



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 09:51 AM EDT

PDB ID : 3KII
Title : AGAO 5-phenoxy-2,3-pentadienylamine complex
Authors : Nguyen, Y.H.; Ernberg, K.E.; Guss, J.M.
Deposited on : 2009-11-02
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

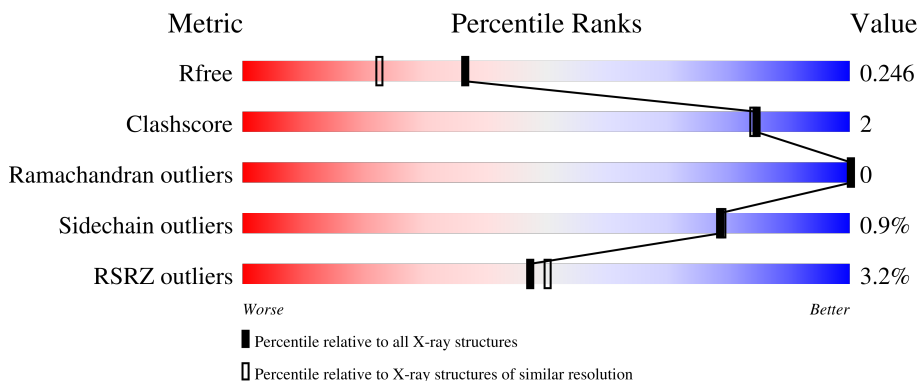
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	646	 4% 90% 5% .
1	B	646	 2% 91% . .

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 10715 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	618	4857	3077	853	918	9	0	5	0
1	B	617	4891	3096	858	927	10	0	6	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	SER	-	SEE REMARK 999	UNP P46881
A	640	ASN	-	SEE REMARK 999	UNP P46881
A	641	TRP	-	SEE REMARK 999	UNP P46881
A	642	SER	-	SEE REMARK 999	UNP P46881
A	643	HIS	-	SEE REMARK 999	UNP P46881
A	644	PRO	-	SEE REMARK 999	UNP P46881
A	645	GLN	-	SEE REMARK 999	UNP P46881
A	646	PHE	-	SEE REMARK 999	UNP P46881
A	647	GLU	-	SEE REMARK 999	UNP P46881
A	648	LYS	-	SEE REMARK 999	UNP P46881
B	639	SER	-	SEE REMARK 999	UNP P46881
B	640	ASN	-	SEE REMARK 999	UNP P46881
B	641	TRP	-	SEE REMARK 999	UNP P46881
B	642	SER	-	SEE REMARK 999	UNP P46881
B	643	HIS	-	SEE REMARK 999	UNP P46881
B	644	PRO	-	SEE REMARK 999	UNP P46881
B	645	GLN	-	SEE REMARK 999	UNP P46881
B	646	PHE	-	SEE REMARK 999	UNP P46881
B	647	GLU	-	SEE REMARK 999	UNP P46881
B	648	LYS	-	SEE REMARK 999	UNP P46881

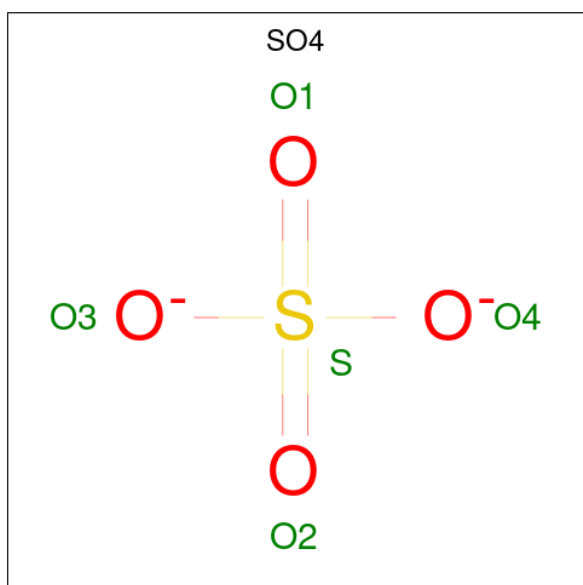
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

