wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2026 – 02:06 PM UTC

PDB ID	:	7Y8W / pdb_00007y8w
Title	:	Crystal structure of DLC-1/SAO-1 complex
Authors	:	Yan, H.; Zhao, C.; Wei, Z.; Yu, C.
Deposited on	:	2022-06-24
Resolution	:	2.40 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:

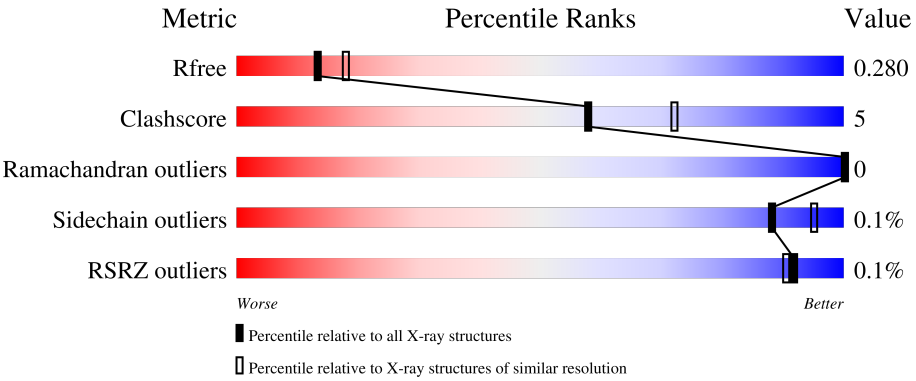
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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.



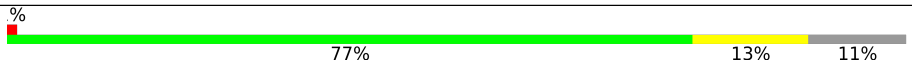
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	95	81% 8% 11%
1	B	95	81% 9% 9%
1	C	95	76% 14% 11%
1	D	95	78% 11% 12%
1	G	95	82% 8% 9%

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Mol	Chain	Length	Quality of chain
1	H	95	
1	I	95	
1	J	95	
1	M	95	
1	N	95	
1	Q	95	
1	R	95	
2	E	30	
2	F	30	
2	K	30	
2	L	30	
2	O	30	
2	P	30	
2	S	30	
2	T	30	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9324 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 Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			690	445	112	129	4			
1	B	86	Total	C	N	O	S	0	0	0
			691	445	112	130	4			
1	C	85	Total	C	N	O	S	0	0	0
			690	446	112	128	4			
1	D	84	Total	C	N	O	S	0	0	0
			673	433	108	128	4			
1	G	86	Total	C	N	O	S	0	0	0
			695	448	113	130	4			
1	H	86	Total	C	N	O	S	0	0	0
			691	445	112	130	4			
1	I	85	Total	C	N	O	S	0	0	0
			686	442	111	129	4			
1	J	84	Total	C	N	O	S	0	0	0
			673	433	108	128	4			
1	M	86	Total	C	N	O	S	0	0	0
			695	448	113	130	4			
1	N	87	Total	C	N	O	S	0	0	0
			701	452	113	132	4			
1	Q	85	Total	C	N	O	S	0	0	0
			690	445	112	129	4			
1	R	87	Total	C	N	O	S	0	0	0
			686	441	110	131	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q22799
A	-4	PRO	-	expression tag	UNP Q22799
A	-3	GLY	-	expression tag	UNP Q22799
A	-2	SER	-	expression tag	UNP Q22799
A	-1	GLU	-	expression tag	UNP Q22799

