



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:01 PM UTC

PDB ID : 8A8Q / pdb_00008a8q
Title : Crystal structure of Protein Scalloped in complex with YAP peptide
Authors : Scheufler, C.; Villard, F.
Deposited on : 2022-06-23
Resolution : 1.47 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

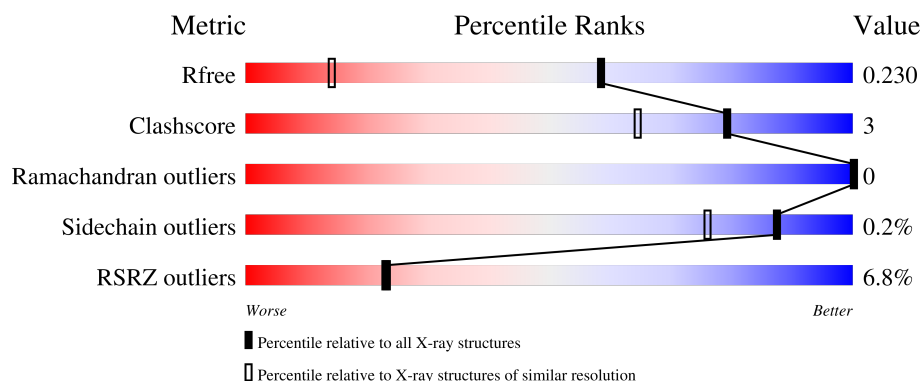
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 $\leq 5\%$. 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	219	
1	B	219	
2	C	51	
2	D	51	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4211 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 Protein scalloped.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	2	0
			1668	1080	273	303	12			
1	B	200	Total	C	N	O	S	0	0	0
			1623	1051	266	295	11			

- Molecule 2 is a protein called Isoform 7 of Transcriptional coactivator YAP1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	43	Total	C	N	O	0	0	0
			336	215	60	61			
2	D	44	Total	C	N	O	0	0	0
			341	219	62	60			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	50	ACE	-	acetylation	UNP P46937
C	73	NLE	MET	conflict	UNP P46937
C	86	NLE	MET	conflict	UNP P46937
C	100	NH2	-	amidation	UNP P46937
D	50	ACE	-	acetylation	UNP P46937
D	73	NLE	MET	conflict	UNP P46937
D	86	NLE	MET	conflict	UNP P46937
D	100	NH2	-	amidation	UNP P46937

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

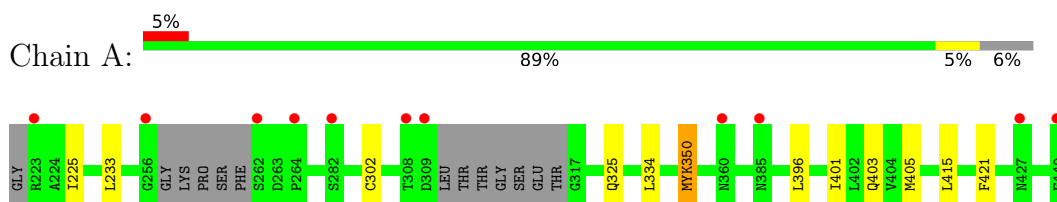
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	85	Total	O	0	0
			85	85		
4	C	27	Total	O	0	0
			27	27		
4	D	20	Total	O	0	0
			20	20		

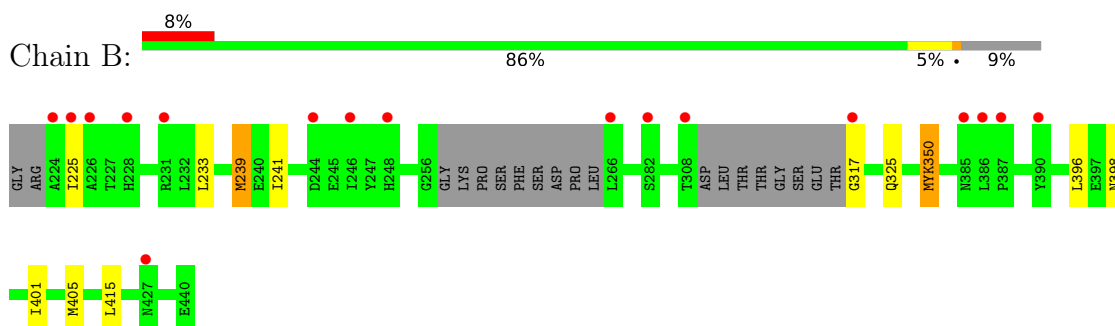
3 Residue-property plots [i](#)

