wwPDB X-ray Structure Validation Summary Report (i)

Apr 25, 2022 – 07:08 pm BST

PDB ID	:	2VE7
Title	:	Crystal structure of a bonsai version of the human Ndc80 complex
Authors	:	Ciferri, C.; Pasqualato, S.; Dos Reis, G.; Screpanti, E.; Maiolica, A.; Polka, J.; De Luca, J.G.; De Wulf, P.; Salek, M.; Rappsilber, J.; Moores, C.A.; Salmon, E.D.; Musacchio, A.
Deposited on	:	2007-10-17
Resolution	:	2.88 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 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	:	2.28
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

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 2.88 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.
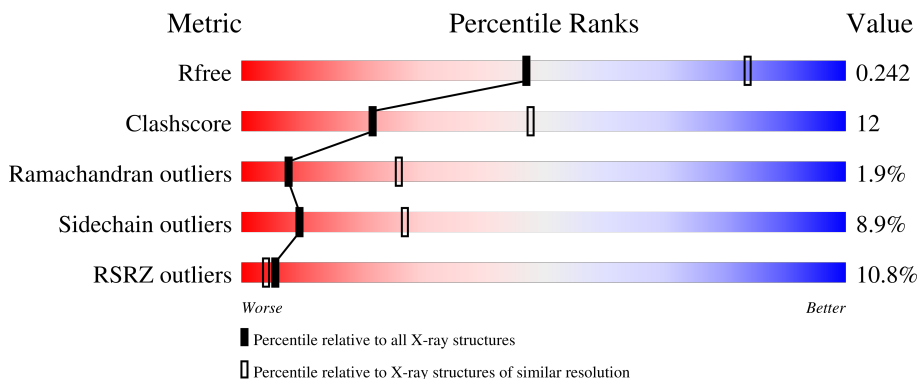
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	315	13% 61% 13% • 22%
1	B	315	7% 72% 19% • •
2	C	250	12% 61% 21% 6% 12%
2	D	250	6% 69% 23% • • •

2　Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8258 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 KINETOCHORE PROTEIN HEC1, KINETOCHORE PROTEIN SPC25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total 1980	C 1265	N 331	O 373	S 11	0	0	0
1	B	303	Total 2447	C 1566	N 406	O 462	S 13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	expression tag	UNP Q9HBM1
B	79	MET	-	expression tag	UNP Q9HBM1
A	1224	GLN	ASN	conflict	UNP Q9HBM1
B	1224	GLN	ASN	conflict	UNP Q9HBM1

- Molecule 2 is a protein called KINETOCHORE PROTEIN NUF2, KINETOCHORE PROTEIN SPC24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total 1800	C 1168	N 303	O 315	S 14	0	0	0
2	D	242	Total 1983	C 1279	N 333	O 357	S 14	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q8NBT2
C	-3	PRO	-	expression tag	UNP Q8NBT2
C	-2	LEU	-	expression tag	UNP Q8NBT2
C	-1	GLY	-	expression tag	UNP Q8NBT2
C	0	SER	-	expression tag	UNP Q8NBT2
D	-4	GLY	-	expression tag	UNP Q8NBT2

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	PRO	-	expression tag	UNP Q8NBT2
D	-2	LEU	-	expression tag	UNP Q8NBT2
D	-1	GLY	-	expression tag	UNP Q8NBT2
D	0	SER	-	expression tag	UNP Q8NBT2
C	1152	GLU	ASP	conflict	UNP Q8NBT2
D	1152	GLU	ASP	conflict	UNP Q8NBT2
C	72	GLY	GLU	engineered mutation	UNP Q9BZD4
D	72	GLY	GLU	engineered mutation	UNP Q9BZD4