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PHE	-	expression tag	UNP Q22799
B	-5	GLY	-	expression tag	UNP Q22799
B	-4	PRO	-	expression tag	UNP Q22799
B	-3	GLY	-	expression tag	UNP Q22799
B	-2	SER	-	expression tag	UNP Q22799
B	-1	GLU	-	expression tag	UNP Q22799
B	0	PHE	-	expression tag	UNP Q22799
C	-5	GLY	-	expression tag	UNP Q22799
C	-4	PRO	-	expression tag	UNP Q22799
C	-3	GLY	-	expression tag	UNP Q22799
C	-2	SER	-	expression tag	UNP Q22799
C	-1	GLU	-	expression tag	UNP Q22799
C	0	PHE	-	expression tag	UNP Q22799
D	-5	GLY	-	expression tag	UNP Q22799
D	-4	PRO	-	expression tag	UNP Q22799
D	-3	GLY	-	expression tag	UNP Q22799
D	-2	SER	-	expression tag	UNP Q22799
D	-1	GLU	-	expression tag	UNP Q22799
D	0	PHE	-	expression tag	UNP Q22799
G	-5	GLY	-	expression tag	UNP Q22799
G	-4	PRO	-	expression tag	UNP Q22799
G	-3	GLY	-	expression tag	UNP Q22799
G	-2	SER	-	expression tag	UNP Q22799
G	-1	GLU	-	expression tag	UNP Q22799
G	0	PHE	-	expression tag	UNP Q22799
H	-5	GLY	-	expression tag	UNP Q22799
H	-4	PRO	-	expression tag	UNP Q22799
H	-3	GLY	-	expression tag	UNP Q22799
H	-2	SER	-	expression tag	UNP Q22799
H	-1	GLU	-	expression tag	UNP Q22799
H	0	PHE	-	expression tag	UNP Q22799
I	-5	GLY	-	expression tag	UNP Q22799
I	-4	PRO	-	expression tag	UNP Q22799
I	-3	GLY	-	expression tag	UNP Q22799
I	-2	SER	-	expression tag	UNP Q22799
I	-1	GLU	-	expression tag	UNP Q22799
I	0	PHE	-	expression tag	UNP Q22799
J	-5	GLY	-	expression tag	UNP Q22799
J	-4	PRO	-	expression tag	UNP Q22799
J	-3	GLY	-	expression tag	UNP Q22799
J	-2	SER	-	expression tag	UNP Q22799
J	-1	GLU	-	expression tag	UNP Q22799

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	PHE	-	expression tag	UNP Q22799
M	-5	GLY	-	expression tag	UNP Q22799
M	-4	PRO	-	expression tag	UNP Q22799
M	-3	GLY	-	expression tag	UNP Q22799
M	-2	SER	-	expression tag	UNP Q22799
M	-1	GLU	-	expression tag	UNP Q22799
M	0	PHE	-	expression tag	UNP Q22799
N	-5	GLY	-	expression tag	UNP Q22799
N	-4	PRO	-	expression tag	UNP Q22799
N	-3	GLY	-	expression tag	UNP Q22799
N	-2	SER	-	expression tag	UNP Q22799
N	-1	GLU	-	expression tag	UNP Q22799
N	0	PHE	-	expression tag	UNP Q22799
Q	-5	GLY	-	expression tag	UNP Q22799
Q	-4	PRO	-	expression tag	UNP Q22799
Q	-3	GLY	-	expression tag	UNP Q22799
Q	-2	SER	-	expression tag	UNP Q22799
Q	-1	GLU	-	expression tag	UNP Q22799
Q	0	PHE	-	expression tag	UNP Q22799
R	-5	GLY	-	expression tag	UNP Q22799
R	-4	PRO	-	expression tag	UNP Q22799
R	-3	GLY	-	expression tag	UNP Q22799
R	-2	SER	-	expression tag	UNP Q22799
R	-1	GLU	-	expression tag	UNP Q22799
R	0	PHE	-	expression tag	UNP Q22799

- Molecule 2 is a protein called Isoform b of Suppressor of aph-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	23	Total	C	N	O	S	0	0	0
			172	103	30	36	3			
2	F	24	Total	C	N	O	S	0	0	0
			179	108	31	37	3			
2	K	23	Total	C	N	O	S	0	0	0
			168	101	29	35	3			
2	L	24	Total	C	N	O	S	0	0	0
			179	108	31	37	3			
2	O	11	Total	C	N	O	S	0	0	0
			84	51	13	18	2			
2	P	12	Total	C	N	O	S	0	0	0
			83	52	13	16	2			
2	S	10	Total	C	N	O	S	0	0	0
			73	44	12	15	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	12	Total	C	N	O	S	0	0	0
			81	50	14	15	2			

There are 48 discrepancies between the modelled and reference sequences:

