



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:26 AM UTC

PDB ID : 4IMK / pdb_00004imk
Title : Uncrossed Fab binding to human Angiopoietin 2
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Deposited on : 2013-01-03
Resolution : 2.20 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

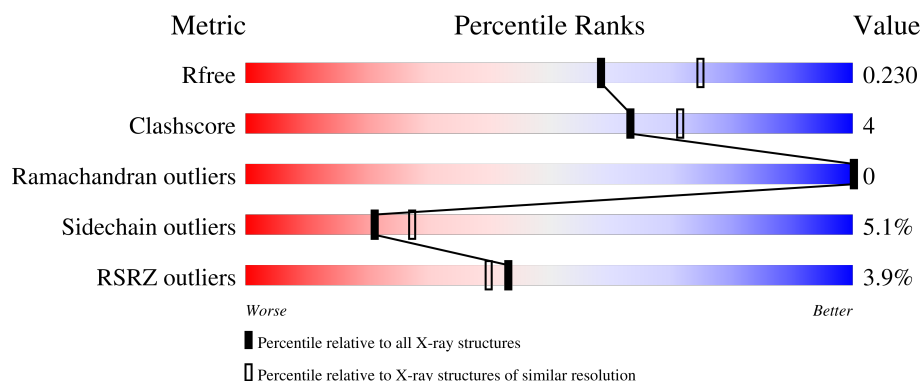
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	230	9% 86% 13%
1	B	230	4% 89% 10% .
2	C	224	% 83% 9% 5%
2	D	224	% 83% 9% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7027 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 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	57	0	0
			1733	1097	288	339	9			
1	B	230	Total	C	N	O	S	82	0	0
			1742	1103	290	340	9			

- Molecule 2 is a protein called Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	29	0	0
			1617	1002	277	333	5			
2	D	210	Total	C	N	O	S	26	0	0
			1598	992	274	328	4			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

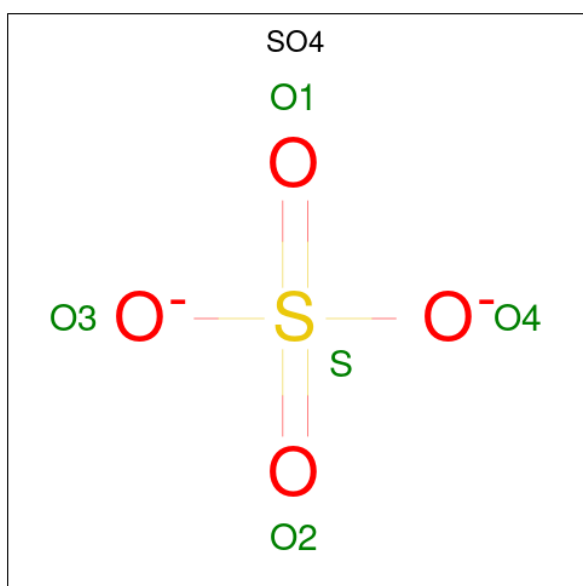
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



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

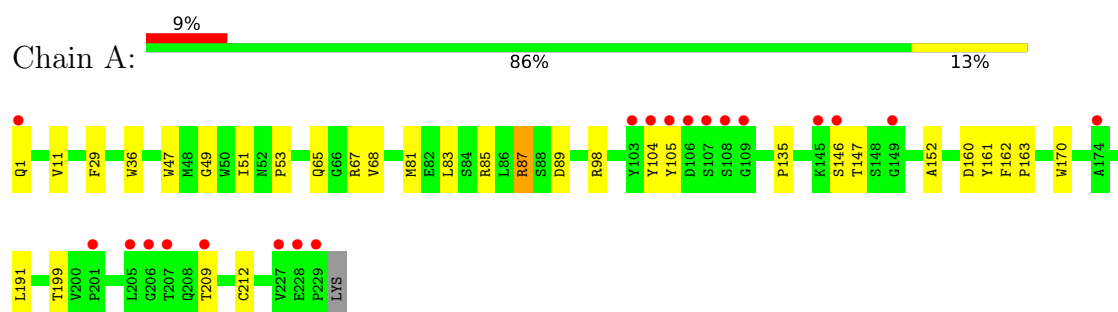
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total 73	O 73	0	0
6	B	50	Total 50	O 50	0	0
6	C	99	Total 99	O 99	0	0
6	D	97	Total 97	O 97	0	0

