



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 04:33 AM EST

PDB ID : 3EGH
Title : Crystal structure of a complex between Protein Phosphatase 1 alpha (PP1), the PP1 binding and PDZ domains of Spinophilin and the small natural molecular toxin Nodularin-R
Authors : Ragusa, M.J.; Page, R.; Peti, W.
Deposited on : 2008-09-10
Resolution : 2.00 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 ⓘ 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

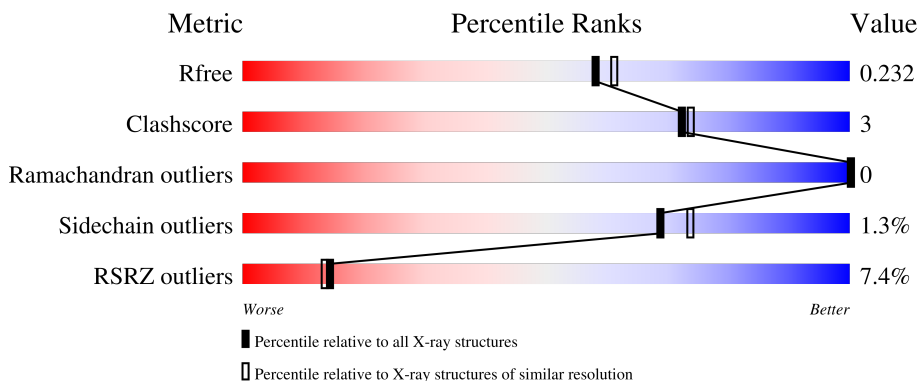
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



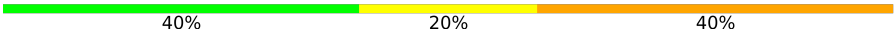
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	329	 81% 7% • 11%
1	B	329	 84% 5% 11%
2	C	170	 25% 83% 10% • 6%
2	D	170	 8% 36% 61% •
3	E	5	 20% 40% 20% 40%

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Mol	Chain	Length	Quality of chain
3	F	5	 40% 20% 40%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 6990 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2358	1520	390	429	19	0	5	0
1	B	294	2346	1509	387	431	19	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P62136
A	3	HIS	-	expression tag	UNP P62136
A	4	MET	-	expression tag	UNP P62136
A	5	GLY	-	expression tag	UNP P62136
A	6	SER	-	expression tag	UNP P62136
B	2	GLY	-	expression tag	UNP P62136
B	3	HIS	-	expression tag	UNP P62136
B	4	MET	-	expression tag	UNP P62136
B	5	GLY	-	expression tag	UNP P62136
B	6	SER	-	expression tag	UNP P62136

- Molecule 2 is a protein called Spinophilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	160	1172	736	201	231	4	0	1	0
2	D	66	496	312	79	104	1	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	414	GLY	-	expression tag	UNP O35274

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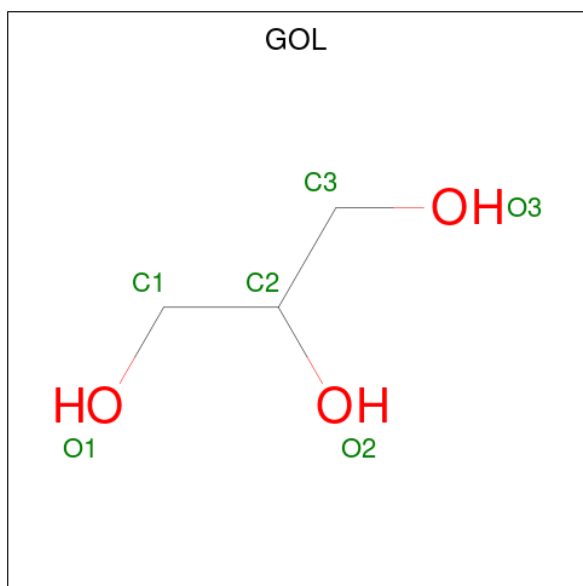
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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	SER	-	expression tag	UNP O35274
C	416	MET	-	expression tag	UNP O35274
D	414	GLY	-	expression tag	UNP O35274
D	415	SER	-	expression tag	UNP O35274
D	416	MET	-	expression tag	UNP O35274

- Molecule 3 is a protein called nodularin R.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
3	E	5	55	40	5	10	0	0	0
3	F	5	54	39	5	10	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Mn 2	0	0
5	B	2	Total 2	Mn 2	0	0

