



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:45 PM UTC

PDB ID : 3EGG / pdb\_00003egg  
Title : Crystal structure of a complex between Protein Phosphatase 1 alpha (PP1) and the PP1 binding and PDZ domains of Spinophilin  
Authors : Ragusa, M.J.; Page, R.; Peti, W.  
Deposited on : 2008-09-10  
Resolution : 1.85 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](mailto: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>.

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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

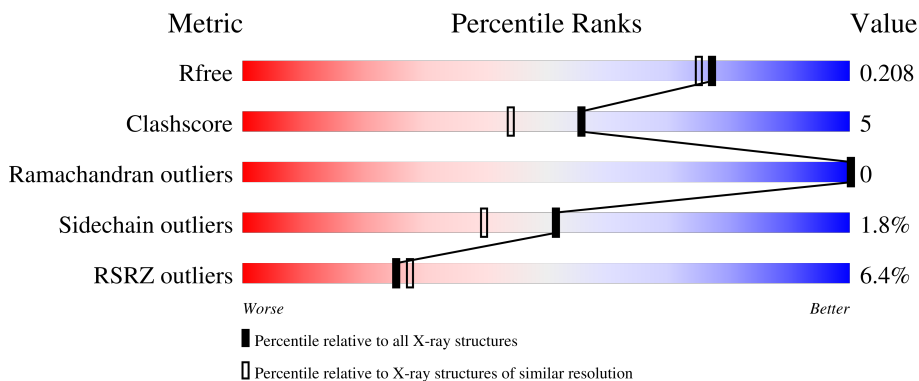
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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  $\geq 3$ , 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	 5% 82% 7% 11%
1	B	329	 % 80% 9% 11%
2	C	170	 11% 85% 8% 6%
2	D	170	 8% 36% 61%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	MES	B	404	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7033 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	2367	1520	387	440	20	0	10	0
1	B	294	2375	1531	390	434	20	0	11	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P62136
A	-3	HIS	-	expression tag	UNP P62136
A	-2	MET	-	expression tag	UNP P62136
A	-1	GLY	-	expression tag	UNP P62136
A	0	SER	-	expression tag	UNP P62136
B	-4	GLY	-	expression tag	UNP P62136
B	-3	HIS	-	expression tag	UNP P62136
B	-2	MET	-	expression tag	UNP P62136
B	-1	GLY	-	expression tag	UNP P62136
B	0	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	1187	746	206	231	4	0	2	0
2	D	66	501	314	82	104	1	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

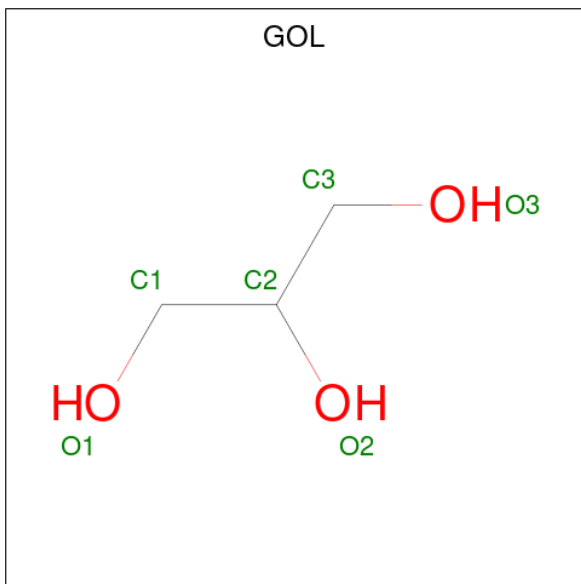
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP O35274

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP O35274
C	0	MET	-	expression tag	UNP O35274
D	-2	GLY	-	expression tag	UNP O35274
D	-1	HIS	-	expression tag	UNP O35274
D	0	MET	-	expression tag	UNP O35274