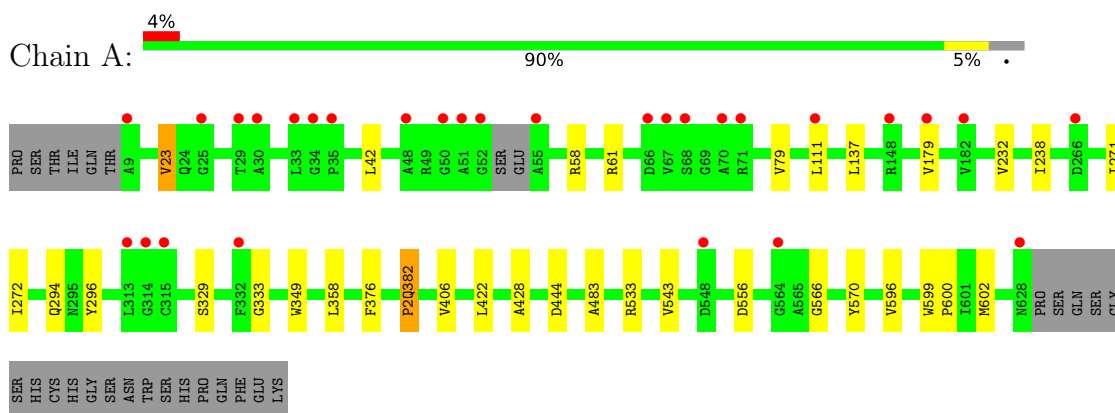
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	385	Total O 385 385	0	0
6	B	498	Total O 498 498	0	0

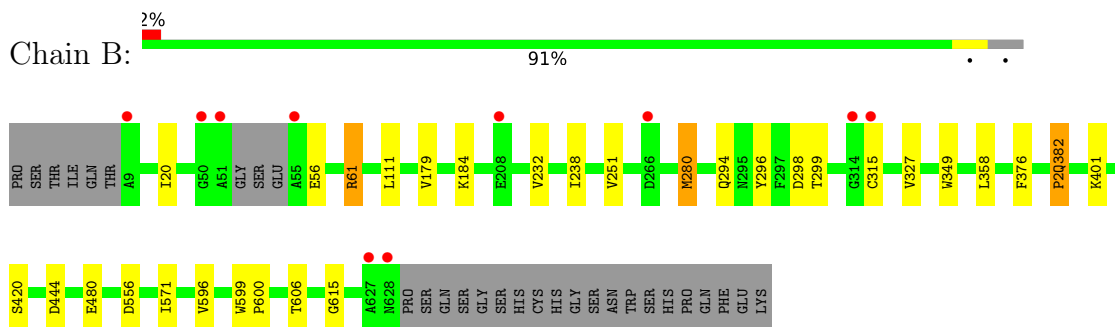
3 Residue-property plots [i](#)

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: Phenylethylamine oxidase



- Molecule 1: Phenylethylamine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.71Å 62.98Å 158.15Å 90.00° 117.39° 90.00°	Depositor
Resolution (Å)	12.99 – 1.90 12.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (12.99-1.90) 99.1 (12.99-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.90Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.218 0.208 , 0.246	Depositor DCC
R_{free} test set	6538 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtrriage
Anisotropy	0.876	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10715	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.65 % 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 2.0525e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, CU, P2Q, GOL, NA

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	0.49	0/4955	0.72	1/6747 (0.0%)
1	B	0.56	0/4993	0.76	1/6797 (0.0%)
All	All	0.53	0/9948	0.75	2/13544 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	533	ARG	NE-CZ-NH1	5.43	123.02	120.30

