



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:22 AM GMT

PDB ID : 3ORX
Title : PDK1 mutant bound to allosteric disulfide fragment inhibitor 1F8
Authors : Sadowsky, J.D.; Wells, J.A.
Deposited on : 2010-09-08
Resolution : 2.20 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
<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

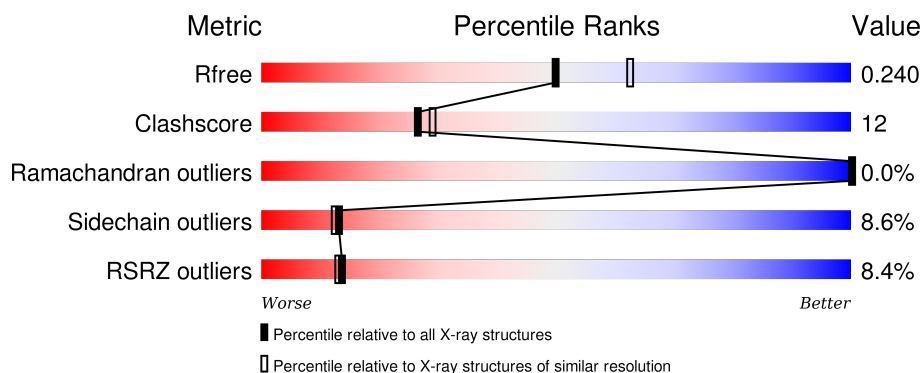
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	316	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	316	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	316	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	316	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	316	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	316	
1	G	316	
1	H	316	

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
2	1F8	A	1	-	-	-	X
2	1F8	B	1	-	-	-	X
2	1F8	E	1	-	-	-	X
2	1F8	G	1	-	-	-	X
2	1F8	H	1	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19043 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 3-phosphoinositide-dependent protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	P	S	0	0	0
			2271	1476	374	412	1	8			
1	B	281	Total	C	N	O	P	S	0	0	0
			2262	1470	368	415	1	8			
1	C	284	Total	C	N	O	P	S	0	0	0
			2264	1469	369	417	1	8			
1	D	283	Total	C	N	O	P	S	0	0	0
			2256	1468	370	409	1	8			
1	E	274	Total	C	N	O	S		0	0	0
			2163	1415	354	386	8				
1	F	275	Total	C	N	O	P	S	0	0	0
			2132	1391	348	384	1	8			
1	G	275	Total	C	N	O	P	S	0	0	0
			2155	1406	352	388	1	8			
1	H	275	Total	C	N	O	P	S	0	0	0
			2114	1379	342	384	1	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLY	-	EXPRESSION TAG	UNP O15530
A	45	ALA	-	EXPRESSION TAG	UNP O15530
A	46	MET	-	EXPRESSION TAG	UNP O15530
A	47	ASP	-	EXPRESSION TAG	UNP O15530
A	48	PRO	-	EXPRESSION TAG	UNP O15530
A	49	GLU	-	EXPRESSION TAG	UNP O15530
A	50	PHE	-	EXPRESSION TAG	UNP O15530
A	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
B	44	GLY	-	EXPRESSION TAG	UNP O15530
B	45	ALA	-	EXPRESSION TAG	UNP O15530
B	46	MET	-	EXPRESSION TAG	UNP O15530
B	47	ASP	-	EXPRESSION TAG	UNP O15530
B	48	PRO	-	EXPRESSION TAG	UNP O15530

