLU	2.2
1	B	64	SER	2.2
1	B	76	ASP	2.2
1	C	209	VAL	2.2
1	D	25	VAL	2.2
1	A	221	HIS	2.1
1	B	244	LEU	2.1
1	A	196	VAL	2.1
1	D	79	PRO	2.1
1	A	43	ILE	2.1
1	B	254	TRP	2.1
1	B	246	ILE	2.1
1	D	32	MET	2.1
1	C	195	LEU	2.0
1	A	292	ALA	2.0
1	D	37	TRP	2.0
1	A	216	ASP	2.0
1	D	65	ASP	2.0
1	C	246	ILE	2.0
1	C	125	SER	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, 95^{th} 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	584	B	401	28/28	0.74	0.22	2.90	64,72,83,84	0
3	PO4	B	402	5/5	0.96	0.15	1.97	63,63,70,70	0
2	584	A	401	28/28	0.83	0.15	0.79	53,64,69,72	0
2	584	C	401	28/28	0.89	0.14	0.60	48,63,73,74	0
3	PO4	D	402	5/5	0.95	0.11	0.08	71,73,75,77	0
2	584	D	401	28/28	0.93	0.12	-0.16	52,63,71,74	0
3	PO4	D	403	5/5	0.98	0.12	-	70,70,72,72	0
3	PO4	C	402	5/5	0.98	0.12	-	62,63,65,69	0

6.5 Other polymers (i)

There are no such residues in this entry.