



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:23 PM GMT

PDB ID : 4OQB
Title : Structure of Human PARP-1 bound to a DNA double strand break in complex with (2Z)-2-{4-[2-(morpholin-4-yl)ethoxy]benzylidene}-3-oxo-2,3-dihydro-1-benzofuran-7-carboxamide
Authors : Pascal, J.M.; Steffen, J.D.
Deposited on : 2014-02-07
Resolution : 3.36 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 (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

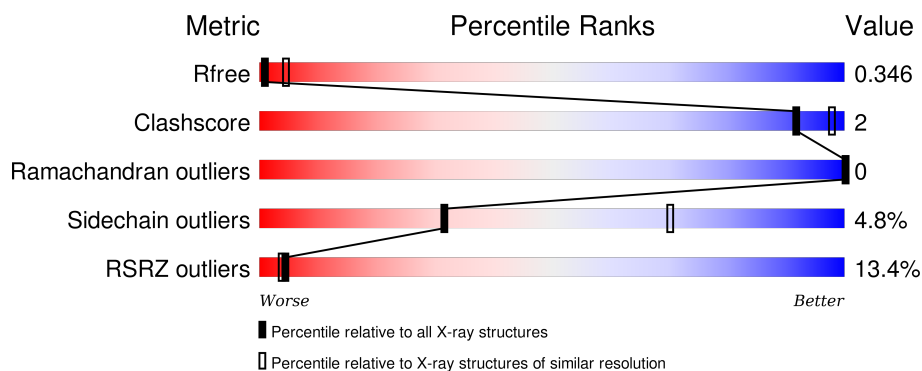
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	267	<div> <div>2%</div> <div>77%</div> <div>5% • 17%</div> </div>
1	D	267	<div> <div>13%</div> <div>78%</div> <div>5% • 17%</div> </div>
2	C	505	<div> <div>12%</div> <div>81%</div> <div>9% 10%</div> </div>
2	F	505	<div> <div>18%</div> <div>81%</div> <div>9% 10%</div> </div>
3	M	26	<div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	N	26	 92%8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11775 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	1	0
			1755	1110	305	327	13			
1	D	222	Total	C	N	O	S	0	1	0
			1755	1110	305	327	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ASP	-	LINKER	UNP P09874
A	206	ILE	-	LINKER	UNP P09874
A	367	LEU	-	EXPRESSION TAG	UNP P09874
A	368	GLU	-	EXPRESSION TAG	UNP P09874
A	369	HIS	-	EXPRESSION TAG	UNP P09874
A	370	HIS	-	EXPRESSION TAG	UNP P09874
A	371	HIS	-	EXPRESSION TAG	UNP P09874
A	372	HIS	-	EXPRESSION TAG	UNP P09874
A	373	HIS	-	EXPRESSION TAG	UNP P09874
A	374	HIS	-	EXPRESSION TAG	UNP P09874
D	205	ASP	-	LINKER	UNP P09874
D	206	ILE	-	LINKER	UNP P09874
D	367	LEU	-	EXPRESSION TAG	UNP P09874
D	368	GLU	-	EXPRESSION TAG	UNP P09874
D	369	HIS	-	EXPRESSION TAG	UNP P09874
D	370	HIS	-	EXPRESSION TAG	UNP P09874
D	371	HIS	-	EXPRESSION TAG	UNP P09874
D	372	HIS	-	EXPRESSION TAG	UNP P09874
D	373	HIS	-	EXPRESSION TAG	UNP P09874
D	374	HIS	-	EXPRESSION TAG	UNP P09874

- Molecule 2 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	456	Total 3586	C 2296	N 605	O 672	S 13	0	0	0
2	F	456	Total 3586	C 2296	N 605	O 672	S 13	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1015	LEU	-	EXPRESSION TAG	UNP P09874
C	1016	GLU	-	EXPRESSION TAG	UNP P09874
C	1017	HIS	-	EXPRESSION TAG	UNP P09874
C	1018	HIS	-	EXPRESSION TAG	UNP P09874
C	1019	HIS	-	EXPRESSION TAG	UNP P09874
C	1020	HIS	-	EXPRESSION TAG	UNP P09874
C	1021	HIS	-	EXPRESSION TAG	UNP P09874
C	1022	HIS	-	EXPRESSION TAG	UNP P09874
F	1015	LEU	-	EXPRESSION TAG	UNP P09874
F	1016	GLU	-	EXPRESSION TAG	UNP P09874
F	1017	HIS	-	EXPRESSION TAG	UNP P09874
F	1018	HIS	-	EXPRESSION TAG	UNP P09874
F	1019	HIS	-	EXPRESSION TAG	UNP P09874
F	1020	HIS	-	EXPRESSION TAG	UNP P09874
F	1021	HIS	-	EXPRESSION TAG	UNP P09874
F	1022	HIS	-	EXPRESSION TAG	UNP P09874