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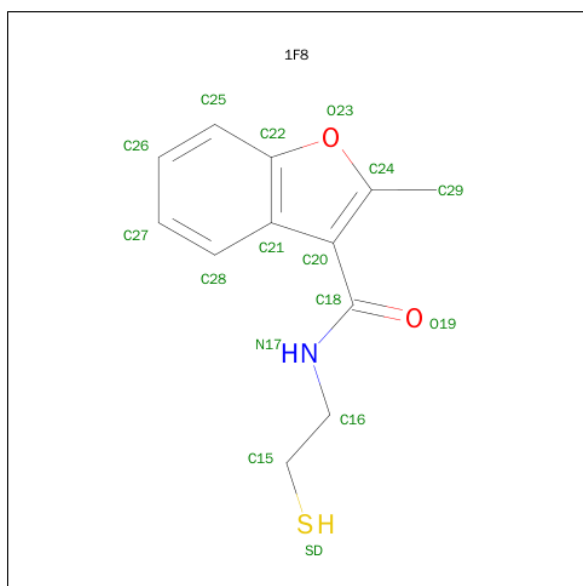
Chain	Residue	Modelled	Actual	Comment	Reference
B	49	GLU	-	EXPRESSION TAG	UNP O15530
B	50	PHE	-	EXPRESSION TAG	UNP O15530
B	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
C	44	GLY	-	EXPRESSION TAG	UNP O15530
C	45	ALA	-	EXPRESSION TAG	UNP O15530
C	46	MET	-	EXPRESSION TAG	UNP O15530
C	47	ASP	-	EXPRESSION TAG	UNP O15530
C	48	PRO	-	EXPRESSION TAG	UNP O15530
C	49	GLU	-	EXPRESSION TAG	UNP O15530
C	50	PHE	-	EXPRESSION TAG	UNP O15530
C	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
D	44	GLY	-	EXPRESSION TAG	UNP O15530
D	45	ALA	-	EXPRESSION TAG	UNP O15530
D	46	MET	-	EXPRESSION TAG	UNP O15530
D	47	ASP	-	EXPRESSION TAG	UNP O15530
D	48	PRO	-	EXPRESSION TAG	UNP O15530
D	49	GLU	-	EXPRESSION TAG	UNP O15530
D	50	PHE	-	EXPRESSION TAG	UNP O15530
D	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
E	44	GLY	-	EXPRESSION TAG	UNP O15530
E	45	ALA	-	EXPRESSION TAG	UNP O15530
E	46	MET	-	EXPRESSION TAG	UNP O15530
E	47	ASP	-	EXPRESSION TAG	UNP O15530
E	48	PRO	-	EXPRESSION TAG	UNP O15530
E	49	GLU	-	EXPRESSION TAG	UNP O15530
E	50	PHE	-	EXPRESSION TAG	UNP O15530
E	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
F	44	GLY	-	EXPRESSION TAG	UNP O15530
F	45	ALA	-	EXPRESSION TAG	UNP O15530
F	46	MET	-	EXPRESSION TAG	UNP O15530
F	47	ASP	-	EXPRESSION TAG	UNP O15530
F	48	PRO	-	EXPRESSION TAG	UNP O15530
F	49	GLU	-	EXPRESSION TAG	UNP O15530
F	50	PHE	-	EXPRESSION TAG	UNP O15530
F	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
G	44	GLY	-	EXPRESSION TAG	UNP O15530
G	45	ALA	-	EXPRESSION TAG	UNP O15530
G	46	MET	-	EXPRESSION TAG	UNP O15530
G	47	ASP	-	EXPRESSION TAG	UNP O15530
G	48	PRO	-	EXPRESSION TAG	UNP O15530
G	49	GLU	-	EXPRESSION TAG	UNP O15530
G	50	PHE	-	EXPRESSION TAG	UNP O15530

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Chain	Residue	Modelled	Actual	Comment	Reference
G	148	CYS	THR	ENGINEERED MUTATION	UNP O15530
H	44	GLY	-	EXPRESSION TAG	UNP O15530
H	45	ALA	-	EXPRESSION TAG	UNP O15530
H	46	MET	-	EXPRESSION TAG	UNP O15530
H	47	ASP	-	EXPRESSION TAG	UNP O15530
H	48	PRO	-	EXPRESSION TAG	UNP O15530
H	49	GLU	-	EXPRESSION TAG	UNP O15530
H	50	PHE	-	EXPRESSION TAG	UNP O15530
H	148	CYS	THR	ENGINEERED MUTATION	UNP O15530

- Molecule 2 is 2-METHYL-N-(2-SULFANYLETHYL)-1-BENZOFURAN-3-CARBOXAMID E (three-letter code: 1F8) (formula: C₁₂H₁₃NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	E	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	F	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	H	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