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.

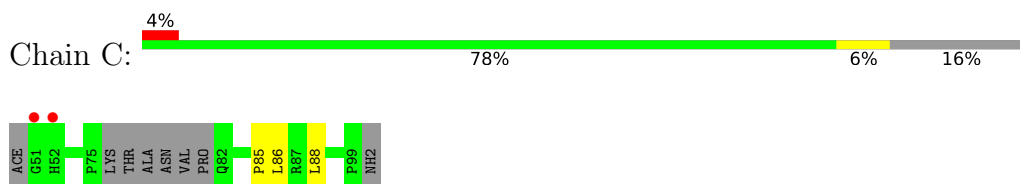
- Molecule 1: Protein scalloped



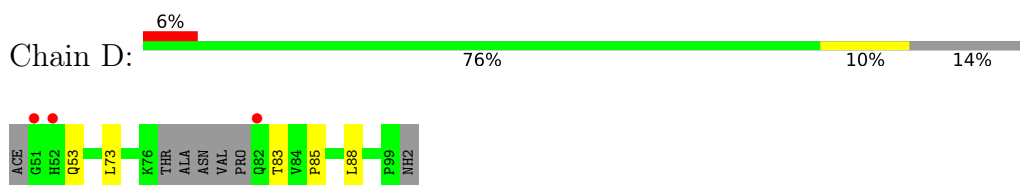
- Molecule 1: Protein scalloped



- Molecule 2: Isoform 7 of Transcriptional coactivator YAP1



- Molecule 2: Isoform 7 of Transcriptional coactivator YAP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.77Å 85.70Å 76.23Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	29.09 – 1.47 29.09 – 1.47	Depositor EDS
% Data completeness (in resolution range)	55.7 (29.09-1.47) 55.7 (29.09-1.47)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.46Å)	Xtriage
Refinement program	BUSTER 2.11.8 (3-FEB-2022)	Depositor
R, R_{free}	0.211 , 0.234 0.204 , 0.230	Depositor DCC
R_{free} test set	2624 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4211	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NLE, MYK, ACT

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	0/1676	0.95	0/2267
1	B	0.68	1/1630 (0.1%)	0.92	0/2203
2	C	0.69	0/326	0.90	0/441
2	D	0.74	0/331	0.94	0/447
All	All	0.69	1/3963 (0.0%)	0.94	0/5358