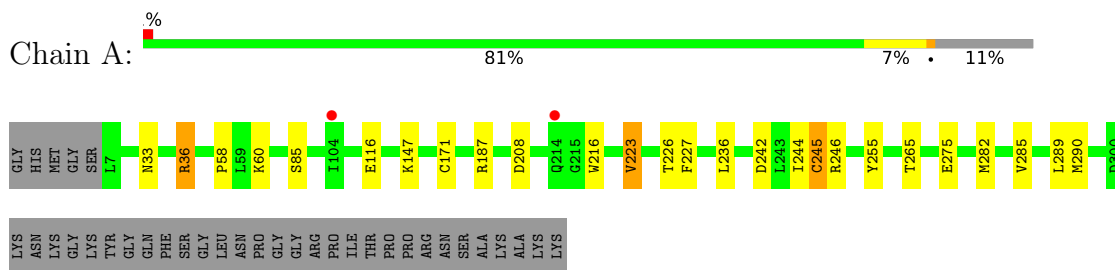
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	179	Total 179	O 179	0	0
6	B	198	Total 198	O 198	0	0
6	C	61	Total 61	O 61	0	0
6	D	38	Total 38	O 38	0	0
6	E	3	Total 3	O 3	0	0
6	F	2	Total 2	O 2	0	0

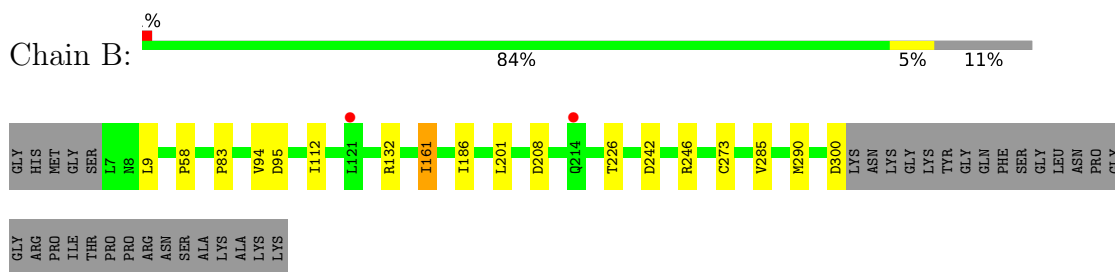
3 Residue-property plots [i](#)

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.

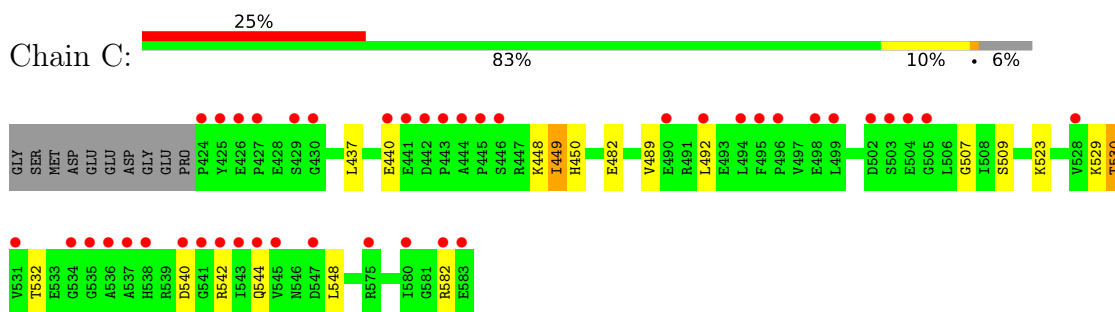
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



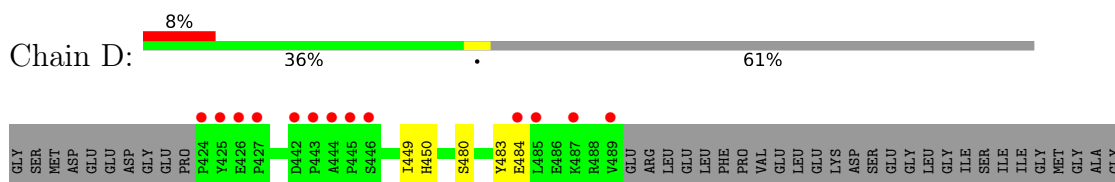
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