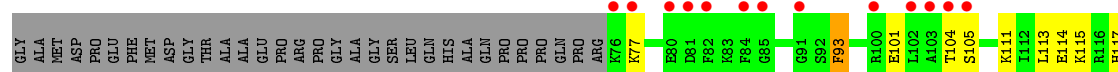
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

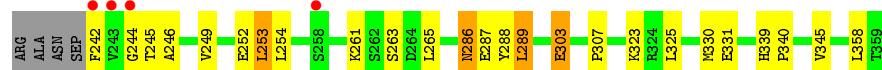
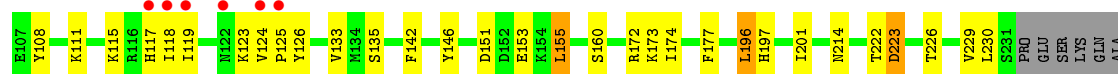
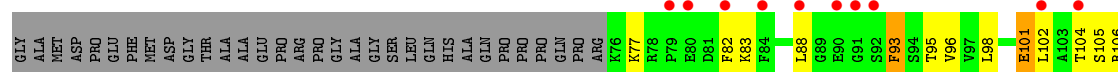
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		
4	B	213	Total	O	0	0
			213	213		
4	C	194	Total	O	0	0
			194	194		
4	D	187	Total	O	0	0
			187	187		
4	E	120	Total	O	0	0
			120	120		
4	F	121	Total	O	0	0
			121	121		
4	G	121	Total	O	0	0
			121	121		
4	H	134	Total	O	0	0
			134	134		



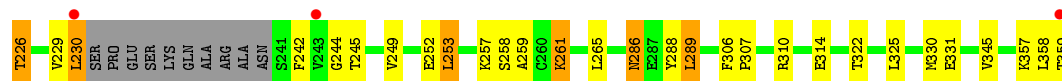
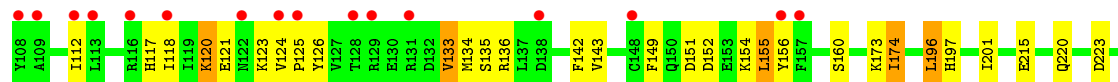
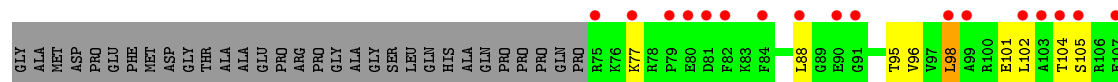
- Molecule 1: 3-phosphoinositide-dependent protein kinase 1



- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

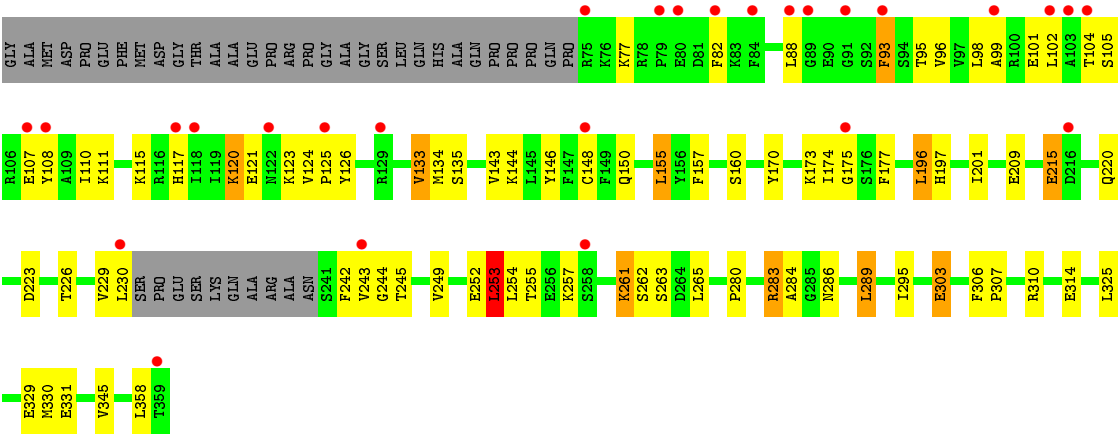


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1

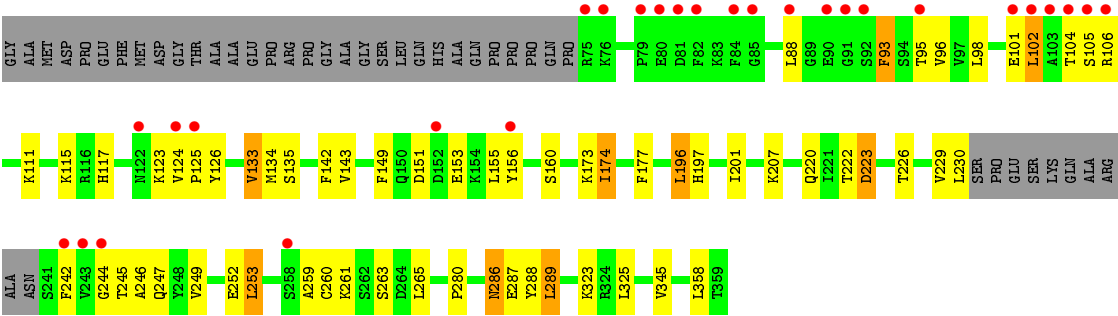


- Molecule 1: 3-phosphoinositide-dependent protein kinase 1





● Molecule 1: 3-phosphoinositide-dependent protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.29Å 115.87Å 145.72Å 91.76° 89.99° 95.41°	Depositor
Resolution (Å)	45.25 – 2.20 45.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.25-2.20) 96.1 (45.25-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2010_01_09_2330)	Depositor
R, R_{free}	0.208 , 0.243 0.207 , 0.240	Depositor DCC
R_{free} test set	6446 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.0	EDS
Estimated twinning fraction	0.073 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 128104 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19043	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 1F8, SEP

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	0.61	0/2315	0.62	1/3125 (0.0%)
1	B	0.54	0/2306	0.62	0/3112
1	C	0.58	0/2308	0.61	0/3120
1	D	0.54	0/2300	0.61	2/3106 (0.1%)
1	E	0.75	0/2217	0.66	0/3003
1	F	0.69	0/2175	0.63	1/2950 (0.0%)
1	G	0.81	0/2199	0.66	2/2980 (0.1%)
1	H	0.70	0/2158	0.63	0/2932
All	All	0.66	0/17978	0.63	6/24328 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	136	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	G	253	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	A	283	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	G	283	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	2271	0	2250	52	0
1	B	2262	0	2245	53	0
1	C	2264	0	2217	54	0
1	D	2256	0	2233	43	0
1	E	2163	0	2101	62	0
1	F	2132	0	2040	56	0
1	G	2155	0	2069	68	0
1	H	2114	0	1982	56	0
2	A	16	0	12	3	0
2	B	16	0	12	3	0
2	C	16	0	12	3	0
2	D	16	0	12	3	0
2	E	16	0	12	2	0
2	F	16	0	12	2	0
2	G	16	0	12	3	0
2	H	16	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	204	0	0	4	0
4	B	213	0	0	9	0
4	C	194	0	0	11	0
4	D	187	0	0	5	0
4	E	120	0	0	1	0
4	F	121	0	0	3	0
4	G	121	0	0	2	0
4	H	134	0	0	3	0
All	All	19043	0	17233	425	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 12.

The worst 5 of 425 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:A:230:LEU:HD21	1:A:235:LYS:HA	1.28	1.12
1:A:323:LYS:NZ	1:G:310:ARG:HH21	1.47	1.10
1:F:253:LEU:N	1:F:253:LEU:HD23	1.69	1.04
1:E:253:LEU:HD23	1:E:253:LEU:N	1.74	1.01
1:G:253:LEU:HD23	1:G:253:LEU:N	1.72	0.99

