



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:16 AM GMT

PDB ID : 2CFG
Title : AGAO IN COMPLEX WITH WC4D3 (RU-WIRE INHIBITOR, 4-CARBON LINKER, DELTA ENANTIOMER, DATA SET 3)
Authors : Langley, D.B.; Duff, A.P.; Freeman, H.C.; Guss, J.M.; Juda, G.A.; Dooley, D.M.; Contakes, S.M.; Halpern-Manners, N.W.; Dunn, A.R.; Gray, H.B.
Deposited on : 2006-02-21
Resolution : 1.55 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
<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

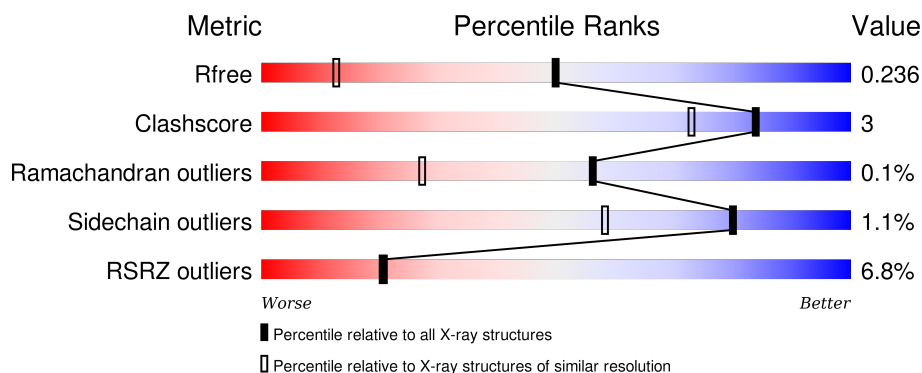
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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	646	<div> <div>8%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	B	646	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>.</div> </div>

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
2	CU	A	1628	-	-	-	X
2	CU	B	1630	-	-	-	X
3	NA	A	1629	-	-	-	X
4	R4A	A	1630	X	-	-	X
4	R4A	B	1632	X	-	-	X
5	GOL	A	1631	-	-	-	X
5	GOL	A	1632	-	-	-	X
5	GOL	A	1634	-	-	-	X
5	GOL	B	1629	-	-	-	X
5	GOL	B	1634	-	-	-	X
5	GOL	B	1635	-	-	-	X
5	GOL	B	1636	-	-	-	X
5	GOL	B	1637	-	-	-	X
5	GOL	B	1638	-	-	-	X
5	GOL	B	1639	-	-	-	X
6	SO4	B	1633	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19843 atoms, of which 9102 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 PHENYLETHYLAMINE OXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	619	Total	C	H	N	O	S	0	4	0
			9355	3080	4480	853	931	11			
1	B	619	Total	C	H	N	O	S	0	5	0
			9362	3082	4485	853	931	11			

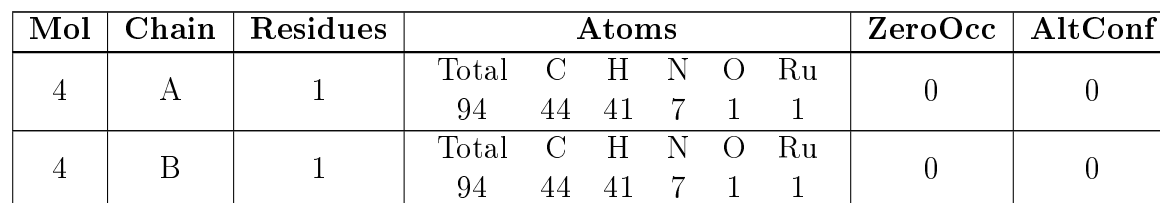
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is BIS[1H,1'H-2,2'-BIPYRIDINATO(2-)-KAPPA 2 N 1 ,N 1']{3-[4-(1,10-DIHYDRO-1,10-PHENANTHROLIN-4-YL-KAPPA 2 N 1 ,N 10)BUTOXY]-N,N-DIMETHYLANILINATO(2-)}RUTHENIUM (three-letter code: R4A) (formula: C₄₄H₆₁N₇ORu).



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- A skeletal structure of 1,2,3-propanetriol (glycerol) is shown. The carbon atoms are labeled C1, C2, and C3 in green. The hydroxyl groups are shown as HO (red) and OH (red). The labels O1, O2, and O3 are in green below the respective oxygen atoms. The structure is drawn with gray lines for the carbon backbone and red lines for the C-O bonds.