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	MET	SD-CE	-6.38	1.63	1.79

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1668	0	1612	8	0
1	B	1623	0	1576	11	0
2	C	336	0	322	1	0
2	D	341	0	331	4	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	103	0	0	0	0
4	B	85	0	0	0	0
4	C	27	0	0	0	0
4	D	20	0	0	0	0
All	All	4211	0	3847	21	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (21) 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:398:ASN:OD1	2:D:83:THR:HG21	1.82	0.80
1:B:350:MYK:HDA	2:D:53:GLN:NE2	2.01	0.74
1:A:334:LEU:HD11	1:A:405:MET:HG3	1.78	0.63
1:B:225:ILE:HG22	1:B:415:LEU:HD21	1.84	0.59
1:B:350:MYK:HI	1:B:401:ILE:HD13	1.83	0.59
1:A:350:MYK:HI	1:A:401:ILE:HD13	1.84	0.57
1:B:405:MET:HE2	1:B:415:LEU:HB3	1.86	0.57
1:A:403:GLN:HG2	1:A:405:MET:HE1	1.92	0.51
1:A:225:ILE:HG22	1:A:415:LEU:HD21	1.93	0.51
1:B:350:MYK:HWA	1:B:396:LEU:HD21	1.93	0.49
1:A:233:LEU:HD12	1:A:325:GLN:HG2	1.93	0.49
1:A:350:MYK:HWA	1:A:396:LEU:HD21	1.94	0.49
2:C:85:PRO:HD2	2:C:88:LEU:HD12	1.94	0.48
1:B:233:LEU:HD12	1:B:325:GLN:HG2	1.94	0.47
2:D:85:PRO:HD2	2:D:88:LEU:HD12	1.96	0.47
1:B:239:MET:CE	1:B:317:GLY:HA3	2.45	0.46
1:B:350:MYK:HYA	1:B:350:MYK:HE	1.76	0.46
1:B:239:MET:HE3	1:B:317:GLY:HA3	1.97	0.46
1:B:350:MYK:HG	2:D:53:GLN:HG3	1.98	0.45
1:A:350:MYK:HYA	1:A:350:MYK:HE	1.78	0.44
1:A:302[A]:CYS:HB2	1:A:421:PHE:CD1	2.55	0.42

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	201/219 (92%)	198 (98%)	3 (2%)	0	100	100
1	B	193/219 (88%)	191 (99%)	2 (1%)	0	100	100
2	C	37/51 (72%)	37 (100%)	0	0	100	100
2	D	38/51 (74%)	38 (100%)	0	0	100	100
All	All	469/540 (87%)	464 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	173/198 (87%)	173 (100%)	0	100	100
1	B	169/198 (85%)	168 (99%)	1 (1%)	78	58
2	C	35/42 (83%)	35 (100%)	0	100	100
2	D	35/42 (83%)	35 (100%)	0	100	100
All	All	412/480 (86%)	411 (100%)	1 (0%)	87	76

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	GLN
1	B	403	GLN
2	C	53	GLN
2	C	74	ASN
2	D	53	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
1	MYK	B	350	1	22,23,24	0.90	0	19,24,26	1.29	3 (15%)
2	NLE	C	86	2	6,7,8	1.21	1 (16%)	2,7,9	0.61	0
2	NLE	D	86	2	6,7,8	0.61	0	2,7,9	0.13	0
1	MYK	A	350	1	22,23,24	0.85	0	19,24,26	1.26	3 (15%)
2	NLE	D	73	2	6,7,8	1.05	1 (16%)	2,7,9	0.44	0
2	NLE	C	73	2	6,7,8	0.71	0	2,7,9	0.36	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
1	MYK	B	350	1	-	12/22/23/25	-
2	NLE	C	86	2	-	2/5/6/8	-
2	NLE	D	86	2	-	2/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MYK	A	350	1	-	12/22/23/25	-
2	NLE	D	73	2	-	1/5/6/8	-
2	NLE	C	73	2	-	1/5/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	86	NLE	CB-CA	2.73	1.57	1.53
2	D	73	NLE	CB-CA	2.34	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	MYK	OX-CX-CY	-2.78	116.98	122.02
1	A	350	MYK	CD-CE-NZ	2.77	119.98	112.20
1	B	350	MYK	CD-CE-NZ	2.64	119.60	112.20
1	A	350	MYK	OX-CX-CY	-2.61	117.29	122.02
1	B	350	MYK	CE-NZ-CX	-2.48	118.20	122.82
1	A	350	MYK	CE-NZ-CX	-2.38	118.39	122.82

