



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:47 PM UTC

PDB ID : 3EGH / pdb_00003egh
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 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

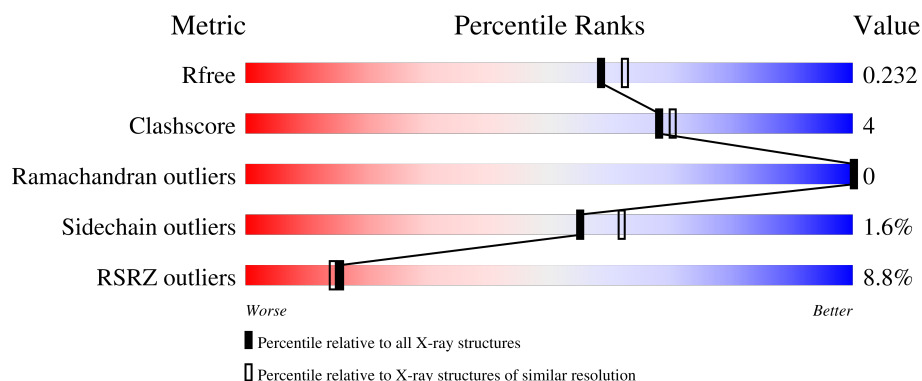
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



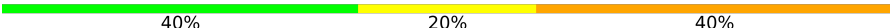
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
1	B	329	
2	C	170	
2	D	170	
3	E	5	

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Mol	Chain	Length	Quality of chain
3	F	5	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment on the left labeled '40%', a yellow segment in the middle labeled '20%', and an orange segment on the right labeled '40%'. The total length of the bar represents 100%.

2 Entry composition

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
1	A	294	Total	C	N	O	S	0	5	0
			2358	1520	390	429	19			
1	B	294	Total	C	N	O	S	0	2	0
			2346	1509	387	431	19			

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
2	C	160	Total	C	N	O	S	0	1	0
			1172	736	201	231	4			
2	D	66	Total	C	N	O	S	0	2	0
			496	312	79	104	1			

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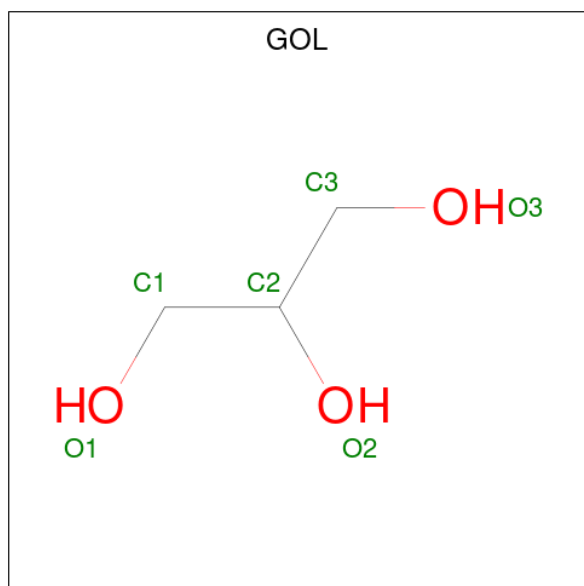
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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	SER	-	expression tag	UNP O35274
C	416	MET	-	expression tag	UNP O35274
D	414	GLY	-	expression tag	UNP O35274
D	415	SER	-	expression tag	UNP O35274
D	416	MET	-	expression tag	UNP O35274

- Molecule 3 is a protein called nodularin R.

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

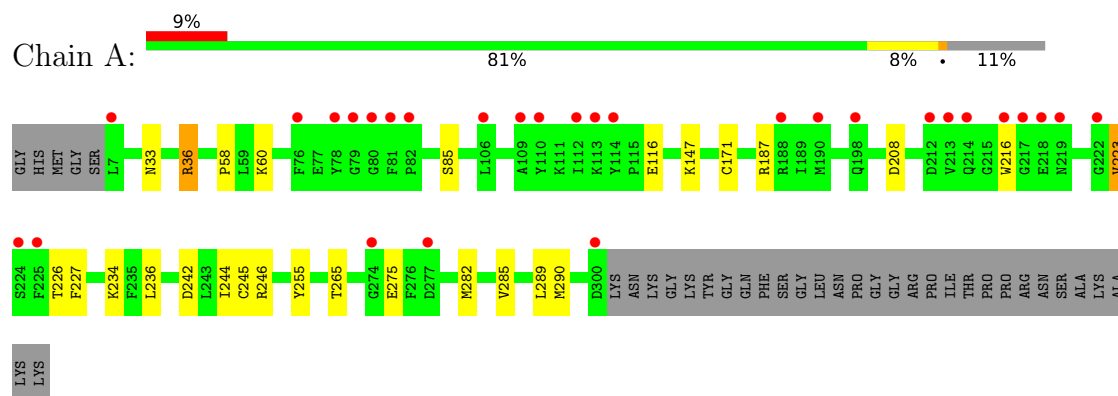
- Molecule 6 is water.