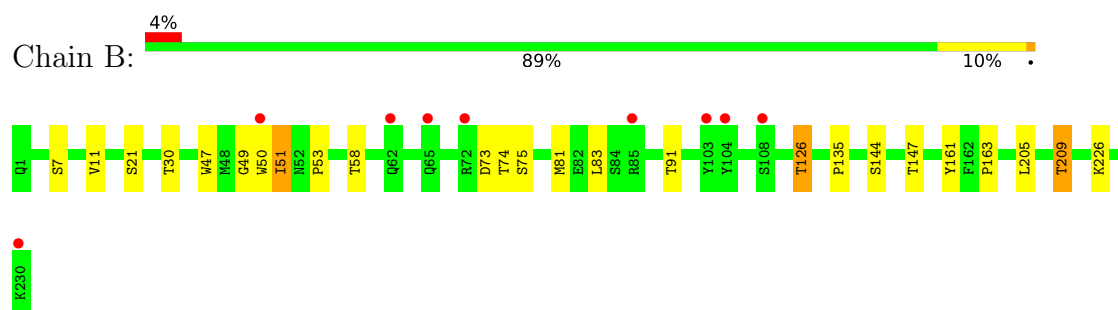
3 Residue-property plots

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.

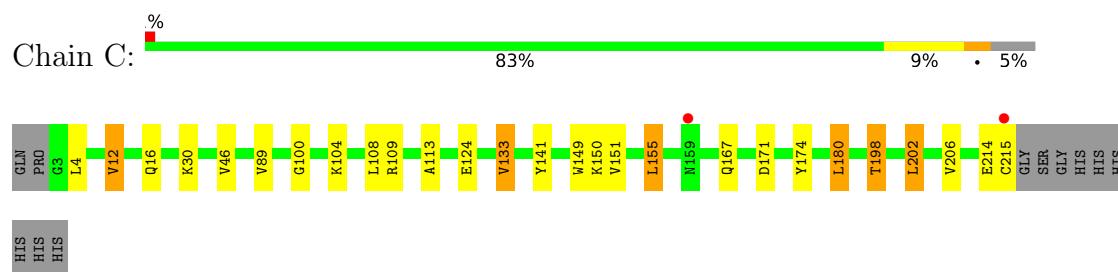
• Molecule 1: Heavy Chain



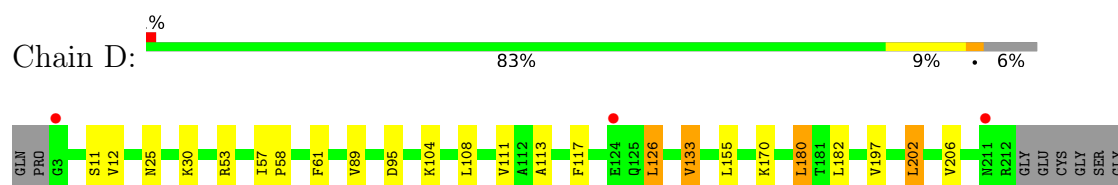
• Molecule 1: Heavy Chain



• Molecule 2: Light Chain



• Molecule 2: Light Chain



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.97 Å 86.67 Å 205.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.76 – 2.20 46.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.76-2.20) 99.8 (46.76-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.226 0.206 , 0.230	Depositor DCC
R_{free} test set	3029 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7027	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: NA, GOL, SO4

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	0.29	0/1782	0.70	0/2431
1	B	0.29	0/1791	0.71	0/2442
2	C	0.30	0/1653	0.71	0/2252
2	D	0.29	0/1634	0.68	0/2227
All	All	0.29	0/6860	0.70	0/9352

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	1733	0	1671	15	0
1	B	1742	0	1685	14	0
2	C	1617	0	1542	14	0
2	D	1598	0	1528	9	0
3	A	1	0	0	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	C	5	0	0	0	0
6	A	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	50	0	0	2	0
6	C	99	0	0	1	0
6	D	97	0	0	1	0
All	All	7027	0	6442	51	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 4.