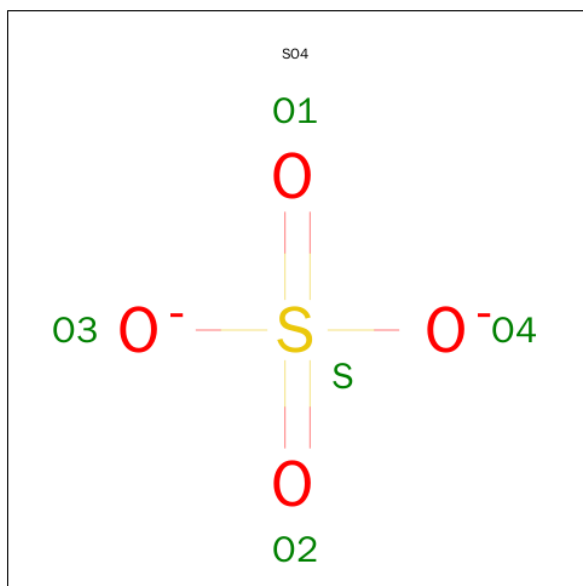
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 11	C 3	H 5	O 3	0	0
5	A	1	Total 11	C 3	H 5	O 3	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			11	3	5	3		
5	A	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	365	Total 365	O 365	0	0
7	B	438	Total 438	O 438	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.37Å 62.95Å 158.13Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	30.01 – 1.55 30.01 – 1.55	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.01-1.55) 92.5 (30.01-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.224 0.220 , 0.236	Depositor DCC
R_{free} test set	11299 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 225428 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19843	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 93.62 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8182e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, R4A, NA, SO4, TPQ, CU

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	0.50	0/4998	0.79	6/6804 (0.1%)
1	B	0.57	0/5006	0.83	8/6815 (0.1%)
All	All	0.54	0/10004	0.81	14/13619 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	540	ASP	CB-CG-OD2	6.58	124.23	118.30
1	A	246	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	298	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	66	ASP	CB-CG-OD2	5.51	123.26	118.30

There are no chirality outliers.

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	4875	4480	4692	19	0
1	B	4877	4485	4693	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	41	47	7	0
4	B	53	41	50	19	0
5	A	24	20	32	1	0
5	B	42	35	56	1	0
6	B	10	0	0	1	0
7	A	365	0	0	1	0
7	B	438	0	0	2	0
All	All	10741	9102	9570	58	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.

The worst 5 of 58 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:105:PHE:CZ	4:B:1632:R4A:HL12	1.38	1.58
1:B:105:PHE:CE2	4:B:1632:R4A:CAL	2.20	1.24
1:B:105:PHE:CZ	4:B:1632:R4A:CL1	2.21	1.22
1:B:105:PHE:CE2	4:B:1632:R4A:CL1	2.33	1.09
1:B:105:PHE:CE2	4:B:1632:R4A:HL12	1.87	1.06

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	620/646 (96%)	598 (96%)	21 (3%)	1 (0%)	52 25
1	B	621/646 (96%)	597 (96%)	24 (4%)	0	100 100
All	All	1241/1292 (96%)	1195 (96%)	45 (4%)	1 (0%)	56 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER

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	516/537 (96%)	512 (99%)	4 (1%)	86	71
1	B	517/537 (96%)	510 (99%)	7 (1%)	74	48
All	All	1033/1074 (96%)	1022 (99%)	11 (1%)	80	58

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	B	146	GLU
1	B	336	ARG
1	A	444	ASP
1	B	263	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	B	306	GLN
1	B	421	GLN
1	B	507	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	TPQ	A	382	1	13,14,15	1.36	2 (15%)	15,19,21	1.72	4 (26%)
1	TPQ	B	382	1	13,14,15	1.32	2 (15%)	15,19,21	1.63	3 (20%)

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	TPQ	A	382	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	382	1	-	0/4/22/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	TPQ	O4-C4	-2.78	1.26	1.34
1	B	382	TPQ	O4-C4	-2.73	1.27	1.34
1	B	382	TPQ	C3-C4	2.54	1.39	1.35
1	A	382	TPQ	C3-C4	2.89	1.40	1.35