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	279/316 (88%)	274 (98%)	5 (2%)	0	100	100
1	B	276/316 (87%)	271 (98%)	5 (2%)	0	100	100
1	C	279/316 (88%)	273 (98%)	6 (2%)	0	100	100
1	D	278/316 (88%)	272 (98%)	5 (2%)	1 (0%)	39	42
1	E	270/316 (85%)	260 (96%)	10 (4%)	0	100	100
1	F	271/316 (86%)	260 (96%)	11 (4%)	0	100	100
1	G	271/316 (86%)	261 (96%)	10 (4%)	0	100	100
1	H	271/316 (86%)	261 (96%)	10 (4%)	0	100	100
All	All	2195/2528 (87%)	2132 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	244	GLY

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	239/273 (88%)	219 (92%)	20 (8%)	14	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	241/273 (88%)	224 (93%)	17 (7%)	18	19
1	C	238/273 (87%)	222 (93%)	16 (7%)	20	21
1	D	237/273 (87%)	221 (93%)	16 (7%)	20	21
1	E	220/273 (81%)	200 (91%)	20 (9%)	12	11
1	F	211/273 (77%)	185 (88%)	26 (12%)	6	5
1	G	215/273 (79%)	193 (90%)	22 (10%)	9	8
1	H	205/273 (75%)	187 (91%)	18 (9%)	12	12
All	All	1806/2184 (83%)	1651 (91%)	155 (9%)	13	12

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	95	THR
1	E	303	GLU
1	H	160	SER
1	E	117	HIS
1	E	173	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	286	ASN
1	D	150	GLN
1	H	247	GLN
1	C	349	ASN
1	D	247	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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
1	SEP	A	241	1	8,9,10	1.53	1 (12%)	8,12,14	1.53	2 (25%)
1	SEP	B	241	1	8,9,10	1.51	1 (12%)	8,12,14	1.43	1 (12%)
1	SEP	C	241	1	8,9,10	0.92	0	8,12,14	1.99	2 (25%)
1	SEP	D	241	1	8,9,10	1.60	1 (12%)	8,12,14	1.46	1 (12%)
1	SEP	F	241	1	8,9,10	1.56	1 (12%)	8,12,14	1.29	1 (12%)
1	SEP	G	241	1	8,9,10	1.59	2 (25%)	8,12,14	1.51	1 (12%)
1	SEP	H	241	1	8,9,10	1.57	1 (12%)	8,12,14	1.19	1 (12%)

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
1	SEP	A	241	1	-	0/6/8/10	0/0/0/0
1	SEP	B	241	1	-	0/6/8/10	0/0/0/0
1	SEP	C	241	1	-	0/6/8/10	0/0/0/0
1	SEP	D	241	1	-	0/6/8/10	0/0/0/0
1	SEP	F	241	1	-	0/6/8/10	0/0/0/0
1	SEP	G	241	1	-	0/6/8/10	0/0/0/0
1	SEP	H	241	1	-	0/6/8/10	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	241	SEP	P-O2P	2.09	1.62	1.54
1	B	241	SEP	P-O1P	3.22	1.61	1.51
1	G	241	SEP	P-O1P	3.23	1.61	1.51
1	A	241	SEP	P-O1P	3.24	1.61	1.51
1	F	241	SEP	P-O1P	3.25	1.61	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	241	SEP	OG-CB-CA	2.08	110.05	108.27
1	A	241	SEP	O2P-P-OG	2.26	113.08	106.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	241	SEP	OG-CB-CA	2.47	110.38	108.27
1	C	241	SEP	O2P-P-OG	2.50	113.77	106.56
1	D	241	SEP	OG-CB-CA	2.76	110.63	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	241	SEP	1	0
1	B	241	SEP	1	0
1	C	241	SEP	1	0
1	D	241	SEP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	1F8	A	1	-	12,17,17	1.07	0	10,23,23	2.06	4 (40%)
2	1F8	B	1	-	12,17,17	1.11	0	10,23,23	2.07	4 (40%)
2	1F8	C	1	-	12,17,17	1.10	0	10,23,23	2.04	4 (40%)
2	1F8	D	1	-	12,17,17	1.09	0	10,23,23	2.06	4 (40%)
2	1F8	E	1	-	12,17,17	1.13	0	10,23,23	1.86	3 (30%)
2	1F8	F	1	-	12,17,17	1.09	0	10,23,23	1.89	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1F8	G	1	-	12,17,17	1.13	0	10,23,23	1.92	3 (30%)
2	1F8	H	1	-	12,17,17	1.11	0	10,23,23	1.99	3 (30%)