- Molecule 2: Spinophilin



- Molecule 2: Spinophilin

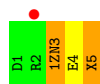


ALA ASP MET GLY LEU LYS LEU GLY ILE PHE VAL LYS THR VAL THR GLU GLY GLY ALA ALA HIS ARG ASP GLY ARG ILE GLN VAL ASN ASP LEU VAL VAL ASP GLY THR SER LEU VAL VAL THR GLN SER PHE ALA ALA SER VAL ARG ASN THR LYS GLY VAL

ARG PHE MET ILE GLY ARG GLU

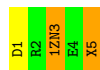
- Molecule 3: nodularin R





- Molecule 3: nodularin R





4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.41Å 84.43Å 109.31Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 39.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.00-2.00) 96.3 (39.37-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.235 0.191 , 0.232	Depositor DCC
R_{free} test set	3528 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6990	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 44.52 % 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 1.5088e-04. 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: MDH, MN, ACB, 1ZN, FGA, 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	0.74	1/2428 (0.0%)	0.75	1/3285 (0.0%)
1	B	0.79	1/2406 (0.0%)	0.77	1/3256 (0.0%)
2	C	0.61	0/1195	0.67	0/1619
2	D	0.70	0/516	0.66	0/705
3	E	0.39	0/6	0.67	0/6
3	F	0.41	0/5	1.02	0/5
All	All	0.73	2/6556 (0.0%)	0.74	2/8876 (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
3	E	0	2
3	F	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	CYS	CB-SG	-5.83	1.72	1.81
1	B	300	ASP	CA-CB	5.25	1.65	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ASP	N-CA-C	6.11	127.49	111.00
1	A	223	VAL	CB-CA-C	-5.65	100.66	111.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	3	1ZN	Mainchain,Peptide
3	F	3	1ZN	Mainchain,Peptide

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	2358	0	2304	20	0
1	B	2346	0	2282	12	0
2	C	1172	0	1126	15	0
2	D	496	0	440	6	0
3	E	55	0	42	1	0
3	F	54	0	40	1	0
4	A	18	0	24	4	0
4	C	6	0	8	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	179	0	0	2	0
6	B	198	0	0	0	0
6	C	61	0	0	0	0
6	D	38	0	0	0	0
6	E	3	0	0	0	0
6	F	2	0	0	0	0
All	All	6990	0	6266	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 3.

The worst 5 of 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:B:290[B]:MET:HE3	2:D:450:HIS:ND1	1.96	0.81
1:A:85:SER:HB3	4:A:402:GOL:H31	1.71	0.73
2:C:509:SER:OG	2:C:530:THR:HB	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290[B]:MET:CE	2:D:450:HIS:ND1	2.58	0.67
1:A:290[B]:MET:HE3	2:C:450:HIS:ND1	2.09	0.66

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	297/329 (90%)	287 (97%)	10 (3%)	0	100	100
1	B	294/329 (89%)	281 (96%)	13 (4%)	0	100	100
2	C	159/170 (94%)	158 (99%)	1 (1%)	0	100	100
2	D	66/170 (39%)	65 (98%)	1 (2%)	0	100	100
All	All	816/998 (82%)	791 (97%)	25 (3%)	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	253/285 (89%)	249 (98%)	4 (2%)	62	67
1	B	252/285 (88%)	249 (99%)	3 (1%)	71	76
2	C	120/141 (85%)	117 (98%)	3 (2%)	47	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	52/141 (37%)	52 (100%)	0	100	100
All	All	677/852 (80%)	667 (98%)	10 (2%)	69	69

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	437	LEU
2	C	449	ILE
2	C	530	THR
1	A	246	ARG
1	B	83	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 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
3	1ZN	E	3	3	23,23,24	0.73	1 (4%)	24,29,31	1.36	3 (12%)
3	FGA	F	4	3	7,8,9	0.88	0	7,9,11	1.14	0
3	ACB	F	1	3	7,8,9	1.12	1 (14%)	8,10,12	1.80	2 (25%)
3	FGA	E	4	3	7,8,9	0.80	0	7,9,11	1.28	1 (14%)
3	ACB	E	1	3	7,8,9	1.10	0	8,10,12	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1ZN	F	3	3	23,23,24	0.86	0	24,29,31	1.20	4 (16%)
3	MDH	E	5	3	4,6,7	1.16	1 (25%)	4,6,8	3.64	2 (50%)
3	MDH	F	5	3	4,6,7	1.87	1 (25%)	4,6,8	2.45	2 (50%)