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

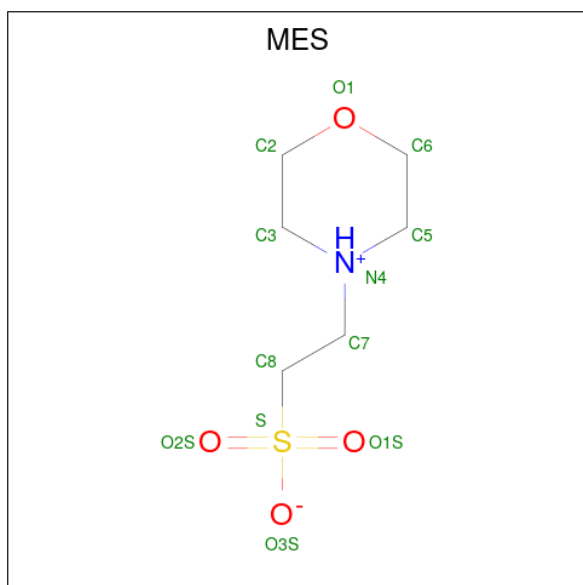


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0
3	B	1	6	3	3	0	0
3	B	1	6	3	3	0	0
3	C	1	6	3	3	0	0
3	D	1	6	3	3	0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 12 6 1 4 1	0	0
5	B	1	Total C N O S 12 6 1 4 1	0	0
5	B	1	Total C N O S 12 6 1 4 1	6	0

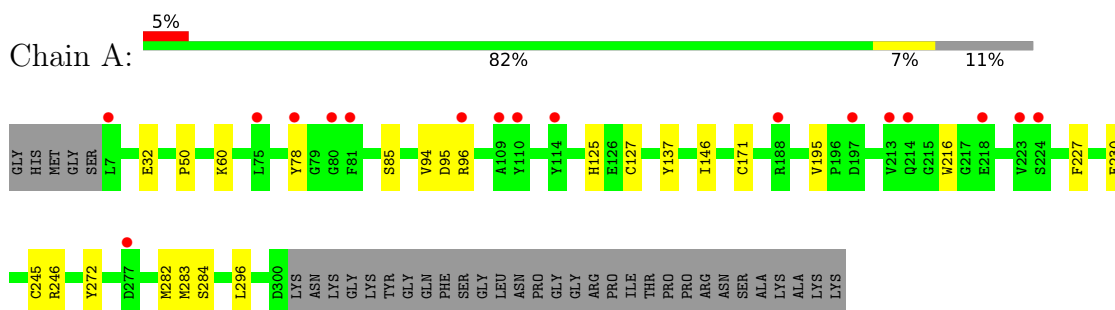
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	160	Total O 160 160	0	0
6	B	287	Total O 287 287	0	0
6	C	67	Total O 67 67	0	0
6	D	7	Total O 7 7	0	0

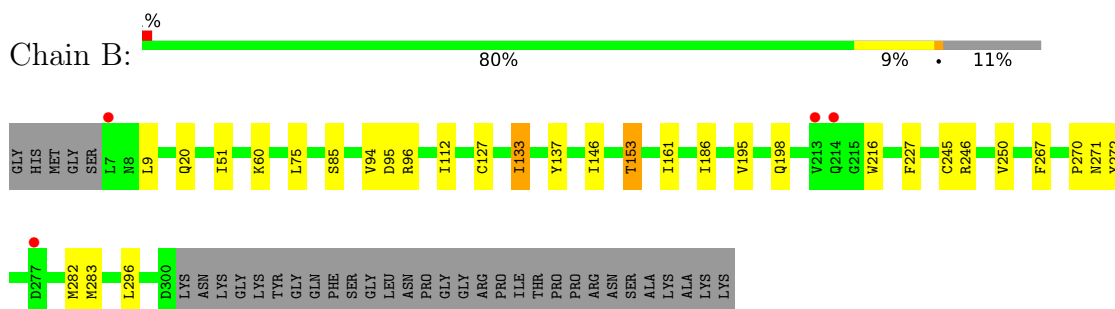
### 3 Residue-property plots [i](#)

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.

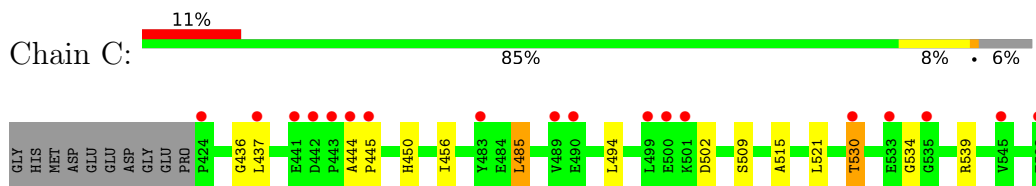
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



