wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 01:52 pm GMT

PDB ID	:	1OL1
Title	:	Cyclin A binding groove inhibitor H-Cit-Cit-Leu-Ile-(p-F-Phe)-NH2
Authors	:	Kontopidis, G.; Andrews, M.; McInnes, C.; Cowan, A.; Powers, H.; Innes, L.; Plater, A.; Griffiths, G.; Paterson, D.; Zheleva, D.; Lane, D.; Green, S.; Walkinshaw, M.; Fischer, P.
Deposited on	:	2003-08-04
Resolution	:	2.90 Å(reported)

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

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

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

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

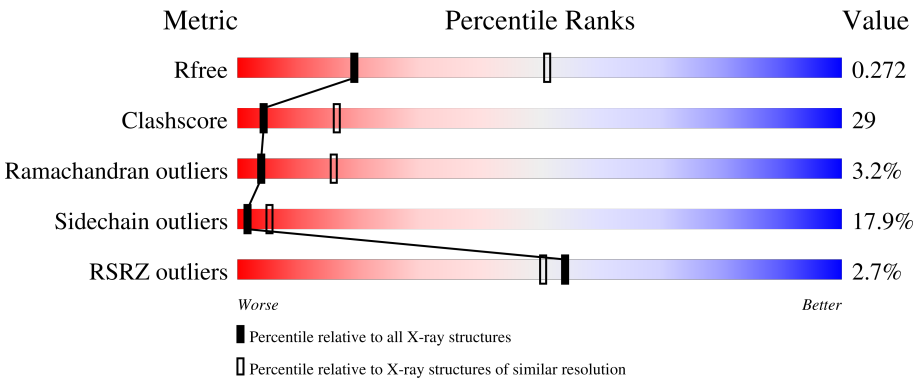
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	298	2%, 45%, 41%, 12%, • •
1	C	298	3%, 49%, 37%, 12%, • •
2	B	260	2%, 57%, 29%, 11%, • •
2	D	260	3%, 44%, 40%, 13%, • •
3	F	6	50%, 17%, 33%

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Mol	Chain	Length	Quality of chain
3	H	6	33% 50% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIR	F	500	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9098 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2378	1547	403	420	8	0	0	0
1	C	296	2378	1547	403	420	8	0	0	0

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	258	2083	1350	339	383	11	0	0	0
2	D	258	2084	1350	339	384	11	0	0	0

- Molecule 3 is a protein called CIR-CIR-LEU-ILE-PFF-NH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	F	N	O			
3	F	6	51	33	1	10	7	0	0	1
3	H	6	51	33	1	10	7	0	0	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	13	13	13	0	0
4	B	16	16	16	0	0
4	C	22	22	22	0	0
4	D	19	19	19	0	0

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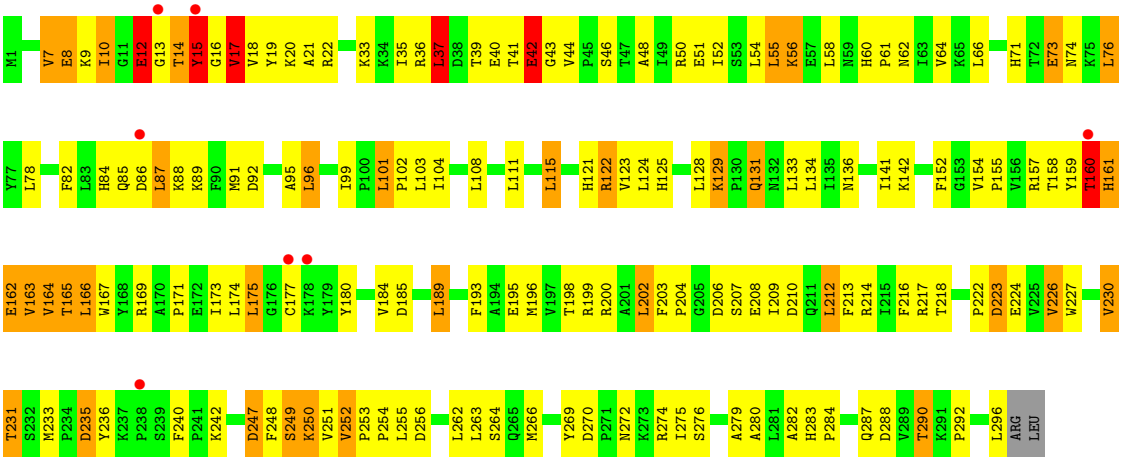
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	F	1	1	1	0	0
			Total	O		
4	H	2	2	2	0	0

