



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:54 AM GMT

PDB ID : 3V4Y
Title : Crystal Structure of the first Nuclear PP1 holoenzyme
Authors : Page, R.; Peti, W.; O'Connell, N.E.; Nichols, S.
Deposited on : 2011-12-15
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

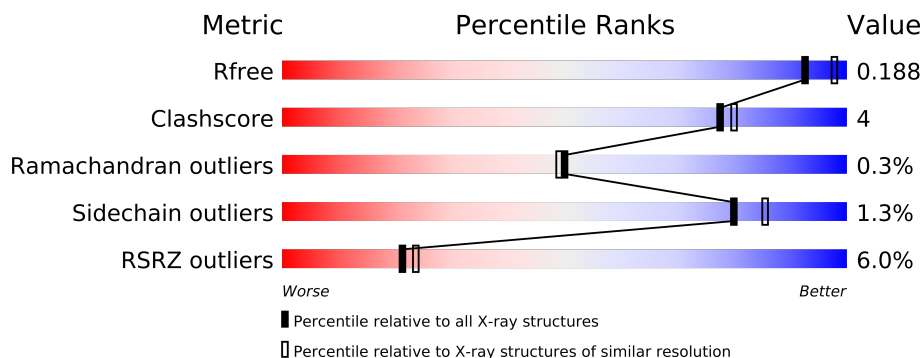
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	306	
1	C	306	
1	E	306	
1	G	306	
2	B	62	
2	D	62	
2	F	62	
2	H	62	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	405	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	C	403	-	X
4	GOL	C	405	-	X
4	GOL	E	404	-	X
4	GOL	E	405	-	X
4	GOL	G	403	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22195 atoms, of which 10645 are hydrogens and 0 are deuterium.

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-proteinphosphatase PP1-alpha catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	293	Total	C	H	N	O	S	0	3	0
			4720	1524	2348	395	435	18			
1	C	295	Total	C	H	N	O	S	0	1	0
			4712	1521	2336	397	440	18			
1	E	293	Total	C	H	N	O	S	0	0	0
			4677	1510	2321	395	433	18			
1	G	297	Total	C	H	N	O	S	0	1	0
			4741	1529	2353	401	438	20			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP P62136
A	-4	HIS	-	EXPRESSION TAG	UNP P62136
A	-3	MET	-	EXPRESSION TAG	UNP P62136
A	-2	GLY	-	EXPRESSION TAG	UNP P62136
A	-1	SER	-	EXPRESSION TAG	UNP P62136
C	-5	GLY	-	EXPRESSION TAG	UNP P62136
C	-4	HIS	-	EXPRESSION TAG	UNP P62136
C	-3	MET	-	EXPRESSION TAG	UNP P62136
C	-2	GLY	-	EXPRESSION TAG	UNP P62136
C	-1	SER	-	EXPRESSION TAG	UNP P62136
E	-5	GLY	-	EXPRESSION TAG	UNP P62136
E	-4	HIS	-	EXPRESSION TAG	UNP P62136
E	-3	MET	-	EXPRESSION TAG	UNP P62136
E	-2	GLY	-	EXPRESSION TAG	UNP P62136
E	-1	SER	-	EXPRESSION TAG	UNP P62136
G	-5	GLY	-	EXPRESSION TAG	UNP P62136
G	-4	HIS	-	EXPRESSION TAG	UNP P62136
G	-3	MET	-	EXPRESSION TAG	UNP P62136
G	-2	GLY	-	EXPRESSION TAG	UNP P62136
G	-1	SER	-	EXPRESSION TAG	UNP P62136

- Molecule 2 is a protein called Nuclear inhibitor of protein phosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	41	Total	C	H	N	O	0	0	0
			640	202	306	54	78			
2	D	39	Total	C	H	N	O	0	0	0
			601	190	284	52	74			
2	F	39	Total	C	H	N	O	0	0	0
			614	194	295	52	73			
2	H	43	Total	C	H	N	O	0	0	0
			669	210	322	57	79			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	EXPRESSION TAG	UNP Q12972
B	-2	ALA	-	EXPRESSION TAG	UNP Q12972
B	-1	MET	-	EXPRESSION TAG	UNP Q12972
D	-3	GLY	-	EXPRESSION TAG	UNP Q12972
D	-2	ALA	-	EXPRESSION TAG	UNP Q12972
D	-1	MET	-	EXPRESSION TAG	UNP Q12972
F	-3	GLY	-	EXPRESSION TAG	UNP Q12972
F	-2	ALA	-	EXPRESSION TAG	UNP Q12972
F	-1	MET	-	EXPRESSION TAG	UNP Q12972
H	-3	GLY	-	EXPRESSION TAG	UNP Q12972
H	-2	ALA	-	EXPRESSION TAG	UNP Q12972
H	-1	MET	-	EXPRESSION TAG	UNP Q12972