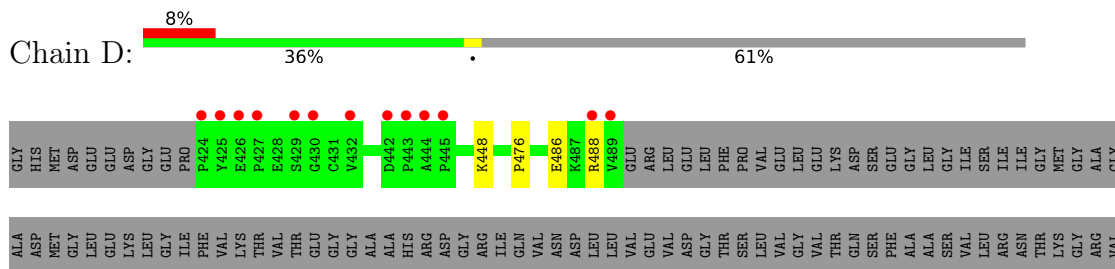
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



- Molecule 2: Spinophilin



- Molecule 2: Spinophilin



ARG  
PHE  
MET  
ILE  
GLY  
ARG  
GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.67Å 84.42Å 109.16Å 90.00° 93.50° 90.00°	Depositor
Resolution (Å)	27.53 – 1.85 27.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (27.53-1.85) 99.0 (27.53-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.85Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.211 0.178 , 0.208	Depositor DCC
$R_{free}$ test set	4548 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 43.73 % 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 1.6904e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MES, MN, 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	0.63	0/2468	0.80	0/3340
1	B	0.68	0/2476	0.82	0/3350
2	C	0.53	0/1212	0.75	0/1639
2	D	0.60	0/521	0.81	0/711
All	All	0.63	0/6677	0.80	0/9040

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	2367	0	2298	20	0
1	B	2375	0	2336	33	0
2	C	1187	0	1158	6	0
2	D	501	0	449	2	0
3	A	18	0	24	2	0
3	B	12	0	16	3	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	12	0	12	3	0
5	B	24	0	24	7	0
6	A	160	0	0	1	0
6	B	287	0	0	4	0
6	C	67	0	0	0	0
6	D	7	0	0	0	0
All	All	7033	0	6333	60	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 5.