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

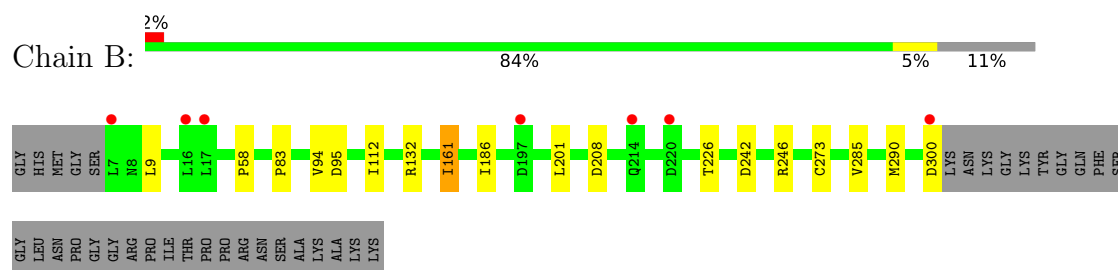
3 Residue-property plots [i](#)

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.

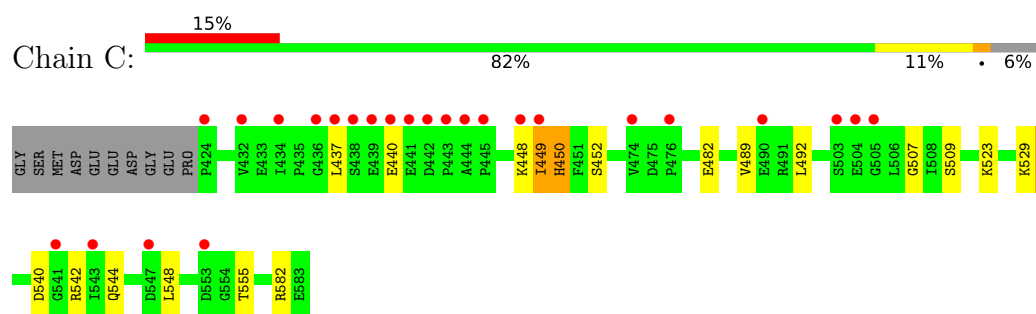
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



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

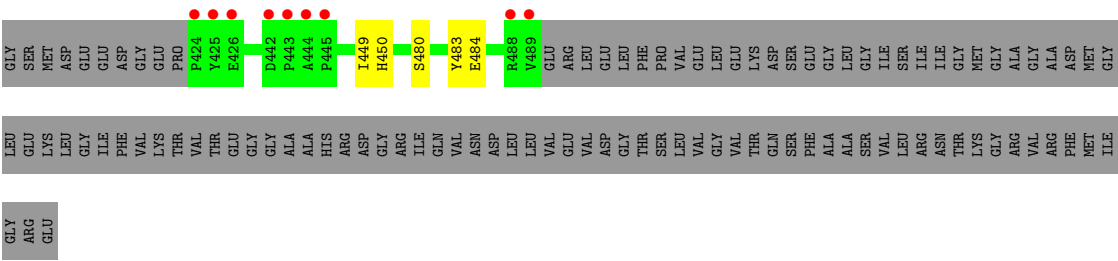


- Molecule 2: Spinophilin



- Molecule 2: Spinophilin





● Molecule 3: nodularin R



● Molecule 3: nodularin R



4 Data and refinement statistics

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 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.00-2.00) 96.2 (40.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.00Å)	Xtriage
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	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6990	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1ZN, GOL, MN, MDH, ACB, FGA