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

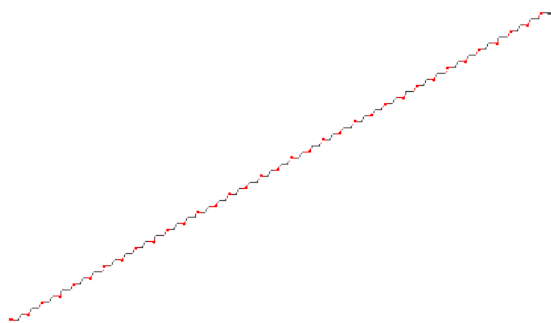
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		
3	C	2	Total	Mn	0	0
			2	2		
3	E	2	Total	Mn	0	0
			2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		
4	G	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: C₆₉H₁₄₀O₃₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	169	Total	O	0	0
			169	169		
6	B	27	Total	O	0	0
			27	27		
6	C	165	Total	O	0	0
			165	165		
6	D	30	Total	O	0	0
			30	30		
6	E	140	Total	O	0	0
			140	140		
6	F	22	Total	O	0	0
			22	22		
6	G	98	Total	O	0	0
			98	98		
6	H	10	Total	O	0	0
			10	10		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

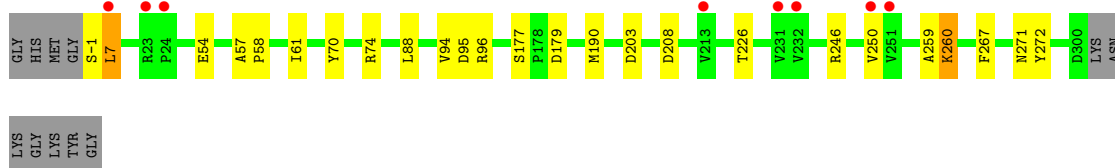
- Molecule 1: Serine/threonine-proteinphosphatase PP1-alpha catalytic subunit

Chain A: 



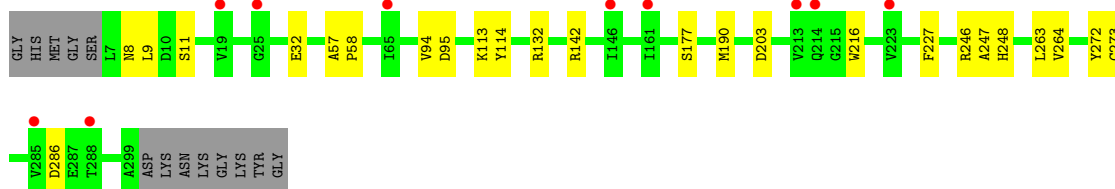
- Molecule 1: Serine/threonine-proteinphosphatase PP1-alpha catalytic subunit

Chain C: 



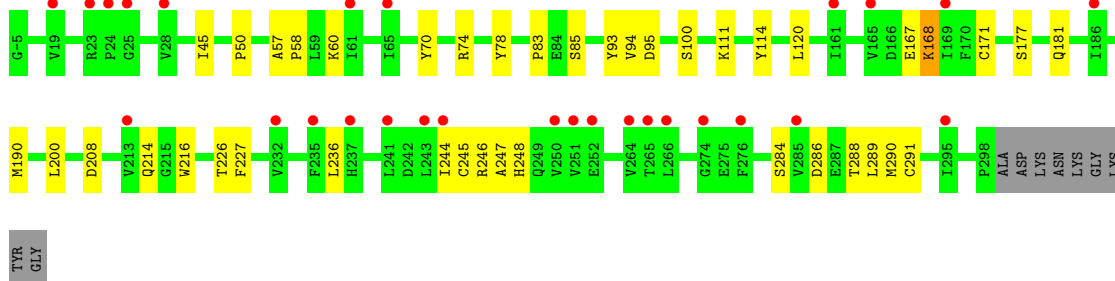
- Molecule 1: Serine/threonine-proteinphosphatase PP1-alpha catalytic subunit

Chain E: 



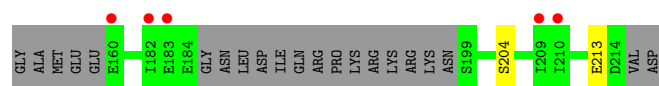
- Molecule 1: Serine/threonine-proteinphosphatase PP1-alpha catalytic subunit

Chain G: 