All (60) 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:96:ARG:HH2	5:B:404:MES:C7	1.77	0.96
1:B:75[B]:LEU:HD23	1:B:296[B]:LEU:HG	1.61	0.82
1:B:96:ARG:NH2	5:B:404:MES:H52	1.95	0.82
1:B:96:ARG:NH2	5:B:404:MES:C5	2.45	0.79
1:B:127[B]:CYS:SG	1:B:195:VAL:HG21	2.24	0.78
1:A:60[A]:LYS:HE2	1:A:284:SER:OG	1.90	0.71
1:A:125:HIS:NE2	5:A:403:MES:H82	2.04	0.71
1:A:127[B]:CYS:SG	1:A:195:VAL:HG21	2.30	0.71
1:B:96:ARG:HH2	5:B:404:MES:C5	2.04	0.70
1:B:96:ARG:HH2	5:B:404:MES:H72	1.56	0.69
2:C:509:SER:OG	2:C:530:THR:HB	1.93	0.69
1:B:153:THR:HG21	6:B:645:HOH:O	1.93	0.68
1:A:230[B]:GLU:HG2	6:A:522:HOH:O	1.93	0.67
1:A:50:PRO:HD3	3:A:333:GOL:H12	1.76	0.67
1:A:96:ARG:HH2	5:A:403:MES:H81	1.60	0.66
1:B:75[B]:LEU:CD2	1:B:296[B]:LEU:HG	2.28	0.62
1:B:161[B]:ILE:HD11	1:B:186:ILE:HG23	1.81	0.61
1:B:137:TYR:CE1	1:B:146:ILE:HD12	2.35	0.61
1:B:133[A]:ILE:HG23	2:D:476:PRO:HA	1.84	0.60
2:C:502:ASP:OD2	2:C:539:ARG:NH2	2.35	0.59
1:A:85[B]:SER:OG	3:A:332:GOL:H31	2.01	0.59
2:C:534:GLY:O	2:C:539:ARG:NH1	2.35	0.59
1:B:127[B]:CYS:SG	1:B:195:VAL:CG2	2.91	0.58
1:A:60[B]:LYS:HD3	1:A:282:MET:SD	2.48	0.54
1:B:245[B]:CYS:SG	1:B:283:MET:HE1	2.48	0.54
1:B:96:ARG:NH2	5:B:404:MES:C7	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127[B]:CYS:SG	1:A:195:VAL:CG2	2.96	0.53
1:B:96:ARG:HH22	5:B:404:MES:H71	1.69	0.52
1:B:94:VAL:O	1:B:95:ASP:HB2	2.11	0.51
1:B:9[A]:LEU:HD11	1:B:112:ILE:HG22	1.93	0.51
1:B:75[B]:LEU:HD23	1:B:296[B]:LEU:CG	2.37	0.50
1:A:245[B]:CYS:SG	1:A:283:MET:HE1	2.50	0.50
1:B:250[B]:VAL:HG12	1:B:267:PHE:CZ	2.47	0.50
1:A:32:GLU:OE2	6:B:573:HOH:O	2.20	0.49
2:D:486:GLU:C	2:D:488:ARG:H	2.20	0.49
1:A:94:VAL:O	1:A:95:ASP:HB2	2.13	0.49
1:A:216:TRP:CZ3	1:A:227:PHE:HB3	2.47	0.49
1:B:85:SER:HB3	3:B:332:GOL:H31	1.95	0.49
1:A:96:ARG:HH22	5:A:403:MES:C8	2.27	0.48
1:B:20:GLN:OE1	3:B:331:GOL:H31	2.12	0.48
2:C:485:LEU:HD23	2:C:515:ALA:HB2	1.97	0.46
1:B:250[B]:VAL:HG11	1:B:272:TYR:CD2	2.50	0.46
1:A:137:TYR:CE1	1:A:146:ILE:HD12	2.51	0.46
1:B:75[B]:LEU:HD23	1:B:296[B]:LEU:CD2	2.47	0.43
1:B:60[A]:LYS:HG3	3:B:332:GOL:H32	1.99	0.43
1:A:96:ARG:NH1	1:A:272:TYR:OH	2.51	0.43
1:B:60[B]:LYS:HD3	1:B:282:MET:SD	2.58	0.43
1:A:78:TYR:CD2	1:A:296[A]:LEU:HD21	2.53	0.43
1:B:153:THR:CG2	6:B:645:HOH:O	2.62	0.42
1:B:51:ILE:HG12	1:B:161[B]:ILE:HG12	2.01	0.42
1:A:78:TYR:HD2	1:A:296[A]:LEU:HD21	1.85	0.42
1:B:270:PRO:O	1:B:271:ASN:C	2.62	0.42
1:B:250[B]:VAL:HG11	1:B:272:TYR:HD2	1.85	0.41
1:B:153:THR:HG22	6:B:646:HOH:O	2.21	0.41
1:B:216:TRP:CZ3	1:B:227:PHE:HB3	2.56	0.41
2:C:436:GLY:HA2	2:C:456:ILE:HG13	2.02	0.40
1:B:250[B]:VAL:HG12	1:B:267:PHE:CE1	2.56	0.40
2:C:444:ALA:HA	2:C:445:PRO:HD3	1.92	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	302/329 (92%)	291 (96%)	11 (4%)	0	100	100
1	B	303/329 (92%)	292 (96%)	11 (4%)	0	100	100
2	C	160/170 (94%)	157 (98%)	3 (2%)	0	100	100
2	D	66/170 (39%)	64 (97%)	2 (3%)	0	100	100
All	All	831/998 (83%)	804 (97%)	27 (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	260/285 (91%)	259 (100%)	1 (0%)	84	82
1	B	263/285 (92%)	258 (98%)	5 (2%)	50	38
2	C	122/141 (86%)	116 (95%)	6 (5%)	22	8
2	D	53/141 (38%)	52 (98%)	1 (2%)	50	38
All	All	698/852 (82%)	685 (98%)	13 (2%)	51	38

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	B	133[A]	ILE
1	B	133[B]	ILE
1	B	153	THR
1	B	198	GLN
1	B	246	ARG
2	C	437	LEU
2	C	450	HIS