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
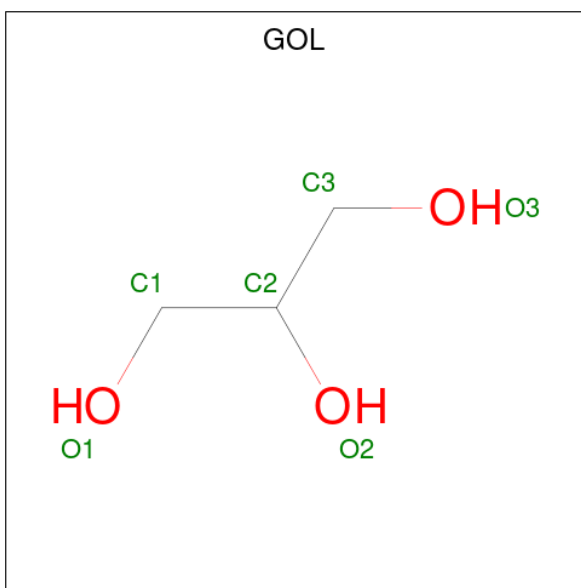
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is PHENOL (three-letter code: IPH) (formula: C_6H_6O).
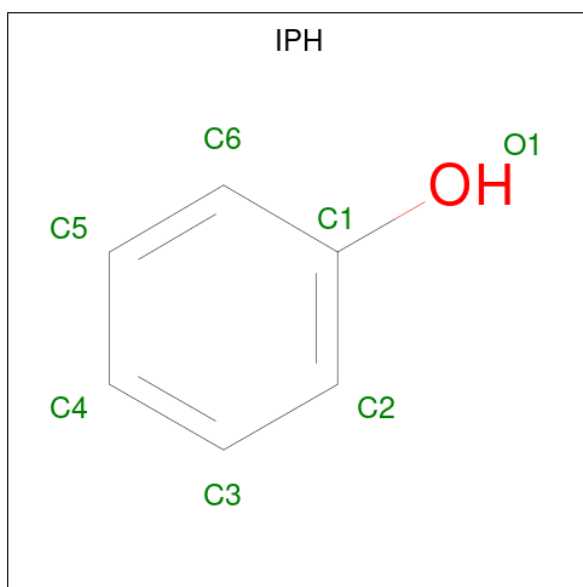
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 7	C 6	O 1	0	0
4	D	1	Total 7	C 6	O 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total 5	O 5	0	0
5	B	10	Total 10	O 10	0	0
5	C	3	Total 3	O 3	0	0
5	D	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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: KINETOCHORE PROTEIN HEC1, KINETOCHORE PROTEIN SPC25
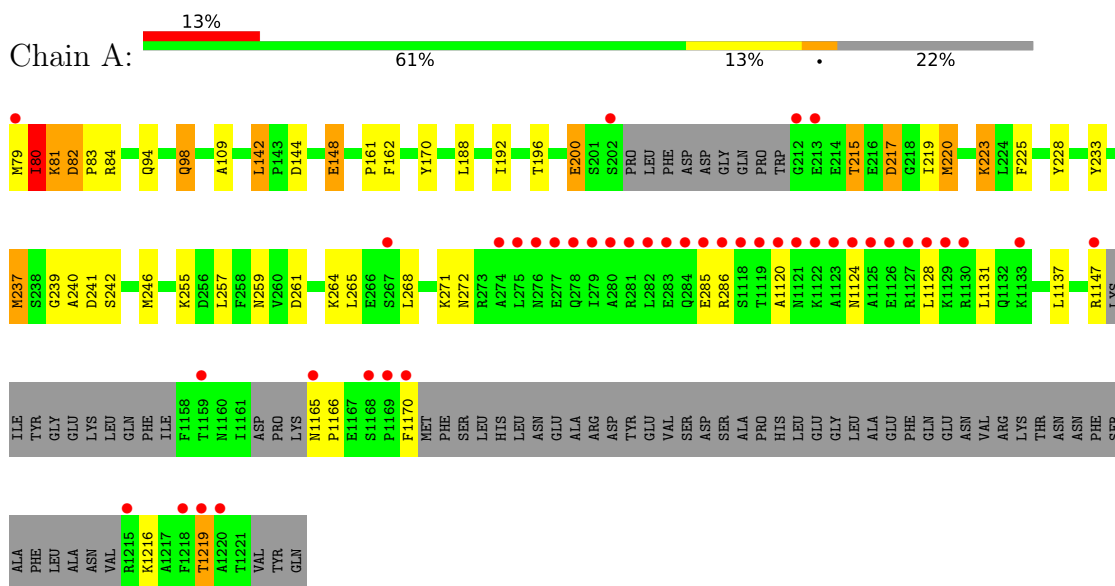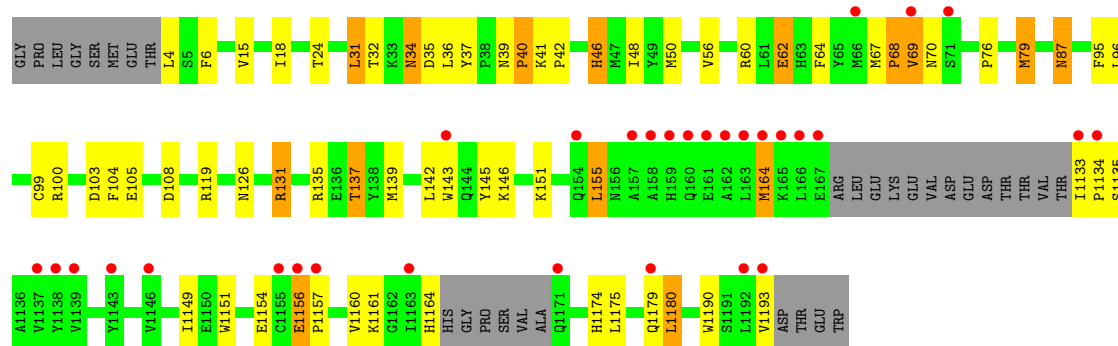