3 Residue-property plots (i)

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

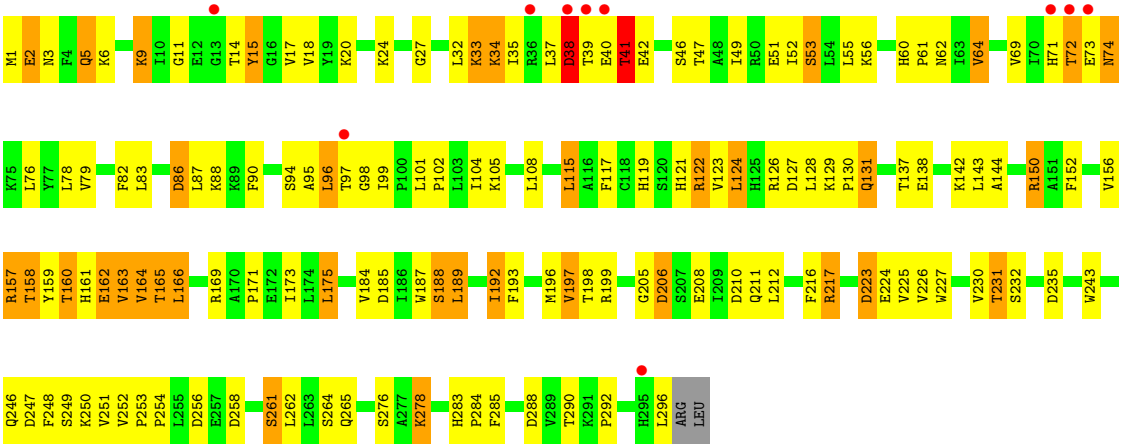
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A: 2% 45% 41% 12%



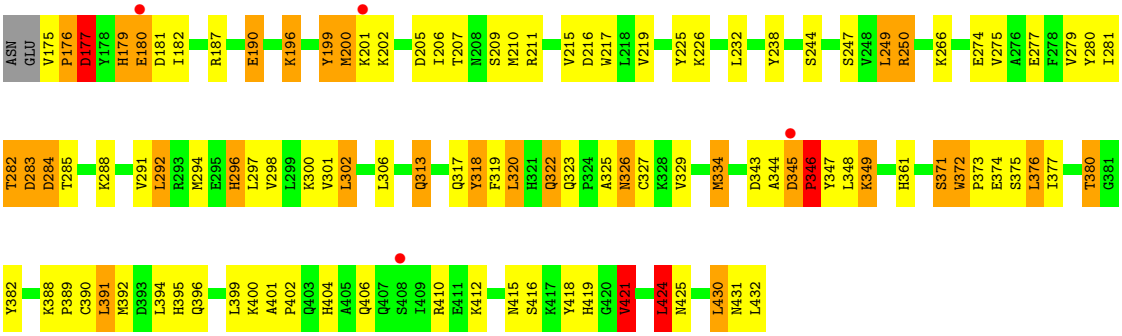
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C: 3% 49% 37% 12%