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	86	NLE	O-C-CA-CB
1	A	350	MYK	CY-CX-NZ-CE
1	B	350	MYK	CY-CX-NZ-CE
1	A	350	MYK	CE-CD-CG-CB
1	B	350	MYK	CE-CD-CG-CB
1	A	350	MYK	CG-CD-CE-NZ
1	B	350	MYK	CG-CD-CE-NZ
1	A	350	MYK	OX-CX-NZ-CE
1	B	350	MYK	OX-CX-NZ-CE
1	A	350	MYK	CP-CR-CU-CQ
1	B	350	MYK	CP-CR-CU-CQ
1	A	350	MYK	CU-CQ-CS-CW
1	B	350	MYK	CU-CQ-CS-CW
1	B	350	MYK	CL-CM-CP-CR
1	A	350	MYK	CL-CM-CP-CR
2	C	86	NLE	CE-CD-CG-CB
1	A	350	MYK	CQ-CS-CW-CV

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Mol	Chain	Res	Type	Atoms
1	B	350	MYK	CQ-CS-CW-CV
2	D	86	NLE	CE-CD-CG-CB
1	B	350	MYK	CK-CI-CT-CY
1	A	350	MYK	CK-CI-CT-CY
1	A	350	MYK	CK-CL-CM-CP
1	B	350	MYK	CK-CL-CM-CP
1	B	350	MYK	CS-CQ-CU-CR
1	A	350	MYK	CS-CQ-CU-CR
2	D	73	NLE	CA-CB-CG-CD
1	B	350	MYK	CI-CK-CL-CM
1	A	350	MYK	CI-CK-CL-CM
2	C	73	NLE	CA-CB-CG-CD
2	D	86	NLE	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	350	MYK	5	0
1	A	350	MYK	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	ACT	A	501	-	3,3,3	0.63	0	3,3,3	1.78	2 (66%)
3	ACT	B	501	-	3,3,3	1.15	0	3,3,3	1.28	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	ACT	O-C-CH3	-2.26	113.26	122.53
3	A	501	ACT	OXT-C-O	2.03	129.55	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	205/219 (93%)	0.26	11 (5%) 31 31	6, 18, 33, 48	2 (0%)
1	B	199/219 (90%)	0.51	17 (8%) 16 17	10, 21, 38, 44	0
2	C	41/51 (80%)	0.25	2 (4%) 35 36	13, 19, 28, 35	0
2	D	42/51 (82%)	0.38	3 (7%) 22 21	13, 20, 31, 38	0
All	All	487/540 (90%)	0.37	33 (6%) 23 23	6, 19, 36, 48	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	308	THR	4.5
1	B	266	LEU	4.0
1	A	262	SER	3.9
1	B	282	SER	3.5
1	B	248	HIS	3.3
1	B	317	GLY	3.1
1	B	390	TYR	3.0
2	D	51	GLY	2.9
1	B	246	ILE	2.9
1	B	427	ASN	2.8
1	B	226	ALA	2.7
1	B	228	HIS	2.7
1	A	264	PRO	2.7
1	A	309	ASP	2.7
1	A	256	GLY	2.6
1	A	385	ASN	2.6
1	B	225	ILE	2.6
1	B	224	ALA	2.5
2	C	52	HIS	2.5
1	A	440	GLU	2.5
1	B	386	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	82	GLN	2.4
1	A	282	SER	2.3
1	A	427	ASN	2.3
1	A	223	ARG	2.2
1	B	231	ARG	2.2
1	A	308	THR	2.2
1	B	244	ASP	2.1
1	A	360	ASN	2.1
2	C	51	GLY	2.1
2	D	52	HIS	2.0
1	B	387	PRO	2.0
1	B	385	ASN	2.0

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
2	NLE	D	73	8/9	0.87	0.12	18,23,25,26	0
1	MYK	B	350	24/25	0.89	0.15	11,31,35,35	0
1	MYK	A	350	24/25	0.89	0.16	10,32,40,40	0
2	NLE	C	73	8/9	0.94	0.09	16,20,25,26	0
2	NLE	C	86	8/9	0.95	0.08	14,16,22,22	0
2	NLE	D	86	8/9	0.97	0.06	15,16,21,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
3	ACT	B	501	4/4	0.91	0.10	23,24,24,25	0
3	ACT	A	501	4/4	0.96	0.06	21,21,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.