- Molecule 3 is a DNA chain called DNA (26-MER).

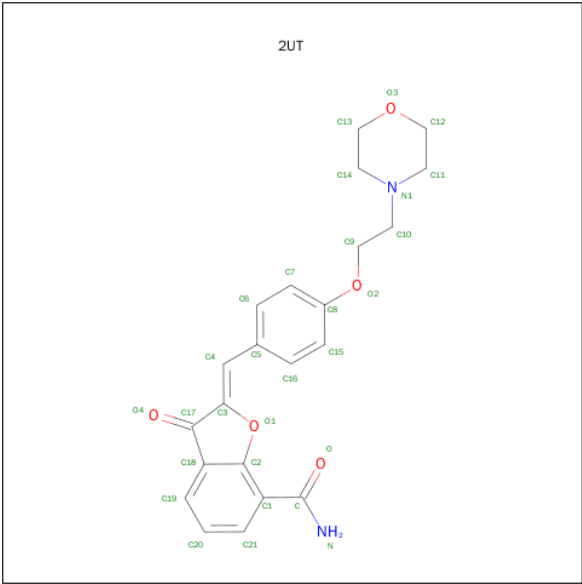
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	26	Total 530	C 251	N 100	O 154	P 25	0	0	0
3	N	26	Total 530	C 251	N 100	O 154	P 25	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Zn 2	0	0
4	D	2	Total 2	Zn 2	0	0

- Molecule 5 is (2Z)-2-{4-[2-(MORPHOLIN-4-YL)ETHOXY]BENZYLIDENE}-3-OXO-2,3-DIHYDRO-1-BENZOFURAN-7-CARBOXAMIDE (three-letter code: 2UT) (formula:

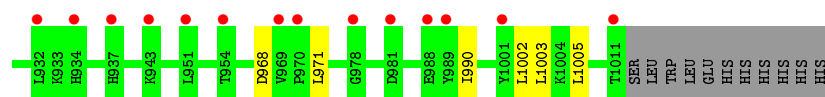
C₂₂H₂₂N₂O₅).



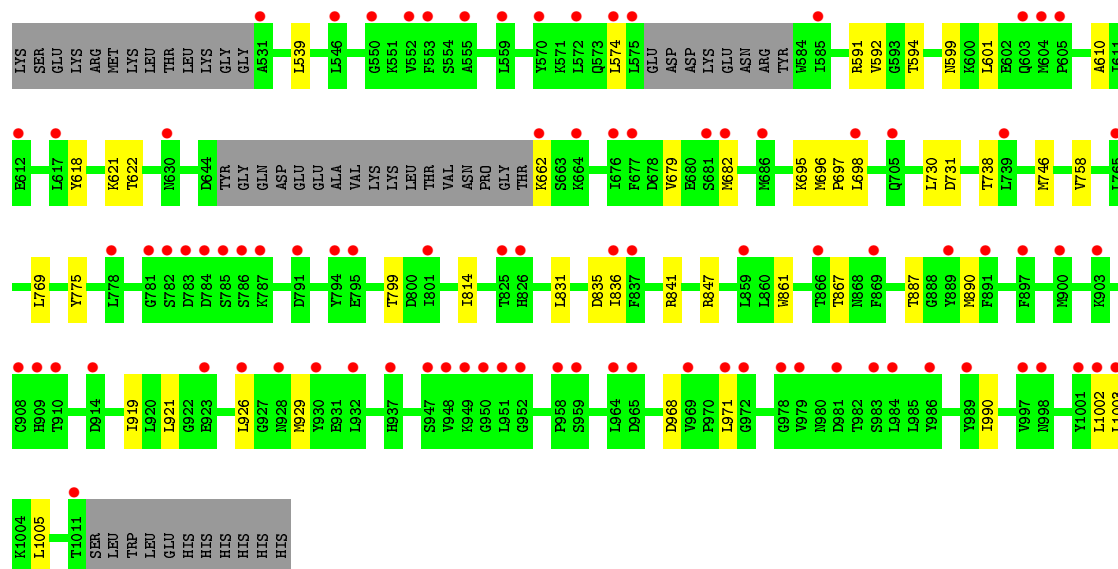
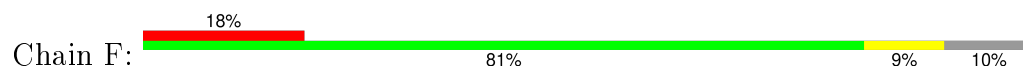
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			29	22	2	5		