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	4857	0	4660	27	0
1	B	4891	0	4712	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	0	0	0
5	A	24	0	32	1	0
5	B	36	0	48	1	0
6	A	385	0	0	0	0
6	B	498	0	0	2	0
All	All	10715	0	9452	44	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 (44) 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:296:TYR:HB3	1:A:382:P2Q:H5	1.67	0.77
1:B:61:ARG:HH22	1:B:556:ASP:CG	1.97	0.66
1:B:296:TYR:CD1	1:B:382:P2Q:H1	2.31	0.65
1:A:23:VAL:HG21	1:A:42:LEU:HD11	1.80	0.64
1:A:296:TYR:CD1	1:A:382:P2Q:H1	2.32	0.64
1:A:137:LEU:HD22	1:A:296:TYR:CZ	2.35	0.62
1:B:56:GLU:OE2	6:B:744:HOH:O	2.16	0.60
1:A:294:GLN:HG3	1:A:296:TYR:CZ	2.38	0.58
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.85	0.58
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.39	0.58
1:A:596[B]:VAL:HG12	1:B:615:GLY:HA2	1.86	0.57
1:A:137:LEU:HD22	1:A:296:TYR:OH	2.04	0.57
1:A:296:TYR:CB	1:A:382:P2Q:H5	2.36	0.55
1:A:232:VAL:HG22	1:A:238:ILE:HD12	1.89	0.55
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.43	0.53
1:A:111:LEU:CD1	1:A:179:VAL:HG11	2.42	0.50
1:A:382:P2Q:H9	1:B:358:LEU:HD23	1.94	0.50
1:A:349:TRP:CH2	5:A:653:GOL:H31	2.48	0.49
1:A:111:LEU:HD13	1:A:179:VAL:CG1	2.43	0.49
1:A:483:ALA:HB1	1:A:543:VAL:HB	1.96	0.48
1:B:596:VAL:HG23	6:B:897:HOH:O	2.13	0.48
1:B:20:ILE:HD12	1:B:327:VAL:HG12	1.95	0.48
1:B:232:VAL:HG22	1:B:238:ILE:HD12	1.96	0.48
1:B:280[B]:MET:HG2	1:B:299:THR:OG1	2.14	0.47
1:A:566:GLY:HA2	1:A:570:TYR:CZ	2.50	0.47
1:B:349:TRP:CZ2	5:B:657:GOL:H2	2.51	0.45
1:A:296:TYR:CG	1:A:382:P2Q:H5	2.52	0.45
1:A:382:P2Q:OC5	1:A:382:P2Q:C3	2.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD12	1:A:179:VAL:HG11	2.00	0.44
1:B:111:LEU:HD21	1:B:184:LYS:HB3	1.98	0.44
1:A:271:ILE:HG22	1:A:272:ILE:HG13	2.00	0.44
1:B:401:LYS:HG2	1:B:606:THR:HG22	2.00	0.44
1:A:61:ARG:HH22	1:A:556:ASP:CG	2.21	0.43
1:B:294:GLN:NE2	1:B:296:TYR:OH	2.44	0.43
1:A:329:SER:OG	1:A:333:GLY:HA2	2.20	0.42
1:A:406:VAL:HG13	1:A:602:MET:HE2	2.02	0.42
1:B:61:ARG:NH2	1:B:556:ASP:OD2	2.48	0.41
1:B:280[B]:MET:HE1	1:B:298:ASP:OD1	2.20	0.41
1:B:111:LEU:HD12	1:B:179:VAL:HG11	2.02	0.41
1:A:58:ARG:HB2	1:A:79:VAL:HG12	2.01	0.41
1:A:58:ARG:O	1:A:79:VAL:HG12	2.20	0.41
1:B:480:GLU:HB3	1:B:571:ILE:HD13	2.02	0.40
1:A:358:LEU:HD23	1:B:382:P2Q:H9	2.03	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	618/646 (96%)	595 (96%)	23 (4%)	0	100	100
1	B	618/646 (96%)	597 (97%)	21 (3%)	0	100	100
All	All	1236/1292 (96%)	1192 (96%)	44 (4%)	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	503/537 (94%)	500 (99%)	3 (1%)	86	87
1	B	513/537 (96%)	506 (99%)	7 (1%)	67	65
All	All	1016/1074 (95%)	1006 (99%)	10 (1%)	78	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	376	PHE
1	A	444	ASP
1	B	251	VAL
1	B	280[A]	MET
1	B	280[B]	MET
1	B	315	CYS
1	B	376	PHE
1	B	420	SER
1	B	444	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	HIS
1	B	294	GLN
1	B	421	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](#)