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Mol	Chain	Res	Type
2	C	485	LEU
2	C	494	LEU
2	C	521	LEU
2	C	530	THR
2	D	448	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	198	GLN
1	B	117	ASN
1	B	262	GLN
2	D	450	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
3	GOL	B	331	-	5,5,5	0.33	0	5,5,5	0.19	0
3	GOL	D	1	-	5,5,5	0.34	0	5,5,5	0.23	0
3	GOL	A	333	-	5,5,5	0.50	0	5,5,5	0.24	0
3	GOL	A	332	-	5,5,5	0.38	0	5,5,5	0.39	0
3	GOL	C	1	-	5,5,5	0.35	0	5,5,5	0.16	0
3	GOL	A	331	-	5,5,5	0.33	0	5,5,5	0.29	0
5	MES	B	404	-	12,12,12	2.20	1 (8%)	15,16,16	2.61	6 (40%)
5	MES	A	403	-	12,12,12	2.21	1 (8%)	15,16,16	2.27	7 (46%)
3	GOL	B	332	-	5,5,5	0.25	0	5,5,5	0.34	0
5	MES	B	405	-	12,12,12	3.61	2 (16%)	15,16,16	4.77	8 (53%)

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	GOL	B	331	-	-	2/4/4/4	-
3	GOL	D	1	-	-	2/4/4/4	-
3	GOL	A	333	-	-	4/4/4/4	-
3	GOL	A	332	-	-	4/4/4/4	-
3	GOL	C	1	-	-	2/4/4/4	-
3	GOL	A	331	-	-	1/4/4/4	-
5	MES	B	404	-	-	4/6/14/14	0/1/1/1
5	MES	A	403	-	-	2/6/14/14	0/1/1/1
3	GOL	B	332	-	-	4/4/4/4	-
5	MES	B	405	-	-	5/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	405	MES	C7-N4	10.70	1.71	1.47
5	A	403	MES	C8-S	-7.33	1.67	1.77
5	B	404	MES	C8-S	-7.25	1.67	1.77
5	B	405	MES	C8-S	-5.87	1.69	1.77

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	405	MES	C7-N4-C3	12.65	144.94	111.24
5	B	405	MES	C7-N4-C5	-9.38	86.24	111.24
5	B	405	MES	C5-N4-C3	6.33	122.47	108.84
5	B	404	MES	C5-N4-C3	5.54	120.77	108.84
5	A	403	MES	C5-N4-C3	5.11	119.84	108.84
5	B	404	MES	O1S-S-C8	4.79	113.97	106.73
5	B	405	MES	O1S-S-C8	3.91	112.63	106.73
5	B	404	MES	C7-N4-C3	3.81	121.40	111.24
5	A	403	MES	C7-N4-C5	3.55	120.71	111.24
5	B	404	MES	C2-C3-N4	-3.42	104.93	110.12
5	A	403	MES	C7-N4-C3	3.08	119.44	111.24
5	B	405	MES	O3S-S-C8	2.84	111.55	106.00
5	A	403	MES	O1S-S-C8	2.78	110.94	106.73
5	B	405	MES	O3S-S-O1S	-2.65	104.78	111.40
5	B	405	MES	O2S-S-O1S	-2.52	105.64	113.82
5	B	404	MES	C7-N4-C5	2.47	117.82	111.24
5	B	405	MES	C2-C3-N4	-2.31	106.61	110.12
5	A	403	MES	C2-C3-N4	-2.25	106.70	110.12
5	A	403	MES	C6-C5-N4	-2.18	106.81	110.12
5	B	404	MES	O2S-S-C8	2.04	109.81	106.73
5	A	403	MES	O3S-S-C8	2.02	109.95	106.00

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	332	GOL	O1-C1-C2-O2
3	A	332	GOL	O1-C1-C2-C3
3	A	333	GOL	O1-C1-C2-C3
3	A	333	GOL	C1-C2-C3-O3
3	B	331	GOL	O1-C1-C2-C3
3	B	332	GOL	O1-C1-C2-C3
3	B	332	GOL	C1-C2-C3-O3
3	D	1	GOL	C1-C2-C3-O3
5	A	403	MES	C8-C7-N4-C3
5	B	404	MES	C8-C7-N4-C3
5	B	405	MES	C8-C7-N4-C5
5	B	405	MES	C7-C8-S-O1S
5	B	405	MES	C7-C8-S-O2S
3	D	1	GOL	O2-C2-C3-O3
5	B	404	MES	C7-C8-S-O3S
3	A	332	GOL	C1-C2-C3-O3
3	C	1	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	333	GOL	O2-C2-C3-O3
3	B	331	GOL	O1-C1-C2-O2
3	B	332	GOL	O2-C2-C3-O3
3	A	333	GOL	O1-C1-C2-O2
5	B	405	MES	C7-C8-S-O3S
3	A	332	GOL	O2-C2-C3-O3
3	B	332	GOL	O1-C1-C2-O2
5	B	404	MES	C7-C8-S-O1S
5	B	404	MES	C7-C8-S-O2S
5	A	403	MES	N4-C7-C8-S
3	C	1	GOL	O1-C1-C2-O2
3	A	331	GOL	C1-C2-C3-O3
5	B	405	MES	C8-C7-N4-C3