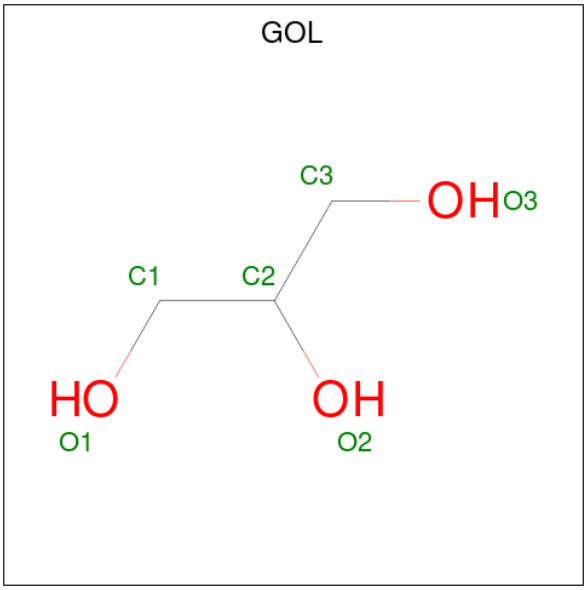
Chain	Residue	Modelled	Actual	Comment	Reference
E	176	GLY	-	expression tag	UNP C6KRN1
E	177	PRO	-	expression tag	UNP C6KRN1
E	178	GLY	-	expression tag	UNP C6KRN1
E	179	SER	-	expression tag	UNP C6KRN1
E	180	GLU	-	expression tag	UNP C6KRN1
E	181	PHE	-	expression tag	UNP C6KRN1
F	176	GLY	-	expression tag	UNP C6KRN1
F	177	PRO	-	expression tag	UNP C6KRN1
F	178	GLY	-	expression tag	UNP C6KRN1
F	179	SER	-	expression tag	UNP C6KRN1
F	180	GLU	-	expression tag	UNP C6KRN1
F	181	PHE	-	expression tag	UNP C6KRN1
K	176	GLY	-	expression tag	UNP C6KRN1
K	177	PRO	-	expression tag	UNP C6KRN1
K	178	GLY	-	expression tag	UNP C6KRN1
K	179	SER	-	expression tag	UNP C6KRN1
K	180	GLU	-	expression tag	UNP C6KRN1
K	181	PHE	-	expression tag	UNP C6KRN1
L	176	GLY	-	expression tag	UNP C6KRN1
L	177	PRO	-	expression tag	UNP C6KRN1
L	178	GLY	-	expression tag	UNP C6KRN1
L	179	SER	-	expression tag	UNP C6KRN1
L	180	GLU	-	expression tag	UNP C6KRN1
L	181	PHE	-	expression tag	UNP C6KRN1
O	176	GLY	-	expression tag	UNP C6KRN1
O	177	PRO	-	expression tag	UNP C6KRN1
O	178	GLY	-	expression tag	UNP C6KRN1
O	179	SER	-	expression tag	UNP C6KRN1
O	180	GLU	-	expression tag	UNP C6KRN1
O	181	PHE	-	expression tag	UNP C6KRN1
P	176	GLY	-	expression tag	UNP C6KRN1
P	177	PRO	-	expression tag	UNP C6KRN1
P	178	GLY	-	expression tag	UNP C6KRN1
P	179	SER	-	expression tag	UNP C6KRN1
P	180	GLU	-	expression tag	UNP C6KRN1
P	181	PHE	-	expression tag	UNP C6KRN1

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Chain	Residue	Modelled	Actual	Comment	Reference
S	176	GLY	-	expression tag	UNP C6KRN1
S	177	PRO	-	expression tag	UNP C6KRN1
S	178	GLY	-	expression tag	UNP C6KRN1
S	179	SER	-	expression tag	UNP C6KRN1
S	180	GLU	-	expression tag	UNP C6KRN1
S	181	PHE	-	expression tag	UNP C6KRN1
T	176	GLY	-	expression tag	UNP C6KRN1
T	177	PRO	-	expression tag	UNP C6KRN1
T	178	GLY	-	expression tag	UNP C6KRN1
T	179	SER	-	expression tag	UNP C6KRN1
T	180	GLU	-	expression tag	UNP C6KRN1
T	181	PHE	-	expression tag	UNP C6KRN1