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	0.87	0/2428	0.95	1/3285 (0.0%)
1	B	0.92	1/2406 (0.0%)	0.96	1/3256 (0.0%)
2	C	0.80	1/1195 (0.1%)	0.92	0/1619
2	D	0.85	0/516	0.94	0/705
3	E	0.39	0/6	0.84	0/6
3	F	0.46	0/5	1.34	0/5
All	All	0.88	2/6556 (0.0%)	0.95	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	B	300	ASP	CA-CB	6.03	1.65	1.53
2	C	555	THR	CA-CB	5.01	1.60	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	5.89	127.49	111.00
1	A	223	VAL	CB-CA-C	-5.70	100.66	110.30

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

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	22	0
1	B	2346	0	2282	12	0
2	C	1172	0	1126	17	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	46	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 (46) 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	1.88	0.88
1:A:290[B]:MET:HE3	2:C:450:HIS:ND1	1.90	0.85
1:A:85:SER:HB3	4:A:402:GOL:H31	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:509:SER:OG	2:C:530:THR:HB	1.89	0.73
1:B:290[B]:MET:CE	2:D:450:HIS:ND1	2.58	0.67
1:B:290[B]:MET:HE3	2:D:450:HIS:CE1	2.34	0.63
1:A:116:GLU:OE1	4:A:403:GOL:H31	2.09	0.53
1:A:289:LEU:HD12	2:C:448:LYS:HD3	1.90	0.52
1:A:216:TRP:CZ3	1:A:227:PHE:HB3	2.46	0.51
2:C:489:VAL:O	2:C:492:LEU:HB2	2.11	0.51
1:A:242:ASP:HB3	2:C:449:ILE:HG12	1.93	0.50
2:D:480:SER:O	2:D:484:GLU:HG2	2.12	0.50
1:B:208:ASP:O	1:B:226:THR:HA	2.11	0.49
1:B:161:ILE:HD12	1:B:201:LEU:HD13	1.95	0.49
4:A:403:GOL:H12	6:A:597:HOH:O	2.12	0.49
1:B:94:VAL:O	1:B:95:ASP:HB2	2.13	0.49
2:C:544:GLN:OE1	2:C:582:ARG:NH2	2.46	0.49
1:A:290[B]:MET:HE3	2:C:450:HIS:CE1	2.48	0.48
2:C:482:GLU:CG	2:C:523:LYS:HD2	2.45	0.47
1:A:187:ARG:HG2	6:A:534:HOH:O	2.14	0.47
1:A:36[A]:ARG:HH22	1:A:147:LYS:CG	2.27	0.47
1:B:161:ILE:HD11	1:B:186:ILE:HG23	1.96	0.46
1:B:58:PRO:HA	1:B:285:VAL:O	2.15	0.46
1:A:290[B]:MET:CE	2:C:450:HIS:ND1	2.72	0.45
2:C:440:GLU:O	2:C:440:GLU:HG3	2.17	0.45
1:A:36[A]:ARG:HH11	1:A:36[A]:ARG:HG3	1.82	0.45
1:A:289:LEU:CD1	2:C:448:LYS:HD3	2.48	0.44
1:B:9:LEU:HD11	1:B:112:ILE:HG22	2.00	0.43
1:A:85:SER:CB	4:A:402:GOL:H31	2.46	0.43
1:A:255:TYR:HA	1:A:265:THR:O	2.18	0.42
1:A:58:PRO:HA	1:A:285:VAL:O	2.20	0.42
1:A:275:GLU:OE1	3:E:5:MDH:HG1	2.19	0.42
2:C:489:VAL:HG22	2:C:548:LEU:HD21	2.02	0.42
1:B:242:ASP:HB3	2:D:449:ILE:HG12	2.02	0.42
1:A:33:ASN:OD1	1:A:36[B]:ARG:NH1	2.53	0.42
1:A:236:LEU:HD21	1:A:244:ILE:HG13	2.01	0.41
1:A:208:ASP:O	1:A:226:THR:HA	2.20	0.41
1:A:60[B]:LYS:HD3	1:A:282:MET:SD	2.61	0.41
2:C:507:GLY:HA2	2:C:532:THR:OG1	2.21	0.41
2:C:529:LYS:HB3	2:C:529:LYS:HE2	1.84	0.41
2:C:540:ASP:OD2	2:C:542:ARG:HD3	2.20	0.41
1:B:273:CYS:SG	3:F:5:MDH:HG1	2.61	0.40
1:A:171:CYS:HA	1:A:245:CYS:O	2.21	0.40
1:A:290[B]:MET:HE2	2:C:452:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HG2	2:D:483:TYR:CG	2.56	0.40
2:C:482:GLU:HG3	2:C:523:LYS:HD2	2.02	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	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%)	248 (98%)	5 (2%)	48	54
1	B	252/285 (88%)	249 (99%)	3 (1%)	63	70
2	C	120/141 (85%)	116 (97%)	4 (3%)	33	34