- Molecule 1: Poly [ADP-ribose] polymerase 1





- Molecule 2: Poly [ADP-ribose] polymerase 1



- Molecule 3: DNA (26-MER)



- Molecule 3: DNA (26-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.10Å 113.08Å 296.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.36 49.37 – 3.36	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.36) 98.9 (49.37-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.322 , 0.349 0.317 , 0.346	Depositor DCC
R_{free} test set	1623 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	136.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 108.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 31745 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11775	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.91% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2UT

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	0.26	0/1795	0.40	0/2416
1	D	0.26	0/1795	0.40	0/2416
2	C	0.26	0/3660	0.42	0/4940
2	F	0.26	0/3660	0.43	0/4940
3	M	0.27	0/594	0.80	0/915
3	N	0.24	0/594	0.78	2/915 (0.2%)
All	All	0.26	0/12098	0.47	2/16542 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	DG	C5'-C4'-O4'	5.23	119.23	109.30
3	N	1	DG	C5'-C4'-C3'	5.08	123.25	114.10

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	1755	0	1712	6	0
1	D	1755	0	1712	6	0
2	C	3586	0	3604	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3586	0	3604	18	0
3	M	530	0	292	1	0
3	N	530	0	292	1	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	C	29	0	22	2	0
All	All	11775	0	11238	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 2.