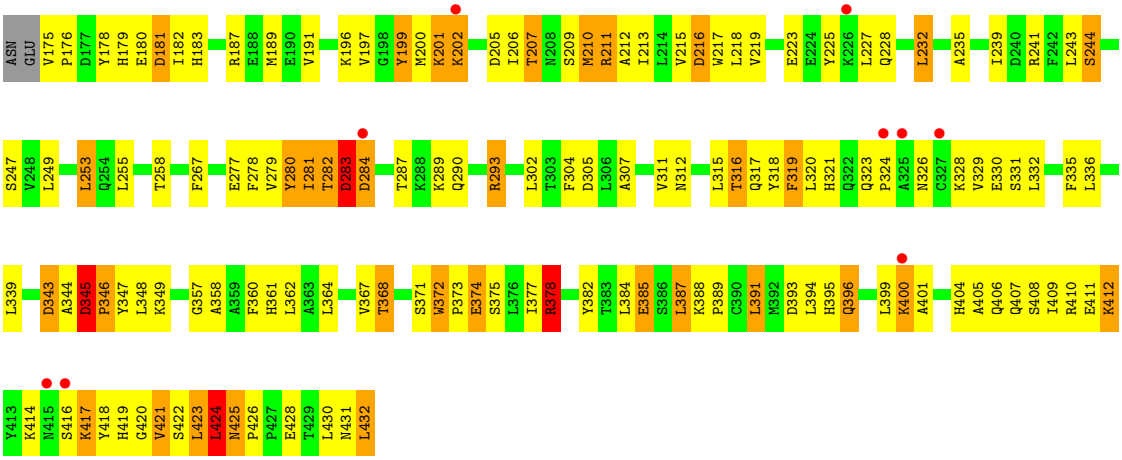
• Molecule 2: CYCLIN A2

Chain B: 2% 57% 29% 11%



- Molecule 2: CYCLIN A2

Chain D:

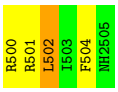


- Molecule 3: CIR-CIR-LEU-ILE-PFF-NH2

Chain F:

- Molecule 3: CIR-CIR-LEU-ILE-PFF-NH2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.50Å 113.47Å 154.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.90 14.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (12.00-2.90) 99.4 (14.99-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.206 , 0.284 0.201 , 0.272	Depositor DCC
R_{free} test set	1206 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9098	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PFF, NH2, CIR

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	0.69	3/2440 (0.1%)	0.86	9/3313 (0.3%)
1	C	0.64	0/2440	0.87	10/3313 (0.3%)
2	B	0.62	0/2133	0.85	7/2897 (0.2%)
2	D	0.63	0/2134	0.83	9/2897 (0.3%)
3	F	0.72	0/15	1.34	0/19
3	H	0.51	0/15	0.79	0/19
All	All	0.65	3/9177 (0.0%)	0.85	35/12458 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	D	0	5
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	GLU	CD-OE2	5.36	1.31	1.25
1	A	21	ALA	CA-CB	-5.30	1.41	1.52
1	A	8	GLU	CD-OE1	5.20	1.31	1.25

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	258	ASP	CB-CG-OD2	8.36	125.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	ASP	CB-CG-OD2	7.95	125.45	118.30
2	D	205	ASP	CB-CG-OD2	7.26	124.84	118.30
1	C	223	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	235	ASP	CB-CG-OD2	6.99	124.59	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	VAL	Peptide
2	B	346	PRO	Peptide
2	D	202	LYS	Peptide
2	D	227	LEU	Peptide
2	D	344	ALA	Peptide

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	2378	0	2426	164	1
1	C	2378	0	2426	144	0
2	B	2083	0	2107	82	1
2	D	2084	0	2107	148	0
3	F	51	0	43	2	0
3	H	51	0	43	3	0
4	A	13	0	0	0	0
4	B	16	0	0	2	0
4	C	22	0	0	0	0
4	D	19	0	0	1	0
4	F	1	0	0	0	0
4	H	2	0	0	0	0
All	All	9098	0	9152	528	1

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 29.

The worst 5 of 528 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:95:ALA:O	1:C:96:LEU:HD12	1.37	1.17
2:B:318:TYR:O	2:B:320:LEU:N	1.76	1.17
2:B:376:LEU:O	2:B:380:THR:HG23	1.48	1.13
1:C:95:ALA:O	1:C:96:LEU:CD1	1.95	1.12
2:D:332:LEU:HD13	2:D:421:VAL:HG12	1.31	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:NZ	2:B:280:TYR:OH[4_455]	2.06	0.14

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	294/298 (99%)	257 (87%)	28 (10%)	9 (3%)	4 16
1	C	294/298 (99%)	267 (91%)	20 (7%)	7 (2%)	6 22
2	B	256/260 (98%)	235 (92%)	12 (5%)	9 (4%)	3 14
2	D	256/260 (98%)	216 (84%)	30 (12%)	10 (4%)	3 12
3	F	2/6 (33%)	2 (100%)	0	0	100 100
3	H	2/6 (33%)	2 (100%)	0	0	100 100
All	All	1104/1128 (98%)	979 (89%)	90 (8%)	35 (3%)	4 16