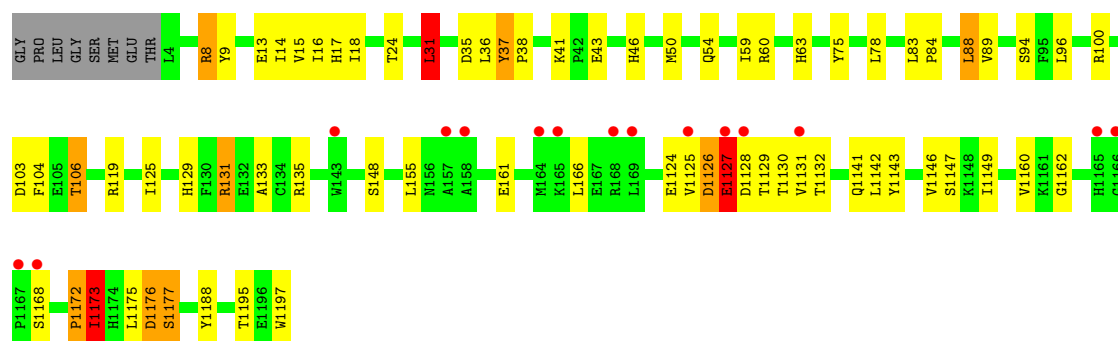• Molecule 1: KINETOCHORE PROTEIN HEC1, KINETOCHORE PROTEIN SPC25
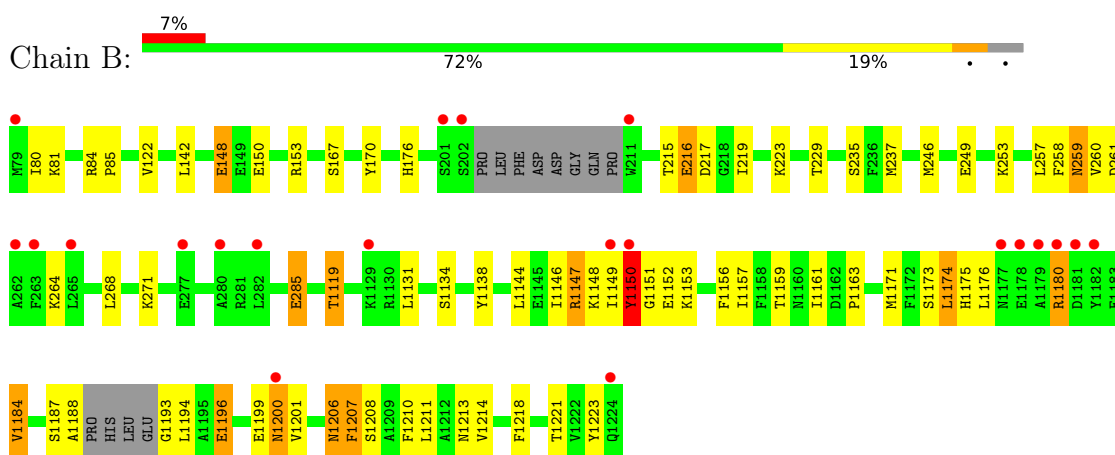
• Molecule 2: KINETOCHORE PROTEIN NUF2, KINETOCHORE PROTEIN SPC24

• Molecule 2: KINETOCHORE PROTEIN NUF2, KINETOCHORE PROTEIN SPC24

Chain D:

4 Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	157.65Å 248.97Å 58.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.88 30.53 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.88) 98.0 (30.53-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.261 0.245 , 0.242	Depositor DCC
R_{free} test set	2678 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8258	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: IPH, 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	0.77	3/2020 (0.1%)	0.78	4/2718 (0.1%)
1	B	0.67	3/2499 (0.1%)	0.68	0/3366
2	C	0.63	1/1848 (0.1%)	0.63	0/2500
2	D	0.67	3/2037 (0.1%)	0.68	1/2763 (0.0%)
All	All	0.69	10/8404 (0.1%)	0.70	5/11347 (0.0%)