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	TPQ	C1-C6-C5	-4.08	120.48	122.97
1	A	382	TPQ	C1-C6-C5	-3.93	120.57	122.97
1	B	382	TPQ	O-C-CA	-2.73	118.37	125.49
1	A	382	TPQ	O2-C2-C1	-2.24	118.90	120.85
1	A	382	TPQ	C3-C2-C1	2.08	119.86	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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$
4	R4A	A	1630	-	53,63,63	4.16	23 (43%)	48,101,101	3.42	25 (52%)
5	GOL	A	1631	-	5,5,5	0.36	0	5,5,5	0.23	0
5	GOL	A	1632	-	5,5,5	0.30	0	5,5,5	0.31	0
5	GOL	A	1633	-	5,5,5	0.36	0	5,5,5	0.29	0
5	GOL	A	1634	-	5,5,5	0.29	0	5,5,5	0.78	0
6	SO4	B	1628	-	4,4,4	0.24	0	6,6,6	0.55	0
5	GOL	B	1629	-	5,5,5	0.29	0	5,5,5	0.20	0
4	R4A	B	1632	-	53,63,63	4.17	24 (45%)	48,101,101	3.43	24 (50%)
6	SO4	B	1633	-	4,4,4	0.25	0	6,6,6	0.45	0
5	GOL	B	1634	-	5,5,5	0.22	0	5,5,5	0.43	0
5	GOL	B	1635	-	5,5,5	0.34	0	5,5,5	0.21	0
5	GOL	B	1636	-	5,5,5	0.27	0	5,5,5	0.46	0
5	GOL	B	1637	-	5,5,5	0.29	0	5,5,5	0.34	0
5	GOL	B	1638	-	5,5,5	0.32	0	5,5,5	0.17	0
5	GOL	B	1639	-	5,5,5	0.24	0	5,5,5	0.64	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
4	R4A	A	1630	-	5/5/19/19	0/12/150/150	0/10/11/11
5	GOL	A	1631	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1632	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1633	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1634	-	-	0/4/4/4	0/0/0/0
6	SO4	B	1628	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1629	-	-	0/4/4/4	0/0/0/0
4	R4A	B	1632	-	5/5/19/19	0/12/150/150	0/10/11/11
6	SO4	B	1633	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1634	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1635	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1636	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1637	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1638	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1639	-	-	0/4/4/4	0/0/0/0

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1630	R4A	CBB-NBA	-13.58	1.27	1.49
4	B	1632	R4A	CBB-NBA	-13.51	1.28	1.49
4	A	1630	R4A	CCB-NCA	-13.39	1.28	1.49
4	B	1632	R4A	CCB-NCA	-13.22	1.28	1.49
4	B	1632	R4A	CBK-NBL	-9.56	1.34	1.49

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1632	R4A	CNF-CNE-NNG	-3.03	117.03	121.22
4	A	1630	R4A	CAC-CAH-CAI	-2.81	118.57	123.91
4	B	1632	R4A	CAC-CAH-CAI	-2.75	118.68	123.91
4	A	1630	R4A	CNF-CNE-NNG	-2.71	117.47	121.22
4	B	1632	R4A	CL1-CAL-CAM	-2.17	117.15	123.84

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1632	R4A	CAK
4	B	1632	R4A	CBG
4	B	1632	R4A	CCF
4	B	1632	R4A	CBF
4	B	1632	R4A	CCG

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1630	R4A	7	0
5	A	1634	GOL	1	0
4	B	1632	R4A	19	0
6	B	1633	SO4	1	0
5	B	1639	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 [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	618/646 (95%)	0.41	49 (7%) 15 15	18, 27, 40, 60	1 (0%)
1	B	618/646 (95%)	0.23	35 (5%) 27 28	16, 24, 35, 58	1 (0%)
All	All	1236/1292 (95%)	0.32	84 (6%) 20 21	16, 25, 38, 60	2 (0%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	GLY	11.9
1	A	53	SER	10.8
1	B	53	SER	10.4
1	A	51	ALA	9.3
1	A	9	ALA	8.8

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. 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
1	TPQ	A	382	14/15	0.94	0.11	-	22,28,35,39	0
1	TPQ	B	382	14/15	0.94	0.12	-	19,26,33,38	0

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	GOL	B	1638	6/6	0.65	0.21	13.50	53,54,55,56	0
5	GOL	A	1632	6/6	0.73	0.23	10.57	66,66,67,67	0
2	CU	A	1628	1/1	1.00	0.16	9.00	32,32,32,32	0
5	GOL	B	1636	6/6	0.74	0.21	7.91	62,63,63,64	0
5	GOL	B	1629	6/6	0.73	0.20	7.82	54,55,55,57	0
5	GOL	B	1639	6/6	0.79	0.20	6.42	46,51,52,54	0
5	GOL	B	1635	6/6	0.73	0.14	4.11	42,46,47,49	0
5	GOL	A	1634	6/6	0.79	0.18	3.53	43,51,52,54	0
5	GOL	B	1634	6/6	0.78	0.16	3.04	33,33,34,35	0
5	GOL	A	1631	6/6	0.71	0.13	2.67	43,49,51,52	0
4	R4A	A	1630	53/53	0.87	0.25	2.62	46,52,53,53	71
3	NA	A	1629	1/1	0.98	0.25	2.42	34,34,34,34	0
2	CU	B	1630	1/1	0.99	0.14	2.39	30,30,30,30	0
5	GOL	B	1637	6/6	0.67	0.23	2.31	56,59,59,60	0
6	SO4	B	1633	5/5	0.93	0.13	2.15	56,56,57,58	0
4	R4A	B	1632	53/53	0.90	0.21	2.14	37,41,43,43	71
5	GOL	A	1633	6/6	0.73	0.20	1.91	59,60,61,61	0
3	NA	B	1631	1/1	0.99	0.17	1.06	30,30,30,30	0
6	SO4	B	1628	5/5	0.96	0.09	0.44	50,50,53,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.