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	1ZN	E	3	3	-	0/22/25/27	0/1/1/1
3	FGA	F	4	3	-	0/7/8/9	-
3	ACB	F	1	3	-	1/9/10/12	-
3	FGA	E	4	3	-	2/7/8/9	-
3	ACB	E	1	3	-	1/9/10/12	-
3	1ZN	F	3	3	-	2/22/25/27	0/1/1/1
3	MDH	E	5	3	-	0/2/6/8	-
3	MDH	F	5	3	-	0/2/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	MDH	C-CA	3.45	1.48	1.43
3	E	3	1ZN	C18-CA	-2.16	1.53	1.55
3	E	5	MDH	C-CA	2.15	1.46	1.43
3	F	1	ACB	CB-CA	-2.11	1.53	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	MDH	O-C-CA	-6.61	116.99	125.39
3	F	5	MDH	O-C-CA	-3.95	120.37	125.39
3	E	3	1ZN	C18-CA-C16	-3.72	107.64	112.98
3	F	1	ACB	C4-CB-CA	3.15	114.29	110.94
3	F	3	1ZN	C4-C3-C2	2.80	117.52	113.42

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	ACB	CA-CB-CG-OD1
3	F	3	1ZN	C19-C18-CA-C16
3	F	3	1ZN	O-C-C18-CA
3	F	1	ACB	CA-CB-CG-OD1
3	E	4	FGA	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	MDH	1	0
3	F	5	MDH	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A	402	-	5,5,5	0.39	0	5,5,5	0.39	0
4	GOL	A	403	-	5,5,5	0.21	0	5,5,5	0.78	0
4	GOL	C	601	-	5,5,5	0.23	0	5,5,5	0.27	0
4	GOL	A	401	-	5,5,5	0.40	0	5,5,5	0.55	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	A	402	-	-	4/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	C	601	-	-	2/4/4/4	-
4	GOL	A	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	GOL	C1-C2-C3-O3
4	A	403	GOL	O1-C1-C2-C3
4	C	601	GOL	O1-C1-C2-C3
4	A	402	GOL	O2-C2-C3-O3
4	A	403	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	GOL	2	0
4	A	403	GOL	2	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	294/329 (89%)	0.09	2 (0%) 87 87	23, 29, 36, 40	5 (1%)
1	B	294/329 (89%)	0.09	2 (0%) 87 87	25, 28, 34, 39	7 (2%)
2	C	160/170 (94%)	1.07	42 (26%) 0 0	22, 31, 40, 45	6 (3%)
2	D	66/170 (38%)	0.83	13 (19%) 1 0	23, 30, 43, 47	1 (1%)
3	E	1/5 (20%)	2.62	1 (100%) 0 0	30, 30, 30, 30	1 (100%)
3	F	1/5 (20%)	0.58	0 100 100	30, 30, 30, 30	1 (100%)
All	All	816/1008 (80%)	0.35	60 (7%) 14 13	22, 29, 37, 47	21 (2%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	442	ASP	6.3
2	C	445	PRO	6.0
2	C	543	ILE	5.6
2	C	494	LEU	5.5
2	C	424	PRO	5.3

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
3	FGA	E	4	9/10	0.78	0.22	29,31,33,36	9
3	FGA	F	4	9/10	0.85	0.23	28,30,31,31	9
3	ACB	F	1	9/10	0.87	0.26	30,32,34,36	9
3	ACB	E	1	9/10	0.88	0.24	27,29,30,30	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1ZN	F	3	23/24	0.88	0.17	22,28,30,31	23
3	MDH	E	5	7/8	0.88	0.26	28,29,30,31	7
3	MDH	F	5	7/8	0.88	0.19	30,31,32,33	7
3	1ZN	E	3	23/24	0.91	0.19	24,27,28,31	23

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(\AA^2)	Q<0.9
4	GOL	A	401	6/6	0.77	0.19	42,43,43,44	6
4	GOL	A	402	6/6	0.85	0.27	25,33,35,40	6
4	GOL	A	403	6/6	0.86	0.15	42,46,48,50	6
4	GOL	C	601	6/6	0.94	0.11	30,32,33,34	6
5	MN	A	404	1/1	0.99	0.05	23,23,23,23	1
5	MN	A	405	1/1	0.99	0.05	27,27,27,27	0
5	MN	B	401	1/1	0.99	0.08	21,21,21,21	1
5	MN	B	402	1/1	1.00	0.06	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.