All (51) 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:51:ILE:HG22	1:B:58:THR:HG22	1.67	0.76
2:C:133:VAL:HG13	2:C:180:LEU:HB3	1.70	0.73
1:A:81:MET:HE1	1:A:83:LEU:HB2	1.74	0.69
1:A:68:VAL:HG23	1:A:81:MET:HE2	1.76	0.67
2:C:12:VAL:HG13	2:C:16:GLN:HB2	1.82	0.62
2:D:133:VAL:HG13	2:D:180:LEU:HB3	1.80	0.62
2:C:109:ARG:NE	2:C:171:ASP:O	2.35	0.57
2:C:4:LEU:HD11	2:C:89:VAL:HG22	1.87	0.55
1:B:135:PRO:HB3	1:B:161:TYR:HB3	1.90	0.53
1:B:73:ASP:HB3	6:B:341:HOH:O	2.10	0.51
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.46	0.50
1:A:135:PRO:HB3	1:A:161:TYR:HB3	1.93	0.49
2:C:30:LYS:NZ	4:C:301:GOL:H11	2.28	0.49
1:A:146:SER:HA	2:D:117:PHE:HD1	1.78	0.48
1:B:30:THR:HA	1:B:53:PRO:HB2	1.96	0.48
2:C:113:ALA:HB1	2:C:202:LEU:HD13	1.95	0.47
1:B:91:THR:HG23	1:B:126:THR:HA	1.98	0.46
1:B:126:THR:HG21	1:B:163:PRO:HB2	1.98	0.45
2:D:113:ALA:HB1	2:D:202:LEU:HD13	1.99	0.45
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.51	0.45
2:C:198:THR:HG23	6:C:477:HOH:O	2.16	0.45
1:B:75:SER:OG	6:B:341:HOH:O	2.20	0.45
1:B:209:THR:HB	1:B:226:LYS:HE3	1.99	0.44
2:D:11:SER:HB3	2:D:108:LEU:HD21	1.99	0.44
1:A:160:ASP:HB3	1:A:191:LEU:HD23	1.99	0.44
1:A:170:TRP:CH2	1:A:212:CYS:HB3	2.53	0.43
1:A:67:ARG:HG2	1:A:85:ARG:NH2	2.33	0.43
2:C:133:VAL:HG22	2:C:149:TRP:CH2	2.53	0.43
2:C:214:GLU:HA	2:C:215:CYS:HA	1.76	0.43
2:D:53:ARG:HD3	2:D:61:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:LYS:HG2	2:C:155:LEU:HD22	2.01	0.43
1:B:144:SER:HA	1:B:147:THR:HG22	2.02	0.42
1:B:81:MET:HE1	1:B:83:LEU:HB2	2.02	0.42
1:A:29:PHE:CE1	1:A:53:PRO:HB3	2.55	0.42
1:A:51:ILE:O	1:A:53:PRO:HD3	2.20	0.42
2:D:126:LEU:HD12	2:D:126:LEU:HA	1.87	0.42
2:C:108:LEU:HA	2:C:141:TYR:OH	2.19	0.42
2:C:167:GLN:HG3	2:C:174:TYR:CZ	2.55	0.42
1:A:87:ARG:HD3	1:A:89:ASP:OD2	2.20	0.41
2:D:57:ILE:HA	2:D:58:PRO:HD3	1.91	0.41
1:B:7:SER:HB3	1:B:21:SER:HB3	2.03	0.41
2:C:202:LEU:HG	2:C:206:VAL:HG23	2.03	0.41
1:A:147:THR:HG22	1:A:152:ALA:HB2	2.02	0.41
2:D:53:ARG:HD2	2:D:57:ILE:HG22	2.02	0.41
2:C:4:LEU:HB2	2:C:100:GLY:HA2	2.03	0.41
1:A:104:TYR:HA	1:A:105:TYR:HA	1.73	0.40
1:B:47:TRP:HZ2	1:B:50:TRP:CD1	2.39	0.40
1:B:47:TRP:CZ2	1:B:49:GLY:HA2	2.55	0.40
2:D:30:LYS:NZ	6:D:479:HOH:O	2.55	0.40
1:A:162:PHE:HA	1:A:163:PRO:HA	1.83	0.40
1:B:51:ILE:O	1:B:53:PRO:HD3	2.22	0.40