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)
2:F:574:LEU:HD11	2:F:610:ALA:HB1	1.69	0.73
2:C:574:LEU:HD11	2:C:610:ALA:HB1	1.70	0.72
1:A:36:ALA:HB2	1:A:51:TRP:CE3	2.39	0.57
1:D:36:ALA:HB2	1:D:51:TRP:CE3	2.39	0.57
2:C:831:LEU:HD12	2:C:1005:LEU:HD23	1.88	0.54
2:F:831:LEU:HD12	2:F:1005:LEU:HD23	1.88	0.54
2:C:898:ALA:HB2	5:C:1101:2UT:H2	1.91	0.53
2:F:814:ILE:HG21	2:F:836:ILE:HD12	1.92	0.52
2:C:814:ILE:HG21	2:C:836:ILE:HD12	1.92	0.51
2:F:679:VAL:HG11	2:F:775:TYR:CZ	2.46	0.50
2:C:679:VAL:HG11	2:C:775:TYR:CZ	2.47	0.50
2:F:919:ILE:HG22	2:F:1005:LEU:HD11	1.94	0.49
2:C:919:ILE:HG22	2:C:1005:LEU:HD11	1.94	0.49
2:F:696:MET:N	2:F:697:PRO:HD2	2.28	0.49
2:C:696:MET:N	2:C:697:PRO:HD2	2.28	0.48
1:D:315:VAL:HG13	1:D:316:THR:HG22	1.95	0.48
2:C:861:TRP:CD2	2:C:921:LEU:HD21	2.49	0.47
1:A:315:VAL:HG13	1:A:316:THR:HG22	1.96	0.47
3:M:22:DT:H2''	3:M:23:DA:C8	2.50	0.47
1:D:319:THR:HG21	2:F:731:ASP:HA	1.96	0.47
2:C:862:HIS:ND1	5:C:1101:2UT:O	2.48	0.46
2:F:861:TRP:CD2	2:F:921:LEU:HD21	2.49	0.46
2:F:926:LEU:HD13	2:F:929:MET:HE3	1.98	0.44
2:C:926:LEU:HD13	2:C:929:MET:HE3	1.99	0.44
1:A:275:GLY:HA2	3:N:23:DA:H3'	1.99	0.44
2:F:799:THR:HG22	2:F:841:ARG:HA	2.00	0.43
2:C:539:LEU:HD11	2:C:601:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:THR:CG2	2:F:731:ASP:HA	2.48	0.42
1:D:64:ILE:HD13	1:D:71:VAL:CG2	2.50	0.42
2:C:814:ILE:CG2	2:C:1003:LEU:HD21	2.50	0.42
1:A:64:ILE:HD13	1:A:71:VAL:CG2	2.50	0.42
2:C:799:THR:HG22	2:C:841:ARG:HA	2.00	0.42
2:F:539:LEU:HD11	2:F:601:LEU:HD21	2.00	0.41
2:C:682:MET:HG2	2:C:867:THR:HG22	2.02	0.41
2:C:734:ASN:O	2:C:738:THR:OG1	2.38	0.41
2:F:696:MET:N	2:F:697:PRO:CD	2.83	0.41
2:F:682:MET:HG2	2:F:867:THR:HG22	2.03	0.41
2:C:990:ILE:HD12	2:C:990:ILE:N	2.36	0.41
2:C:696:MET:N	2:C:697:PRO:CD	2.83	0.41
1:A:319:THR:HG22	2:C:734:ASN:HD22	1.86	0.41
2:C:618:TYR:CE2	2:C:622:THR:HG21	2.56	0.41
2:F:591:ARG:HD3	2:F:746:MET:HE1	2.03	0.41
2:F:814:ILE:CG2	2:F:1003:LEU:HD21	2.50	0.41
1:D:36:ALA:HB2	1:D:51:TRP:CZ3	2.56	0.41
2:F:990:ILE:HD12	2:F:990:ILE:N	2.36	0.41
2:C:618:TYR:O	2:C:622:THR:HG22	2.21	0.40
1:A:36:ALA:HB2	1:A:51:TRP:CZ3	2.56	0.40
2:F:618:TYR:O	2:F:622:THR:HG22	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	219/267 (82%)	212 (97%)	7 (3%)	0	100	100
1	D	219/267 (82%)	212 (97%)	7 (3%)	0	100	100
2	C	450/505 (89%)	423 (94%)	27 (6%)	0	100	100
2	F	450/505 (89%)	422 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1338/1544 (87%)	1269 (95%)	69 (5%)	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	189/237 (80%)	179 (95%)	10 (5%)	28	66
1	D	189/237 (80%)	179 (95%)	10 (5%)	28	66
2	C	391/443 (88%)	373 (95%)	18 (5%)	33	71
2	F	391/443 (88%)	373 (95%)	18 (5%)	33	71
All	All	1160/1360 (85%)	1104 (95%)	56 (5%)	31	70

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	CYS
1	A	22	LYS
1	A	37	ILE
1	A	40	GLN
1	A	47	LYS
1	A	48	VAL
1	A	280	LEU
1	A	301	GLN
1	A	316	THR
1	A	319	THR
2	C	592	VAL
2	C	594	THR
2	C	599	ASN
2	C	621	LYS
2	C	662	LYS
2	C	695	LYS
2	C	698	LEU

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Mol	Chain	Res	Type
2	C	730	LEU
2	C	738	THR
2	C	758	VAL
2	C	769	LEU
2	C	835	ASP
2	C	847	ARG
2	C	887	THR
2	C	890	MET
2	C	968	ASP
2	C	971	LEU
2	C	1002	LEU
1	D	21	CYS
1	D	22	LYS
1	D	37	ILE
1	D	40	GLN
1	D	47	LYS
1	D	48	VAL
1	D	280	LEU
1	D	301	GLN
1	D	316	THR
1	D	319	THR
2	F	592	VAL
2	F	594	THR
2	F	599	ASN
2	F	621	LYS
2	F	662	LYS
2	F	695	LYS
2	F	698	LEU
2	F	730	LEU
2	F	738	THR
2	F	758	VAL
2	F	769	LEU
2	F	835	ASP
2	F	847	ARG
2	F	887	THR
2	F	890	MET
2	F	968	ASP
2	F	971	LEU
2	F	1002	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	573	GLN
2	C	599	ASN
2	C	613	HIS
2	C	820	ASN
2	C	856	ASN
2	C	906	ASN
2	C	961	ASN
2	F	573	GLN
2	F	599	ASN
2	F	613	HIS
2	F	820	ASN
2	F	856	ASN
2	F	906	ASN
2	F	961	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	2UT	C	1101	-	32,32,32	0.24	0	41,44,44	2.18	7 (17%)