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	P2Q	A	382	1	26,28,29	1.03	1 (3%)	26,36,38	1.57	4 (15%)
1	P2Q	B	382	1	26,28,29	1.08	3 (11%)	26,36,38	1.75	4 (15%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	P2Q	A	382	1	-	7/16/19/21	0/2/2/2
1	P2Q	B	382	1	-	8/16/19/21	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	P2Q	C4-C3	-2.70	1.37	1.49
1	A	382	P2Q	C4-C3	-2.40	1.39	1.49
1	B	382	P2Q	CB-CG	-2.24	1.48	1.51
1	B	382	P2Q	C2-C3	2.06	1.40	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	P2Q	CD1-CE1-NAS	-4.95	114.40	121.81
1	B	382	P2Q	CB-CA-C	-4.85	102.38	111.47
1	B	382	P2Q	CD1-CE1-NAS	-4.73	114.73	121.81
1	A	382	P2Q	CB-CA-C	-3.01	105.83	111.47
1	B	382	P2Q	CG-CB-CA	2.71	118.71	114.53
1	B	382	P2Q	CD1-CG-CD2	2.69	121.41	118.17
1	A	382	P2Q	CD1-CG-CD2	2.30	120.93	118.17
1	A	382	P2Q	CG-CB-CA	2.11	117.80	114.53

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382	P2Q	C5-C1-C2-C3
1	A	382	P2Q	NAS-C1-C2-C3
1	A	382	P2Q	C2-C1-NAS-CE1
1	A	382	P2Q	CZ-CE1-NAS-C1
1	B	382	P2Q	C5-C1-C2-C3
1	B	382	P2Q	NAS-C1-C2-C3
1	B	382	P2Q	C2-C1-NAS-CE1
1	B	382	P2Q	CZ-CE1-NAS-C1
1	B	382	P2Q	CD1-CE1-NAS-C1
1	A	382	P2Q	CD1-CE1-NAS-C1
1	A	382	P2Q	N-CA-CB-CG
1	B	382	P2Q	C11-C6-OAT-C4
1	B	382	P2Q	C7-C6-OAT-C4
1	A	382	P2Q	C5-C1-NAS-CE1
1	B	382	P2Q	C5-C1-NAS-CE1