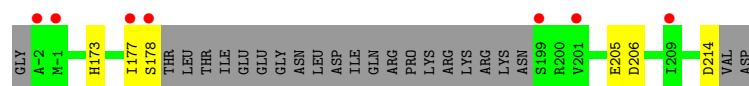
- Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain B: 



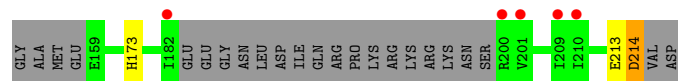
- Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain D: 



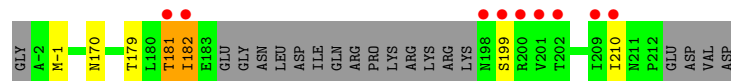
- Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain F: 



- Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.64Å 116.03Å 168.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 47.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-2.10) 95.7 (47.75-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.154 , 0.196 0.149 , 0.188	Depositor DCC
R_{free} test set	4237 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 88292 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22195	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, 15P

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	0.41	0/2435	0.54	0/3290
1	C	0.42	0/2433	0.56	0/3287
1	E	0.40	0/2410	0.52	0/3256
1	G	0.33	0/2446	0.49	0/3302
2	B	0.36	0/336	0.47	0/454
2	D	0.36	0/319	0.48	0/429
2	F	0.30	0/321	0.48	0/434
2	H	0.30	0/349	0.45	0/471
All	All	0.38	0/11049	0.52	0/14923