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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%)	665 (98%)	12 (2%)	55	58

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36[A]	ARG
1	A	36[B]	ARG
1	A	223	VAL
1	A	234	LYS
1	A	246	ARG
1	B	83	PRO
1	B	161	ILE
1	B	246	ARG
2	C	437	LEU
2	C	449	ILE
2	C	450	HIS
2	C	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	181	GLN
1	A	271	ASN
1	B	117	ASN
1	B	271	ASN
2	C	464	ASN
2	C	538	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	FGA	E	4	3	6,8,9	0.86	0	6,9,11	0.85	0
3	1ZN	F	3	3	21,23,24	0.82	0	25,29,31	1.25	4 (16%)
3	ACB	E	1	3	7,8,9	0.93	0	8,10,12	1.48	1 (12%)
3	ACB	F	1	3	7,8,9	0.82	0	8,10,12	1.73	2 (25%)
3	FGA	F	4	3	6,8,9	0.94	0	6,9,11	0.98	0
3	MDH	F	5	3	4,6,7	1.68	1 (25%)	4,6,8	2.56	3 (75%)
3	MDH	E	5	3	4,6,7	1.04	0	4,6,8	3.76	2 (50%)
3	1ZN	E	3	3	21,23,24	0.46	0	25,29,31	1.33	3 (12%)

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	FGA	E	4	3	-	2/8/8/9	-
3	1ZN	F	3	3	-	3/23/25/27	0/1/1/1
3	ACB	E	1	3	-	2/10/10/12	-
3	ACB	F	1	3	-	2/10/10/12	-
3	FGA	F	4	3	-	0/8/8/9	-
3	MDH	F	5	3	-	0/2/6/8	-
3	MDH	E	5	3	-	0/2/6/8	-
3	1ZN	E	3	3	-	1/23/25/27	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	MDH	C-CA	3.02	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	MDH	O-C-CA	-6.70	116.99	125.39
3	F	5	MDH	O-C-CA	-4.00	120.37	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	1ZN	C18-CA-C16	-3.72	107.64	112.98
3	E	5	MDH	CM-N-CA	-2.97	119.48	123.98
3	E	3	1ZN	O-C-C18	-2.90	117.57	124.96
3	F	3	1ZN	C4-C3-C2	2.81	117.52	113.23
3	F	1	ACB	C-CA-N	2.77	115.31	109.49
3	E	1	ACB	C-CA-N	2.72	115.20	109.49
3	E	3	1ZN	CA-C16-C15	-2.51	119.54	123.62
3	F	3	1ZN	O-C-C18	-2.36	118.96	124.96
3	F	3	1ZN	C11-C10-C12	-2.27	106.22	110.08
3	F	5	MDH	CB-CA-N	-2.18	119.96	122.70
3	F	3	1ZN	C16-C15-C13	-2.17	121.66	126.32
3	F	1	ACB	CB-CA-C	-2.14	107.37	110.54
3	F	5	MDH	CM-N-CA	-2.11	120.78	123.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	ACB	CA-CB-CG-OD1
3	E	1	ACB	C4-CB-CG-OD1
3	F	1	ACB	C4-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
3	E	4	FGA	OXT-C-CA-N
3	E	3	1ZN	C10-C2-C3-C4
3	F	3	1ZN	C10-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	C	601	-	5,5,5	0.24	0	5,5,5	0.30	0
4	GOL	A	401	-	5,5,5	0.42	0	5,5,5	0.56	0
4	GOL	A	402	-	5,5,5	0.40	0	5,5,5	0.41	0
4	GOL	A	403	-	5,5,5	0.21	0	5,5,5	0.83	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	601	-	-	2/4/4/4	-
4	GOL	A	401	-	-	0/4/4/4	-
4	GOL	A	402	-	-	3/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) 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
4	C	601	GOL	O1-C1-C2-O2
4	A	402	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 ⓘ