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	227/230 (99%)	223 (98%)	4 (2%)	0	100	100
1	B	228/230 (99%)	224 (98%)	4 (2%)	0	100	100
2	C	211/224 (94%)	208 (99%)	3 (1%)	0	100	100
2	D	208/224 (93%)	205 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	874/908 (96%)	860 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	192/193 (100%)	185 (96%)	7 (4%)	31	42
1	B	193/193 (100%)	187 (97%)	6 (3%)	35	48
2	C	184/193 (95%)	174 (95%)	10 (5%)	20	25
2	D	182/193 (94%)	167 (92%)	15 (8%)	10	12
All	All	751/772 (97%)	713 (95%)	38 (5%)	21	27

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	11	VAL
1	A	65	GLN
1	A	87	ARG
1	A	98	ARG
1	A	199	THR
1	A	209	THR
1	B	11	VAL
1	B	51	ILE
1	B	74	THR
1	B	126	THR
1	B	205	LEU
1	B	209	THR
2	C	12	VAL
2	C	46	VAL
2	C	104	LYS
2	C	124	GLU

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Mol	Chain	Res	Type
2	C	133	VAL
2	C	151	VAL
2	C	155	LEU
2	C	180	LEU
2	C	198	THR
2	C	202	LEU
2	D	12	VAL
2	D	25	ASN
2	D	89	VAL
2	D	95	ASP
2	D	104	LYS
2	D	111	VAL
2	D	126	LEU
2	D	133	VAL
2	D	155	LEU
2	D	170	LYS
2	D	180	LEU
2	D	182	LEU
2	D	197	VAL
2	D	202	LEU
2	D	206	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	54	ASN
1	A	65	GLN
1	A	187	GLN
2	C	161	GLN
2	D	211	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	GOL	C	301	-	5,5,5	0.44	0	5,5,5	0.53	0
5	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.08	0
4	GOL	D	301	-	5,5,5	0.33	0	5,5,5	0.44	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	GOL	C	301	-	-	2/4/4/4	-
4	GOL	D	301	-	-	2/4/4/4	-

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
4	C	301	GOL	O1-C1-C2-C3
4	D	301	GOL	O1-C1-C2-C3
4	D	301	GOL	O1-C1-C2-O2
4	C	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	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	229/230 (99%)	0.44	20 (8%) 16 13	23, 49, 82, 100	18 (7%)
1	B	229/230 (99%)	0.32	9 (3%) 43 40	33, 55, 82, 99	22 (9%)
2	C	213/224 (95%)	-0.02	2 (0%) 81 79	29, 45, 63, 110	12 (5%)
2	D	210/224 (93%)	0.09	3 (1%) 73 71	30, 48, 74, 93	9 (4%)
All	All	881/908 (97%)	0.21	34 (3%) 43 40	23, 49, 79, 110	61 (6%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	TYR	7.0
1	A	106	ASP	6.8
1	A	104	TYR	5.4
2	D	3	GLY	4.9
1	A	107	SER	4.5
1	B	108	SER	3.8
1	A	209	THR	3.7
1	A	229	PRO	3.6
1	A	206	GLY	3.5
1	A	149	GLY	3.1
1	A	205	LEU	3.1
1	B	65	GLN	3.0
1	A	228	GLU	2.9
1	B	104	TYR	2.8
2	C	215	CYS	2.7
1	A	108	SER	2.7
1	B	103	TYR	2.7
2	C	159	ASN	2.6
1	A	207	THR	2.5
1	B	230	LYS	2.5
1	A	109	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	85	ARG	2.2
2	D	124	GLU	2.2
1	A	1	GLN	2.2
1	A	174	ALA	2.2
1	A	145	LYS	2.2
1	A	227	VAL	2.1
1	B	62	GLN	2.1
1	B	72	ARG	2.1
1	A	103	TYR	2.1
1	B	50	TRP	2.1
1	A	146	SER	2.0
2	D	211	ASN	2.0
1	A	201	PRO	2.0

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, 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
5	SO4	C	302	5/5	0.83	0.17	92,94,95,96	0
4	GOL	C	301	6/6	0.89	0.15	72,73,73,74	0
3	NA	A	301	1/1	0.90	0.14	64,64,64,64	0
4	GOL	D	301	6/6	0.92	0.11	46,48,58,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.