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2372	2348	0	13	0
1	C	2376	2336	0	17	0
1	E	2356	2321	0	14	0
1	G	2388	2353	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	334	306	0	1	0
2	D	317	284	0	7	0
2	F	319	295	0	3	0
2	H	347	322	0	10	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	18	24	0	1	0
4	C	18	24	0	1	0
4	E	18	24	0	0	0
4	G	6	8	0	1	0
5	A	12	0	14	1	0
6	A	169	0	0	0	0
6	B	27	0	0	0	0
6	C	165	0	0	2	1
6	D	30	0	0	0	0
6	E	140	0	0	2	1
6	F	22	0	0	0	0
6	G	98	0	0	1	0
6	H	10	0	0	1	0
All	All	11550	10645	14	79	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (79) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:-1:SER:O	1:C:7:LEU:HB2	1.79	0.81
1:E:32:GLU:OE2	6:E:568:HOH:O	2.13	0.66
1:C:190:MET:HE2	2:D:173:HIS:ND1	2.11	0.66
1:A:7:LEU:HD11	1:A:12:ILE:CD1	2.27	0.64
1:E:57:ALA:HB1	1:E:58:PRO:HA	1.81	0.60
2:H:179:THR:O	2:H:179:THR:HG22	2.03	0.59
1:A:56:GLU:H	4:A:403:GOL:H32	1.68	0.58
1:C:271:ASN:HB3	6:C:655:HOH:O	2.04	0.56
1:C:190:MET:HE2	2:D:173:HIS:CE1	2.40	0.56
1:C:54:GLU:O	4:C:403:GOL:H31	2.04	0.56
1:C:94:VAL:O	1:C:95:ASP:HB2	2.06	0.56
1:G:286:ASP:OD2	1:G:290:MET:HB3	2.06	0.55
1:E:272:TYR:O	1:E:273:CYS:HB2	2.07	0.55
2:B:213:GLU:O	2:B:213:GLU:HG2	2.05	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:236:LEU:HD21	1:G:244:ILE:HG13	1.88	0.55
1:G:288:THR:O	1:G:289:LEU:HB2	2.07	0.54
1:G:167:GLU:O	1:G:168:LYS:HD3	2.08	0.54
1:A:137:TYR:CE2	1:A:146[A]:ILE:HD12	2.43	0.53
1:G:57:ALA:HB1	1:G:58:PRO:HA	1.91	0.53
1:A:177:SER:HB2	1:A:203:ASP:HB2	1.91	0.52
1:E:177:SER:HB2	1:E:203:ASP:HB2	1.92	0.52
1:E:94:VAL:O	1:E:95:ASP:HB2	2.10	0.52
1:C:190:MET:HE2	2:D:173:HIS:CG	2.45	0.51
2:H:179:THR:HG22	2:H:182:ILE:HG12	1.92	0.51
1:G:181:GLN:CG	2:H:181:THR:HG21	2.40	0.51
1:A:7:LEU:HD11	1:A:12:ILE:HD11	1.91	0.50
1:G:94:VAL:O	1:G:95:ASP:HB2	2.11	0.50
1:A:94:VAL:O	1:A:95:ASP:HB2	2.11	0.50
2:H:182:ILE:HG22	2:H:182:ILE:O	2.11	0.50
1:A:247:ALA:O	1:A:248:HIS:HB3	2.12	0.50
1:C:177:SER:HB2	1:C:203:ASP:HB2	1.94	0.48
6:C:656:HOH:O	2:D:173:HIS:HE1	1.97	0.48
1:G:78:TYR:CD1	2:H:210:ILE:HG12	2.49	0.48
1:C:259:ALA:O	1:C:260:LYS:HB2	2.14	0.48
2:H:179:THR:HG22	2:H:182:ILE:CG1	2.44	0.48
1:A:141:LYS:HB2	1:A:146[A]:ILE:HD11	1.95	0.48
1:E:113:LYS:HE2	1:E:114:TYR:HH	1.79	0.47
1:G:78:TYR:CG	2:H:210:ILE:HG12	2.50	0.47
1:A:177:SER:HB2	1:A:203:ASP:CB	2.45	0.47
1:E:247:ALA:O	1:E:248:HIS:HB3	2.15	0.46
1:G:60:LYS:HE3	1:G:85:SER:HG	1.80	0.46
1:G:50:PRO:HD2	4:G:403:GOL:H12	1.96	0.46
1:E:263:LEU:HD23	1:E:263:LEU:C	2.36	0.46
1:G:216:TRP:CZ3	1:G:227:PHE:HB3	2.51	0.46
2:F:173:HIS:HE1	6:G:568:HOH:O	1.99	0.46
1:C:250:VAL:HG22	1:C:267:PHE:CZ	2.51	0.45
1:G:93:TYR:HH	1:G:120:LEU:HB3	1.80	0.45
1:C:179:ASP:OD2	2:D:177:ILE:HG23	2.17	0.45
1:G:208:ASP:O	1:G:226:THR:HA	2.17	0.45
5:A:406:15P:H28	5:A:406:15P:H16	1.59	0.45
1:C:190:MET:CE	2:D:173:HIS:CG	3.00	0.45
1:C:96:ARG:HG3	1:C:272:TYR:OH	2.18	0.44
1:E:263:LEU:HD23	1:E:264:VAL:N	2.33	0.44
1:A:272:TYR:O	1:A:273:CYS:HB2	2.16	0.44
1:C:70:TYR:O	1:C:74:ARG:HG3	2.18	0.44
1:C:57:ALA:HB1	1:C:58:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:179:THR:HB	6:H:305:HOH:O	2.18	0.43
1:E:8:ASN:ND2	1:E:11:SER:CB	2.82	0.43
2:F:213:GLU:O	2:F:214:ASP:HB2	2.18	0.43
1:A:7:LEU:HD11	1:A:12:ILE:HD12	2.00	0.43
1:E:216:TRP:CZ3	1:E:227:PHE:HB3	2.54	0.42
1:G:190[B]:MET:HE2	2:H:170:ASN:OD1	2.19	0.42
1:G:70:TYR:O	1:G:74:ARG:HG3	2.20	0.42
1:C:208:ASP:O	1:C:226:THR:HA	2.20	0.42
1:G:177:SER:HG	1:G:200:LEU:HA	1.85	0.42
1:E:142:ARG:NH1	6:E:629:HOH:O	2.24	0.42
1:A:95:ASP:OD2	1:A:125:HIS:ND1	2.52	0.42
1:E:190:MET:HE1	2:F:173:HIS:CG	2.55	0.41
2:H:179:THR:CG2	2:H:182:ILE:HG12	2.49	0.41
1:G:83:PRO:HD3	1:G:114:TYR:CZ	2.55	0.41
1:G:45:ILE:HG21	1:G:111:LYS:HE3	2.02	0.41
1:A:7:LEU:HD12	1:A:8:ASN:N	2.36	0.41
1:G:95:ASP:H	1:G:100:SER:HG	1.69	0.41
2:D:177:ILE:O	2:D:178:SER:CB	2.69	0.41
1:G:247:ALA:O	1:G:248:HIS:HB3	2.21	0.41
1:E:286:ASP:OD1	1:E:286:ASP:C	2.60	0.41
1:C:61:ILE:HA	1:C:88:LEU:O	2.21	0.40
1:G:284:SER:O	1:G:291:CYS:HA	2.21	0.40
1:G:171:CYS:HA	1:G:245:CYS:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:653:HOH:O	6:E:622:HOH:O[4_556]	2.04	0.16