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382	P2Q	6	0
1	B	382	P2Q	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	SO4	B	650	-	4,4,4	0.18	0	6,6,6	0.30	0
5	GOL	B	656	-	5,5,5	0.44	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	652	-	5,5,5	0.33	0	5,5,5	0.47	0
5	GOL	A	650	-	5,5,5	0.47	0	5,5,5	0.73	0
5	GOL	A	651	-	5,5,5	0.37	0	5,5,5	0.46	0
5	GOL	A	653	-	5,5,5	0.49	0	5,5,5	0.59	0
5	GOL	B	657	-	5,5,5	0.43	0	5,5,5	0.83	0
4	SO4	B	649	-	4,4,4	0.12	0	6,6,6	0.33	0
5	GOL	A	652	-	5,5,5	0.51	0	5,5,5	0.16	0
4	SO4	B	651	-	4,4,4	0.14	0	6,6,6	0.16	0
5	GOL	B	655	-	5,5,5	0.21	0	5,5,5	0.56	0
4	SO4	A	649	-	4,4,4	0.16	0	6,6,6	0.19	0
5	GOL	B	653	-	5,5,5	0.43	0	5,5,5	0.31	0
5	GOL	B	654	-	5,5,5	0.36	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
5	GOL	B	656	-	-	0/4/4/4	-
5	GOL	B	652	-	-	2/4/4/4	-
5	GOL	A	650	-	-	2/4/4/4	-
5	GOL	A	651	-	-	2/4/4/4	-
5	GOL	A	653	-	-	2/4/4/4	-
5	GOL	B	657	-	-	0/4/4/4	-
5	GOL	A	652	-	-	2/4/4/4	-
5	GOL	B	655	-	-	0/4/4/4	-
5	GOL	B	653	-	-	4/4/4/4	-
5	GOL	B	654	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	650	GOL	C1-C2-C3-O3
5	A	652	GOL	C1-C2-C3-O3
5	A	653	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	652	GOL	O1-C1-C2-C3
5	B	653	GOL	O1-C1-C2-C3
5	B	653	GOL	C1-C2-C3-O3
5	B	654	GOL	C1-C2-C3-O3
5	A	650	GOL	O2-C2-C3-O3
5	A	653	GOL	O2-C2-C3-O3
5	B	652	GOL	O1-C1-C2-O2
5	B	653	GOL	O2-C2-C3-O3
5	A	652	GOL	O2-C2-C3-O3
5	B	653	GOL	O1-C1-C2-O2
5	A	651	GOL	C1-C2-C3-O3
5	A	651	GOL	O2-C2-C3-O3
5	B	654	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	653	GOL	1	0
5	B	657	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, 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	617/646 (95%)	0.17	29 (4%) 31 34	22, 38, 63, 84	0
1	B	616/646 (95%)	-0.22	10 (1%) 72 74	19, 32, 49, 69	0
All	All	1233/1292 (95%)	-0.02	39 (3%) 47 50	19, 34, 59, 84	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	6.3
1	B	51	ALA	5.7
1	A	55	ALA	5.4
1	A	52	GLY	5.4
1	A	68	SER	5.3
1	A	51	ALA	4.7
1	A	266	ASP	4.3
1	A	35	PRO	4.2
1	A	315	CYS	4.1
1	B	55	ALA	4.1
1	A	313	LEU	3.8
1	B	628	ASN	3.8
1	B	266	ASP	3.6
1	A	182	VAL	3.4
1	A	67	VAL	3.4
1	B	50	GLY	3.4
1	A	50	GLY	3.4
1	B	314	GLY	3.4
1	B	9	ALA	3.2
1	A	564	GLY	3.0
1	A	34	GLY	3.0
1	A	314	GLY	2.8
1	A	30	ALA	2.7
1	A	628	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	66	ASP	2.6
1	A	25	GLY	2.5
1	B	315	CYS	2.4
1	A	70	ALA	2.4
1	A	71	ARG	2.4
1	A	111	LEU	2.4
1	A	548	ASP	2.4
1	A	29	THR	2.4
1	A	33	LEU	2.3
1	B	208	GLU	2.3
1	A	332	PHE	2.2
1	A	48	ALA	2.1
1	B	627	ALA	2.1
1	A	148	ARG	2.1
1	A	179	VAL	2.1

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
1	P2Q	A	382	27/28	0.88	0.15	28,51,78,79	0
1	P2Q	B	382	27/28	0.91	0.14	24,47,67,69	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
5	GOL	B	652	6/6	0.73	0.23	47,58,60,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	655	6/6	0.74	0.22	50,53,58,63	0
5	GOL	A	651	6/6	0.79	0.14	50,60,62,63	0
4	SO4	A	649	5/5	0.80	0.29	102,106,108,108	0
5	GOL	A	653	6/6	0.83	0.23	53,60,62,63	0
4	SO4	B	649	5/5	0.85	0.19	82,85,91,93	0
4	SO4	B	651	5/5	0.85	0.26	92,95,98,99	0
5	GOL	A	652	6/6	0.86	0.19	47,50,55,61	0
5	GOL	A	650	6/6	0.90	0.15	47,49,50,50	0
4	SO4	B	650	5/5	0.90	0.18	86,88,93,96	0
5	GOL	B	657	6/6	0.92	0.18	36,46,55,56	0
5	GOL	B	653	6/6	0.93	0.20	46,67,69,70	0
5	GOL	B	656	6/6	0.94	0.14	51,54,57,58	0
5	GOL	B	654	6/6	0.94	0.12	31,35,38,38	0
3	NA	A	702	1/1	0.95	0.09	35,35,35,35	0
3	NA	B	702	1/1	0.95	0.10	31,31,31,31	0
2	CU	A	701	1/1	1.00	0.06	33,33,33,33	0
2	CU	B	701	1/1	1.00	0.04	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.