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
5	2UT	C	1101	-	-	0/13/34/34	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1101	2UT	O1-C3-C4	-7.63	112.75	123.83
5	C	1101	2UT	C18-C17-C3	-5.44	100.75	104.15
5	C	1101	2UT	C18-C2-C1	-2.68	121.65	124.92
5	C	1101	2UT	C2-C1-C	-2.45	121.86	125.82
5	C	1101	2UT	O1-C3-C17	2.71	111.79	109.50
5	C	1101	2UT	O4-C17-C3	6.19	132.27	126.41
5	C	1101	2UT	C2-C18-C17	6.62	109.63	107.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1101	2UT	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 ⓘ

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	222/267 (83%)	0.18	6 (2%) 58 58	136, 174, 261, 285	0
1	D	222/267 (83%)	0.70	34 (15%) 3 3	176, 243, 321, 342	0
2	C	456/505 (90%)	0.85	59 (12%) 5 4	135, 195, 248, 286	0
2	F	456/505 (90%)	1.06	89 (19%) 1 2	169, 241, 300, 331	0
3	M	26/26 (100%)	-0.58	0 100 100	161, 187, 226, 228	0
3	N	26/26 (100%)	-0.61	0 100 100	157, 203, 226, 230	0
All	All	1408/1596 (88%)	0.74	188 (13%) 4 4	135, 214, 293, 342	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	349	LYS	10.9
1	D	348	LEU	8.7
2	F	951	LEU	7.1
2	C	786	SER	6.8
2	F	930	TYR	6.4
2	F	989	TYR	6.4
2	F	786	SER	5.8
1	D	225	LYS	5.7
2	C	785	SER	5.6
2	C	575	LEU	5.5
2	C	934	HIS	5.3
1	D	58	TRP	5.1
2	C	989	TYR	5.1
2	F	928	ASN	5.0
2	F	958	PRO	5.0
2	F	1001	TYR	5.0
2	C	574	LEU	4.9
2	F	1011	THR	4.9
2	F	605	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	309	TYR	4.8
1	D	359	PRO	4.7
1	D	35	MET	4.6
2	F	783	ASP	4.5
2	F	785	SER	4.4
2	F	923	GLU	4.4
2	C	539	LEU	4.3
2	F	998	ASN	4.3
2	F	781	GLY	4.2
2	F	932	LEU	4.2
2	F	782	SER	4.1
2	F	572	LEU	4.0
2	F	937	HIS	4.0
2	F	794	TYR	4.0
2	F	612	GLU	3.9
2	F	531	ALA	3.9
2	F	900	MET	3.8
2	C	951	LEU	3.8
2	C	553	PHE	3.8
2	F	603	GLN	3.8
2	C	1011	THR	3.7
2	F	1003	LEU	3.7
2	F	836	ILE	3.7
2	F	984	LEU	3.6
2	F	997	VAL	3.6
1	D	33	LEU	3.6
2	F	959	SER	3.6
2	F	574	LEU	3.6
2	F	948	VAL	3.6
1	D	229	ASP	3.6
2	F	986	TYR	3.5
2	F	801	ILE	3.5
2	F	662	LYS	3.5
2	F	978	GLY	3.4
2	C	543	ALA	3.4
1	D	224	SER	3.3
2	C	787	LYS	3.3
2	C	970	PRO	3.3
2	F	891	PHE	3.3
2	F	555	ALA	3.3
2	F	553	PHE	3.3
2	F	705	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	575	LEU	3.2
1	A	309	TYR	3.2
2	C	788	ASP	3.2
2	C	903	LYS	3.1
1	D	283	VAL	3.1
2	F	559	LEU	3.1
1	D	13	TYR	3.1
2	F	889	TYR	3.0
2	F	971	LEU	3.0
1	D	280	LEU	3.0
2	C	686	MET	3.0
2	F	550	GLY	3.0
1	D	62	HIS	3.0