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	331	GOL	1	0
3	A	333	GOL	1	0
3	A	332	GOL	1	0
5	B	404	MES	7	0
5	A	403	MES	3	0
3	B	332	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	294/329 (89%)	0.72	17 (5%) 29 31	16, 24, 30, 34	17 (5%)
1	B	294/329 (89%)	0.21	4 (1%) 73 77	15, 24, 29, 33	17 (5%)
2	C	160/170 (94%)	1.14	18 (11%) 10 9	14, 26, 35, 38	7 (4%)
2	D	66/170 (38%)	1.22	13 (19%) 3 2	17, 25, 36, 37	3 (4%)
All	All	814/998 (81%)	0.66	52 (6%) 25 27	14, 25, 32, 38	44 (5%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	583	GLU	7.0
2	D	442	ASP	5.8
2	D	489	VAL	4.7
2	D	425	TYR	4.6
2	C	442	ASP	4.0
2	D	445	PRO	3.9
1	A	213	VAL	3.8
2	C	444	ALA	3.6
1	A	214	GLN	3.5
2	C	443	PRO	3.4
2	D	424	PRO	3.4
1	B	277	ASP	3.3
1	A	7	LEU	3.2
2	C	437	LEU	3.1
1	A	96	ARG	3.1
2	C	545	VAL	3.0
2	D	430	GLY	3.0
1	A	197	ASP	2.9
2	D	444	ALA	2.9
2	C	535	GLY	2.8
2	D	426	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	489	VAL	2.8
2	C	483	TYR	2.7
1	A	109	ALA	2.7
1	A	223	VAL	2.7
1	A	78	TYR	2.7
2	D	432	VAL	2.6
1	A	277	ASP	2.6
2	D	488	ARG	2.6
2	D	427	PRO	2.6
2	C	424	PRO	2.5
1	A	81	PHE	2.5
2	C	445	PRO	2.5
1	A	80	GLY	2.4
2	C	441	GLU	2.4
2	C	499	LEU	2.4
1	A	75[A]	LEU	2.4
2	C	490	GLU	2.4
2	C	533	GLU	2.3
1	A	224	SER	2.3
2	D	429	SER	2.3
1	A	218[A]	GLU	2.3
1	B	7	LEU	2.3
2	D	443	PRO	2.3
1	B	214	GLN	2.3
1	A	114	TYR	2.2
1	A	188	ARG	2.2
2	C	501	LYS	2.1
1	B	213	VAL	2.1
2	C	530	THR	2.0
2	C	500	GLU	2.0
1	A	110	TYR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	A	331	6/6	0.63	0.20	44,45,46,47	6
3	GOL	D	1	6/6	0.65	0.18	49,53,53,54	0
3	GOL	B	331	6/6	0.74	0.20	42,43,44,44	6
3	GOL	A	333	6/6	0.74	0.18	39,41,42,43	0
5	MES	B	405	12/12	0.80	0.18	20,20,47,47	6
3	GOL	A	332	6/6	0.81	0.19	24,28,30,33	6
5	MES	A	403	12/12	0.81	0.25	18,28,31,32	12
3	GOL	B	332	6/6	0.81	0.19	22,28,32,34	6
5	MES	B	404	12/12	0.88	0.24	13,30,35,36	12
3	GOL	C	1	6/6	0.93	0.11	25,27,27,28	6
4	MN	A	400	1/1	0.96	0.24	28,28,28,28	1
4	MN	B	401	1/1	0.97	0.23	25,25,25,25	1
4	MN	A	402	1/1	0.98	0.12	19,19,19,19	0
4	MN	B	403	1/1	1.00	0.14	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.