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	1F8	A	1	-	-	0/4/8/8	0/1/2/2
2	1F8	B	1	-	-	0/4/8/8	0/1/2/2
2	1F8	C	1	-	-	0/4/8/8	0/1/2/2
2	1F8	D	1	-	-	0/4/8/8	0/1/2/2
2	1F8	E	1	-	-	0/4/8/8	0/1/2/2
2	1F8	F	1	-	-	0/4/8/8	0/1/2/2
2	1F8	G	1	-	-	0/4/8/8	0/1/2/2
2	1F8	H	1	-	-	0/4/8/8	0/1/2/2

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	1F8	C15-C16-N17	-4.34	103.80	112.37
2	A	1	1F8	C15-C16-N17	-4.29	103.90	112.37
2	C	1	1F8	C15-C16-N17	-4.20	104.08	112.37
2	D	1	1F8	C15-C16-N17	-4.18	104.12	112.37
2	F	1	1F8	C15-C16-N17	-3.25	105.96	112.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	1F8	3	0
2	B	1	1F8	3	0
2	C	1	1F8	3	0
2	D	1	1F8	3	0
2	E	1	1F8	2	0
2	F	1	1F8	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	1F8	3	0
2	H	1	1F8	2	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	283/316 (89%)	0.15	15 (5%)	30 29	16, 32, 69, 100	0
1	B	280/316 (88%)	0.23	15 (5%)	29 29	17, 32, 70, 88	0
1	C	283/316 (89%)	0.25	22 (7%)	16 15	16, 32, 73, 98	0
1	D	282/316 (89%)	0.33	24 (8%)	13 12	17, 33, 72, 96	0
1	E	274/316 (86%)	0.36	20 (7%)	18 17	17, 41, 85, 109	0
1	F	274/316 (86%)	0.56	36 (13%)	5 4	18, 41, 86, 108	0
1	G	274/316 (86%)	0.43	27 (9%)	9 8	17, 42, 85, 109	0
1	H	274/316 (86%)	0.52	28 (10%)	9 8	17, 42, 86, 109	0
All	All	2224/2528 (87%)	0.35	187 (8%)	14 13	16, 37, 82, 109	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	82	PHE	7.9
1	E	243	VAL	7.6
1	H	124	VAL	7.6
1	H	102	LEU	6.7
1	H	82	PHE	6.7

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	SEP	F	241	10/11	0.83	0.36	-	70,81,94,96	0
1	SEP	D	241	10/11	0.91	0.15	-	45,60,82,85	0
1	SEP	C	241	10/11	0.91	0.18	-	48,64,81,86	0
1	SEP	B	241	10/11	0.93	0.12	-	46,61,81,86	0
1	SEP	A	241	10/11	0.93	0.16	-	45,61,78,84	0
1	SEP	H	241	10/11	0.75	0.29	-	64,81,89,93	0
1	SEP	G	241	10/11	0.71	0.35	-	66,78,100,109	0

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(\AA^2)	Q<0.9
2	1F8	H	1	16/16	0.65	0.39	5.17	87,98,109,112	0
2	1F8	G	1	16/16	0.64	0.31	3.82	87,98,108,110	0
2	1F8	B	1	16/16	0.80	0.34	3.56	72,89,110,121	0
2	1F8	E	1	16/16	0.65	0.34	2.47	87,96,108,111	0
2	1F8	A	1	16/16	0.71	0.37	2.31	72,88,110,120	0
2	1F8	F	1	16/16	0.66	0.35	1.95	87,97,109,111	0
2	1F8	C	1	16/16	0.73	0.29	1.07	71,88,109,120	0
2	1F8	D	1	16/16	0.78	0.30	0.86	73,88,110,120	0
3	CL	A	2	1/1	0.97	0.22	-	45,45,45,45	0
3	CL	C	6	1/1	0.99	0.16	-	46,46,46,46	0
3	CL	B	5	1/1	0.94	0.17	-	44,44,44,44	0
3	CL	D	360	1/1	0.96	0.21	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.