2	F	949	LYS	3.0
2	F	1002	LEU	3.0
2	F	826	HIS	3.0
1	D	226	LYS	2.9
2	C	969	VAL	2.9
2	F	546	LEU	2.9
2	C	677	PHE	2.9
2	C	943	LYS	2.9
2	C	914	ASP	2.9
2	C	572	LEU	2.9
2	F	677	PHE	2.8
2	F	950	GLY	2.8
1	A	302	LEU	2.8
1	D	15	LYS	2.8
2	F	825	THR	2.8
2	F	739	LEU	2.8
2	C	817	TYR	2.8
1	D	6	ASP	2.8
2	C	605	PRO	2.8
2	C	777	LEU	2.8
2	C	954	THR	2.8
2	C	937	HIS	2.8
1	A	35	MET	2.8
2	C	537	SER	2.8
1	D	51	TRP	2.8
2	F	682	MET	2.8
1	D	353	GLN	2.8
2	F	910	THR	2.7
2	F	585	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	57	PHE	2.7
1	D	74	PHE	2.7
2	F	791	ASP	2.7
2	C	698	LEU	2.7
2	C	681	SER	2.6
2	F	686	MET	2.6
2	F	909	HIS	2.6
2	F	979	VAL	2.6
2	C	842	GLU	2.6
2	C	682	MET	2.5
2	C	869	PHE	2.6
2	F	698	LEU	2.5
1	D	19	ALA	2.5
2	F	866	THR	2.5
2	C	932	LEU	2.5
2	C	988	GLU	2.5
1	D	356	ILE	2.5
2	F	778	LEU	2.5
2	F	664	LYS	2.5
2	F	787	LYS	2.5
2	F	914	ASP	2.5
2	F	972	GLY	2.5
1	D	287	MET	2.5
2	C	685	ALA	2.4
2	C	732	LEU	2.4
2	F	765	LEU	2.4
2	C	978	GLY	2.4
1	D	350	VAL	2.4
2	F	952	GLY	2.4
2	C	570	TYR	2.4
2	F	908	CYS	2.4
2	F	964	LEU	2.4
2	F	903	LYS	2.4
2	F	897	PHE	2.4
2	F	784	ASP	2.4
2	C	917	GLY	2.4
2	C	729	ILE	2.4
2	C	736	PHE	2.4
1	D	69	VAL	2.3
1	A	265	LEU	2.3
1	D	54	PHE	2.3
1	A	64	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	347	LYS	2.3
2	F	969	VAL	2.3
2	C	909	HIS	2.3
1	A	291	ALA	2.3
2	F	859	LEU	2.3
2	C	531	ALA	2.2
1	D	276	GLU	2.2
2	F	965	ASP	2.2
2	C	910	THR	2.2
2	F	630	ASN	2.2
2	F	570	TYR	2.2
2	C	630	ASN	2.2
2	F	926	LEU	2.2
2	C	814	ILE	2.2
1	D	333	TRP	2.2
1	D	299	SER	2.2
2	C	891	PHE	2.2
2	C	545	VAL	2.2
2	C	604	MET	2.2
2	C	981	ASP	2.2
2	F	983	SER	2.2
2	F	552	VAL	2.2
2	C	692	ASP	2.2
2	C	742	HIS	2.2
1	D	285	ASP	2.1
2	C	1001	TYR	2.1
2	F	676	ILE	2.1
1	D	231	ASP	2.1
1	D	34	ARG	2.1
2	C	724	SER	2.1
2	C	897	PHE	2.0
2	F	869	PHE	2.0
2	C	825	THR	2.0
2	F	795	GLU	2.0
2	C	555	ALA	2.0
2	C	853	GLN	2.0
2	F	947	SER	2.0
2	F	604	MET	2.0
2	C	778	LEU	2.0
2	F	617	LEU	2.0
2	F	837	PHE	2.0
2	F	981	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	681	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, 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
5	2UT	C	1101	29/29	0.80	0.28	-0.47	121,127,140,140	0
4	ZN	D	402	1/1	0.88	0.04	-1.44	132,132,132,132	0
4	ZN	A	402	1/1	0.95	0.04	-2.76	62,62,62,62	0
4	ZN	A	401	1/1	0.96	0.04	-	78,78,78,78	0
4	ZN	D	401	1/1	0.91	0.07	-	118,118,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.