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	1	Total O 1 1	0	0
4	C	2	Total O 2 2	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	7	Total O 7 7	0	0
4	H	3	Total O 3 3	0	0
4	K	2	Total O 2 2	0	0
4	L	2	Total O 2 2	0	0
4	N	1	Total O 1 1	0	0

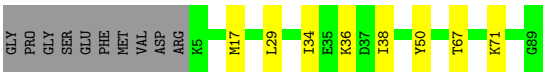
3 Residue-property plots (i)

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: Dynein light chain 1, cytoplasmic

Chain A:

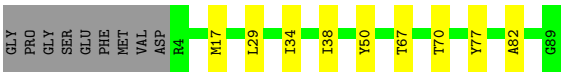




• Molecule 1: Dynein light chain 1, cytoplasmic

Chain B:

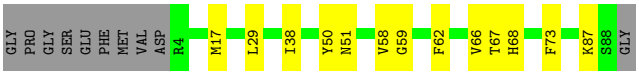




• Molecule 1: Dynein light chain 1, cytoplasmic

Chain C:





• Molecule 1: Dynein light chain 1, cytoplasmic

Chain D:

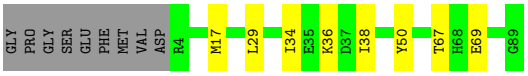




• Molecule 1: Dynein light chain 1, cytoplasmic

Chain G:

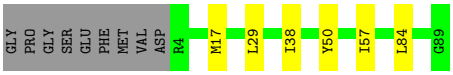




• Molecule 1: Dynein light chain 1, cytoplasmic

Chain H:





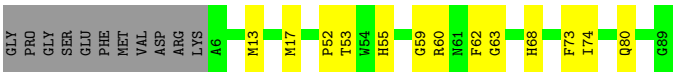
• Molecule 1: Dynein light chain 1, cytoplasmic

Chain I:



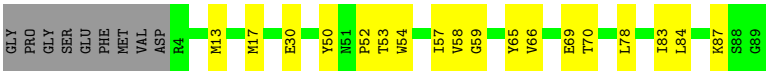
• Molecule 1: Dynein light chain 1, cytoplasmic

Chain J:



• Molecule 1: Dynein light chain 1, cytoplasmic

Chain M:



• Molecule 1: Dynein light chain 1, cytoplasmic

Chain N:



• Molecule 1: Dynein light chain 1, cytoplasmic

Chain Q:





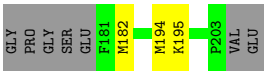
• Molecule 1: Dynein light chain 1, cytoplasmic

Chain R:



• Molecule 2: Isoform b of Suppressor of aph-1

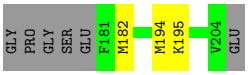
Chain E:



• Molecule 2: Isoform b of Suppressor of aph-1

Chain F:

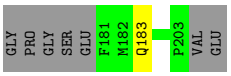




• Molecule 2: Isoform b of Suppressor of aph-1

Chain K:

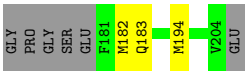




• Molecule 2: Isoform b of Suppressor of aph-1

Chain L:

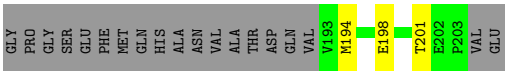




• Molecule 2: Isoform b of Suppressor of aph-1

Chain O:

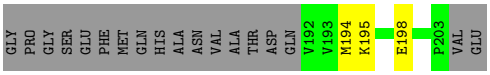




• Molecule 2: Isoform b of Suppressor of aph-1

Chain P:

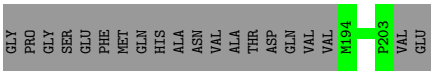




• Molecule 2: Isoform b of Suppressor of aph-1

Chain S:





• Molecule 2: Isoform b of Suppressor of aph-1

Chain T:




GLY
PRO
GLY
SER
GLU
PHE
MET
GLN
HIS
ALA
ASN
VAL
ALA
THR
ASP
GLN
V192
V193
M194
K195
P203
VAL
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	40.27Å 163.51Å 229.13Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.40) 84.8 (50.00-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.253 , 0.285 0.254 , 0.280	Depositor DCC
R_{free} test set	1982 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 29.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.440 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9324	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: GOL