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	2	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1199	GLU	CD-OE2	8.26	1.34	1.25
1	B	1199	GLU	CD-OE1	7.80	1.34	1.25
1	A	286	ARG	CZ-NH1	7.31	1.42	1.33
2	D	161	GLU	CD-OE2	6.59	1.32	1.25
1	A	1170	PHE	CG-CD1	6.40	1.48	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1147	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	A	1147	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	286	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	80	ILE	N-CA-C	-6.11	94.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	31	LEU	CA-CB-CG	5.23	127.32	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	82	ASP	CA
1	A	237	MET	CA

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	1980	0	1943	57	0
1	B	2447	0	2403	56	0
2	C	1800	0	1792	50	0
2	D	1983	0	1959	52	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	C	7	0	6	3	0
4	D	7	0	6	1	0
5	A	5	0	0	0	0
5	B	10	0	0	0	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	8258	0	8125	194	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 194 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:240:ALA:HB1	1:A:241:ASP:CA	1.49	1.42
1:A:240:ALA:CB	1:A:241:ASP:HA	1.44	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:HB2	1:A:83:PRO:CD	1.69	1.20
1:A:82:ASP:CB	1:A:83:PRO:HD2	1.87	1.04
2:D:35:ASP:HB2	2:D:41:LYS:HD2	1.40	1.03

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	236/315 (75%)	228 (97%)	7 (3%)	1 (0%)	34	64
1	B	297/315 (94%)	269 (91%)	21 (7%)	7 (2%)	6	20
2	C	213/250 (85%)	188 (88%)	21 (10%)	4 (2%)	8	26
2	D	240/250 (96%)	221 (92%)	12 (5%)	7 (3%)	4	16
All	All	986/1130 (87%)	906 (92%)	61 (6%)	19 (2%)	8	26

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1150	TYR
1	B	1223	TYR
1	B	259	ASN
1	B	1151	GLY
2	D	1176	ASP

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	215/279 (77%)	194 (90%)	21 (10%)	8	22
1	B	266/279 (95%)	243 (91%)	23 (9%)	10	29
2	C	199/226 (88%)	184 (92%)	15 (8%)	13	35
2	D	220/226 (97%)	199 (90%)	21 (10%)	8	24
All	All	900/1010 (89%)	820 (91%)	80 (9%)	9	27

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	164	MET
2	D	131	ARG
2	D	8	ARG
2	D	43	GLU
2	D	1141	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1174	HIS
2	D	129	HIS
2	D	63	HIS
2	D	144	GLN
1	B	1206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	A	2222	-	5,5,5	0.27	0	5,5,5	0.37	0
3	GOL	B	2225	-	5,5,5	0.28	0	5,5,5	0.43	0
4	IPH	C	2194	-	7,7,7	0.49	0	8,8,8	0.37	0
4	IPH	D	2198	-	7,7,7	0.57	0	8,8,8	0.68	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	A	2222	-	-	1/4/4/4	-
3	GOL	B	2225	-	-	<mark>3/4/4/4</mark>	-
4	IPH	C	2194	-	-	-	0/1/1/1
4	IPH	D	2198	-	-	-	0/1/1/1

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	B	2225	GOL	O1-C1-C2-O2
3	B	2225	GOL	O1-C1-C2-C3
3	A	2222	GOL	O1-C1-C2-C3
3	B	2225	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2194	IPH	3	0
4	D	2198	IPH	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	246/315 (78%)	0.65	42 (17%)	1	1	10, 52, 153, 176	0
1	B	303/315 (96%)	0.34	21 (6%)	16	13	12, 56, 131, 162	0
2	C	219/250 (87%)	0.62	31 (14%)	2	2	19, 48, 164, 233	0
2	D	242/250 (96%)	0.33	15 (6%)	20	16	17, 50, 125, 155	0
All	All	1010/1130 (89%)	0.47	109 (10%)	5	4	10, 52, 143, 233	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1125	ALA	7.8
1	A	1128	LEU	7.6
2	C	1155	CYS	7.2
1	A	1129	LYS	6.9
1	A	1126	GLU	6.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	GOL	A	2222	6/6	0.88	0.27	63,66,66,67	0
3	GOL	B	2225	6/6	0.88	0.28	68,70,70,71	0
4	IPH	D	2198	7/7	0.93	0.26	54,56,57,57	0
4	IPH	C	2194	7/7	0.94	0.22	44,45,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.