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	294/329 (89%)	0.79	29 (9%) 13 11	13, 29, 35, 40	10 (3%)
1	B	294/329 (89%)	0.23	7 (2%) 59 59	15, 28, 34, 39	9 (3%)
2	C	160/170 (94%)	1.20	26 (16%) 4 4	18, 31, 40, 45	7 (4%)
2	D	66/170 (38%)	0.85	9 (13%) 7 6	19, 30, 43, 47	3 (4%)
3	E	1/5 (20%)	2.68	1 (100%) 0 0	22, 22, 22, 22	1 (100%)
3	F	1/5 (20%)	1.48	0 100 100	23, 23, 23, 23	1 (100%)
All	All	816/1008 (80%)	0.68	72 (8%) 15 14	13, 29, 37, 47	31 (3%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	ASP	8.7
1	A	300	ASP	8.0
2	C	504	GLU	6.6
2	C	438[A]	SER	4.9
1	A	214	GLN	4.8
2	D	424	PRO	4.5
2	D	442	ASP	4.3
1	B	214	GLN	4.0
2	C	439	GLU	3.9
2	C	443	PRO	3.9
2	C	440	GLU	3.5
1	A	109	ALA	3.5
2	C	437	LEU	3.4
1	A	213	VAL	3.4
2	C	436	GLY	3.2
1	B	7	LEU	3.2
2	C	445	PRO	3.2
1	A	224	SER	3.1
1	A	222	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	274	GLY	3.0
1	A	78	TYR	3.0
2	C	543	ILE	3.0
1	A	198	GLN	2.9
2	C	441	GLU	2.9
2	D	489	VAL	2.9
1	A	277	ASP	2.8
2	C	553	ASP	2.8
2	C	442	ASP	2.8
1	B	17	LEU	2.8
2	C	505	GLY	2.8
1	A	110	TYR	2.7
3	E	2	ARG	2.7
1	A	114	TYR	2.7
1	A	225	PHE	2.6
2	C	424	PRO	2.6
2	C	537	ALA	2.6
2	C	448	LYS	2.6
2	D	425	TYR	2.5
1	A	7	LEU	2.5
1	A	113	LYS	2.5
1	A	79	GLY	2.5
2	C	434	ILE	2.5
1	B	220	ASP	2.5
1	A	80	GLY	2.5
1	A	81	PHE	2.4
1	A	219	ASN	2.4
2	C	474	VAL	2.4
1	A	188	ARG	2.4
1	B	16	LEU	2.4
1	A	76	PHE	2.4
1	A	217	GLY	2.4
2	C	503	SER	2.4
2	C	490	GLU	2.3
1	A	212	ASP	2.3
1	A	106	LEU	2.3
1	A	82	PRO	2.3
2	C	547	ASP	2.3
2	D	444	ALA	2.3
2	D	488	ARG	2.2
2	D	443	PRO	2.2
2	C	444	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	216	TRP	2.2
1	B	197	ASP	2.2
1	A	218	GLU	2.1
2	D	445	PRO	2.1
2	D	426	GLU	2.1
2	C	449	ILE	2.1
2	C	432	VAL	2.1
1	A	190	MET	2.1
1	A	112	ILE	2.0
2	C	476	PRO	2.0
2	C	541	GLY	2.0

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	0.68	0.20	29,31,33,36	9
3	MDH	E	5	7/8	0.72	0.17	28,29,30,31	7
3	ACB	E	1	9/10	0.77	0.17	27,29,30,30	9
3	ACB	F	1	9/10	0.78	0.17	30,32,34,36	9
3	MDH	F	5	7/8	0.79	0.17	30,31,32,33	7
3	1ZN	F	3	23/24	0.81	0.16	22,28,30,31	23
3	FGA	F	4	9/10	0.82	0.18	28,30,31,31	9
3	1ZN	E	3	23/24	0.83	0.15	24,27,28,31	23

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
4	GOL	A	403	6/6	0.80	0.18	42,46,48,50	6
4	GOL	A	401	6/6	0.81	0.14	42,43,43,44	6
4	GOL	A	402	6/6	0.85	0.20	25,33,35,40	6
4	GOL	C	601	6/6	0.92	0.12	30,32,33,34	6
5	MN	A	404	1/1	0.99	0.16	23,23,23,23	1
5	MN	A	405	1/1	0.99	0.14	27,27,27,27	0
5	MN	B	401	1/1	1.00	0.17	21,21,21,21	1
5	MN	B	402	1/1	1.00	0.15	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.