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	0.28	0/706	0.68	0/950
1	B	0.29	0/707	0.70	0/953
1	C	0.28	0/706	0.70	0/952
1	D	0.27	0/689	0.72	0/931
1	G	0.29	0/711	0.69	0/957
1	H	0.28	0/707	0.70	0/953
1	I	0.26	0/702	0.70	0/946
1	J	0.28	0/689	0.74	0/931
1	M	0.30	0/711	0.76	0/957
1	N	0.27	0/717	0.75	0/969
1	Q	0.28	0/706	0.72	0/950
1	R	0.29	0/701	0.81	0/948
2	E	0.38	0/173	0.57	0/234
2	F	0.25	0/180	0.61	0/244
2	K	0.23	0/169	0.56	0/229
2	L	0.25	0/180	0.63	0/244
2	O	0.23	0/84	0.51	0/112
2	P	0.25	0/83	0.52	0/112
2	S	0.23	0/73	0.50	0/97
2	T	0.36	0/80	0.59	0/107
All	All	0.28	0/9474	0.71	0/12776

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 (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	690	0	667	4	0
1	B	691	0	658	6	0
1	C	690	0	666	9	0
1	D	673	0	632	9	0
1	G	695	0	669	5	0
1	H	691	0	658	3	0
1	I	686	0	656	9	0
1	J	673	0	632	12	0
1	M	695	0	669	13	0
1	N	701	0	668	7	0
1	Q	690	0	667	9	0
1	R	686	0	643	10	0
2	E	172	0	162	3	0
2	F	179	0	171	3	0
2	K	168	0	156	1	0
2	L	179	0	171	3	0
2	O	84	0	83	3	0
2	P	83	0	82	3	0
2	S	73	0	70	0	0
2	T	81	0	78	2	0
3	A	12	0	16	1	0
3	G	6	0	8	0	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	1	0
4	H	3	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	N	1	0	0	0	0
All	All	9324	0	8882	82	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 5.

The worst 5 of 82 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:N:13:MET:HE2	1:N:17:MET:HB3	1.59	0.85
1:R:13:MET:HE2	1:R:17:MET:HB3	1.59	0.84
1:D:13:MET:HE2	1:D:17:MET:HB3	1.64	0.77
1:J:13:MET:HE2	1:J:17:MET:HB3	1.68	0.75
1:Q:70:THR:HG22	2:T:195:LYS:HE3	1.71	0.73

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	83/95 (87%)	81 (98%)	2 (2%)	0	100	100
1	B	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
1	C	83/95 (87%)	81 (98%)	2 (2%)	0	100	100
1	D	82/95 (86%)	80 (98%)	2 (2%)	0	100	100
1	G	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
1	H	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
1	I	83/95 (87%)	81 (98%)	2 (2%)	0	100	100
1	J	82/95 (86%)	80 (98%)	2 (2%)	0	100	100
1	M	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
1	N	85/95 (90%)	83 (98%)	2 (2%)	0	100	100
1	Q	83/95 (87%)	81 (98%)	2 (2%)	0	100	100
1	R	85/95 (90%)	83 (98%)	2 (2%)	0	100	100
2	E	21/30 (70%)	21 (100%)	0	0	100	100
2	F	22/30 (73%)	22 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	21/30 (70%)	21 (100%)	0	0	100	100
2	L	22/30 (73%)	22 (100%)	0	0	100	100
2	O	9/30 (30%)	9 (100%)	0	0	100	100
2	P	10/30 (33%)	10 (100%)	0	0	100	100
2	S	8/30 (27%)	8 (100%)	0	0	100	100
2	T	10/30 (33%)	10 (100%)	0	0	100	100
All	All	1125/1380 (82%)	1101 (98%)	24 (2%)	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	72/81 (89%)	71 (99%)	1 (1%)	59	79
1	B	71/81 (88%)	71 (100%)	0	100	100
1	C	72/81 (89%)	72 (100%)	0	100	100
1	D	69/81 (85%)	69 (100%)	0	100	100
1	G	72/81 (89%)	72 (100%)	0	100	100
1	H	71/81 (88%)	71 (100%)	0	100	100
1	I	71/81 (88%)	71 (100%)	0	100	100
1	J	69/81 (85%)	69 (100%)	0	100	100
1	M	72/81 (89%)	72 (100%)	0	100	100
1	N	73/81 (90%)	73 (100%)	0	100	100
1	Q	72/81 (89%)	72 (100%)	0	100	100
1	R	70/81 (86%)	70 (100%)	0	100	100
2	E	20/26 (77%)	20 (100%)	0	100	100
2	F	21/26 (81%)	21 (100%)	0	100	100
2	K	19/26 (73%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	21/26 (81%)	21 (100%)	0	100	100
2	O	11/26 (42%)	11 (100%)	0	100	100
2	P	10/26 (38%)	10 (100%)	0	100	100
2	S	9/26 (35%)	9 (100%)	0	100	100
2	T	9/26 (35%)	9 (100%)	0	100	100
All	All	974/1180 (82%)	973 (100%)	1 (0%)	88	95