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	96	LEU
1	A	160	THR
1	A	165	THR

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Mol	Chain	Res	Type
2	B	179	HIS

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	261/263 (99%)	211 (81%)	50 (19%)	1 4
1	C	261/263 (99%)	217 (83%)	44 (17%)	2 6
2	B	232/234 (99%)	190 (82%)	42 (18%)	1 5
2	D	232/234 (99%)	193 (83%)	39 (17%)	2 6
3	F	2/2 (100%)	1 (50%)	1 (50%)	0 0
3	H	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	990/998 (99%)	813 (82%)	177 (18%)	2 5

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	157	ARG
2	D	210	MET
1	C	175	LEU
1	C	248	PHE
2	D	280	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	60	HIS
1	C	246	GLN
2	D	419	HIS
1	C	131	GLN
2	D	208	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)

6 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	$\#\|Z\| > 2$
3	CIR	F	500	3	9,10,11	2.69	4 (44%)	6,11,13	2.23	3 (50%)
3	CIR	H	500	3	9,10,11	2.75	3 (33%)	6,11,13	2.36	5 (83%)
3	CIR	H	501	3	9,10,11	0.73	0	6,11,13	1.54	1 (16%)
3	PFF	H	504	3	11,12,13	0.60	0	12,15,17	1.09	0
3	CIR	F	501	3	9,10,11	0.74	0	6,11,13	0.92	0
3	PFF	F	504	3	11,12,13	0.98	1 (9%)	12,15,17	1.10	1 (8%)

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
3	CIR	F	500	3	-	6/8/9/11	-
3	CIR	H	500	3	-	1/8/9/11	-
3	CIR	H	501	3	-	5/8/9/11	-
3	PFF	H	504	3	-	1/5/6/8	0/1/1/1
3	CIR	F	501	3	-	2/8/9/11	-
3	PFF	F	504	3	-	2/5/6/8	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	500	CIR	C5-N6	-5.22	1.34	1.46
3	H	500	CIR	C5-N6	-5.15	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	500	CIR	C4-C5	-4.55	1.33	1.51
3	H	500	CIR	C4-C3	-4.33	1.33	1.52
3	F	500	CIR	C4-C3	-3.97	1.35	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	500	CIR	C4-C5-N6	3.28	121.57	112.21
3	F	500	CIR	C5-N6-C7	-3.13	119.01	122.73
3	H	500	CIR	C4-C5-N6	3.04	120.90	112.21
3	F	500	CIR	C3-C4-C5	2.93	120.85	112.05
3	H	500	CIR	N8-C7-N6	2.69	119.69	116.85

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	500	CIR	O-C-CA-C3
3	F	500	CIR	O7-C7-N6-C5
3	F	500	CIR	N8-C7-N6-C5
3	H	501	CIR	C4-C3-CA-N
3	F	500	CIR	C3-C4-C5-N6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	504	PFF	2	0
3	F	504	PFF	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	296/298 (99%)	-0.15	7 (2%)	59	56	21, 52, 85, 113	0
1	C	296/298 (99%)	-0.22	10 (3%)	45	40	25, 50, 95, 129	0
2	B	258/260 (99%)	-0.24	4 (1%)	72	71	26, 52, 80, 105	0
2	D	258/260 (99%)	-0.26	9 (3%)	44	38	27, 53, 83, 95	0
3	F	2/6 (33%)	-1.01	0	100	100	58, 58, 58, 62	0
3	H	2/6 (33%)	0.05	0	100	100	56, 56, 56, 61	0
All	All	1112/1128 (98%)	-0.22	30 (2%)	54	50	21, 51, 86, 129	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	TYR	4.6
1	C	39	THR	4.5
1	A	13	GLY	4.5
2	D	284	ASP	4.0
2	B	345	ASP	3.5

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. 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
3	PFF	H	504	12/13	0.86	0.20	46,60,72,73	0
3	CIR	F	500	11/12	0.88	0.26	53,67,75,77	0
3	CIR	H	500	11/12	0.89	0.21	45,64,94,102	0
3	CIR	H	501	11/12	0.91	0.37	42,63,94,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CIR	F	501	11/12	0.93	0.25	45,75,122,125	0
3	PFF	F	504	12/13	0.94	0.16	36,50,80,93	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.