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

Mol	Chain	Res	Type
1	A	71	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	191	GLN
1	I	10	ASN
1	Q	19	GLN
1	M	61	ASN
1	N	19	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	GOL	G	101	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	A	102	-	5,5,5	0.42	0	5,5,5	0.37	0
3	GOL	A	101	-	5,5,5	0.38	0	5,5,5	0.33	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
3	GOL	G	101	-	-	2/4/4/4	-
3	GOL	A	102	-	-	2/4/4/4	-
3	GOL	A	101	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	102	GOL	O1-C1-C2-C3
3	G	101	GOL	C1-C2-C3-O3
3	A	102	GOL	O1-C1-C2-O2
3	G	101	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	101	GOL	1	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, 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	85/95 (89%)	-1.08	0 100 100	19, 36, 52, 56	0
1	B	86/95 (90%)	-1.03	0 100 100	23, 46, 68, 93	0
1	C	85/95 (89%)	-0.78	0 100 100	43, 69, 88, 100	0
1	D	84/95 (88%)	-0.53	0 100 100	53, 76, 98, 103	0
1	G	86/95 (90%)	-1.08	0 100 100	21, 36, 54, 69	0
1	H	86/95 (90%)	-0.98	0 100 100	23, 47, 71, 92	0
1	I	85/95 (89%)	-0.72	0 100 100	51, 69, 84, 102	0
1	J	84/95 (88%)	-0.49	0 100 100	49, 79, 99, 106	0
1	M	86/95 (90%)	-0.03	0 100 100	74, 87, 100, 112	0
1	N	87/95 (91%)	-0.06	0 100 100	74, 82, 98, 102	0
1	Q	85/95 (89%)	-0.04	1 (1%) 76 73	73, 85, 99, 106	0
1	R	87/95 (91%)	-0.29	0 100 100	59, 82, 96, 117	0
2	E	23/30 (76%)	-0.89	0 100 100	33, 63, 82, 86	0
2	F	24/30 (80%)	-0.90	0 100 100	32, 54, 84, 91	0
2	K	23/30 (76%)	-0.87	0 100 100	31, 59, 83, 86	0
2	L	24/30 (80%)	-0.96	0 100 100	30, 48, 80, 89	0
2	O	11/30 (36%)	-0.41	0 100 100	82, 84, 95, 102	0
2	P	12/30 (40%)	-0.45	0 100 100	57, 81, 87, 97	0
2	S	10/30 (33%)	-0.61	0 100 100	69, 77, 87, 87	0
2	T	12/30 (40%)	-0.52	0 100 100	58, 75, 79, 97	0
All	All	1165/1380 (84%)	-0.61	1 (0%) 92 90	19, 73, 96, 117	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	56	CYS	3.5

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 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, 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	B-factors(Å^2)	Q<0.9
3	GOL	A	101	6/6	0.97	0.08	60,63,64,64	0
3	GOL	A	102	6/6	0.97	0.07	73,73,74,74	0
3	GOL	G	101	6/6	0.97	0.08	63,68,70,72	0

6.5 Other polymers (i)

There are no such residues in this entry.