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	294/306 (96%)	284 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	294/306 (96%)	278 (95%)	14 (5%)	2 (1%)	30	23
1	E	291/306 (95%)	277 (95%)	14 (5%)	0	100	100
1	G	296/306 (97%)	280 (95%)	16 (5%)	0	100	100
2	B	37/62 (60%)	35 (95%)	2 (5%)	0	100	100
2	D	35/62 (56%)	34 (97%)	1 (3%)	0	100	100
2	F	35/62 (56%)	34 (97%)	1 (3%)	0	100	100
2	H	39/62 (63%)	36 (92%)	1 (3%)	2 (5%)	3	0
All	All	1321/1472 (90%)	1258 (95%)	59 (4%)	4 (0%)	50	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	LEU
2	H	181	THR
1	C	260	LYS
2	H	182	ILE

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	261/267 (98%)	259 (99%)	2 (1%)	89	93
1	C	261/267 (98%)	260 (100%)	1 (0%)	95	97
1	E	258/267 (97%)	255 (99%)	3 (1%)	82	87
1	G	262/267 (98%)	259 (99%)	3 (1%)	84	88
2	B	40/58 (69%)	39 (98%)	1 (2%)	60	63
2	D	37/58 (64%)	34 (92%)	3 (8%)	17	12
2	F	38/58 (66%)	37 (97%)	1 (3%)	59	62
2	H	41/58 (71%)	39 (95%)	2 (5%)	35	31
All	All	1198/1300 (92%)	1182 (99%)	16 (1%)	80	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	246	ARG
2	B	204	SER
1	C	246	ARG
2	D	205	GLU
2	D	206	ASP
2	D	214	ASP
1	E	9	LEU
1	E	132	ARG
1	E	246	ARG
2	F	214	ASP
1	G	168	LYS
1	G	214	GLN
1	G	246	ARG
2	H	-1	MET
2	H	199	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	262	GLN
1	C	68	GLN
1	C	262	GLN
2	D	170	ASN
1	E	117	ASN
1	E	198	GLN
1	E	249	GLN
1	E	262	GLN
2	F	173	HIS
1	G	8	ASN
1	G	214	GLN
1	G	239	HIS
2	H	173	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	403	-	5,5,5	0.31	0	5,5,5	0.35	0
4	GOL	A	404	-	5,5,5	0.31	0	5,5,5	0.40	0
4	GOL	A	405	-	5,5,5	0.37	0	5,5,5	0.19	0
5	15P	A	406	-	11,11,103	4.24	1 (9%)	9,10,102	1.49	1 (11%)
4	GOL	C	403	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GOL	C	404	-	5,5,5	0.32	0	5,5,5	0.26	0
4	GOL	C	405	-	5,5,5	0.38	0	5,5,5	0.37	0
4	GOL	E	403	-	5,5,5	0.35	0	5,5,5	0.41	0
4	GOL	E	404	-	5,5,5	0.28	0	5,5,5	0.38	0
4	GOL	E	405	-	5,5,5	0.39	0	5,5,5	0.21	0
4	GOL	G	403	-	5,5,5	0.26	0	5,5,5	0.35	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	403	-	-	0/4/4/4	0/0/0/0
4	GOL	A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	A	405	-	-	0/4/4/4	0/0/0/0
5	15P	A	406	-	-	0/9/9/101	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	403	-	-	0/4/4/4	0/0/0/0
4	GOL	C	404	-	-	0/4/4/4	0/0/0/0
4	GOL	C	405	-	-	0/4/4/4	0/0/0/0
4	GOL	E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	E	404	-	-	0/4/4/4	0/0/0/0
4	GOL	E	405	-	-	0/4/4/4	0/0/0/0
4	GOL	G	403	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	15P	C1-C2	-13.87	1.49	1.55

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	406	15P	C2-O1-C3	2.11	119.45	112.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å²)	Q<0.9	
1	A	293/306 (95%)	0.10	9 (3%)	47	52	12, 23, 52, 113	0
1	C	295/306 (96%)	0.14	8 (2%)	52	57	11, 23, 55, 102	0
1	E	293/306 (95%)	0.08	10 (3%)	43	47	14, 28, 56, 105	0
1	G	297/306 (97%)	0.52	28 (9%)	9	9	18, 38, 78, 119	0
2	B	41/62 (66%)	0.76	5 (12%)	5	5	14, 37, 78, 81	0
2	D	39/62 (62%)	0.56	7 (17%)	2	2	18, 37, 76, 96	0
2	F	39/62 (62%)	0.59	5 (12%)	4	5	22, 43, 79, 91	0
2	H	43/62 (69%)	1.36	9 (20%)	1	1	25, 63, 105, 119	0
All	All	1340/1472 (91%)	0.29	81 (6%)	21	24	11, 29, 69, 119	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	6.1
2	H	182	ILE	5.9
2	H	200	ARG	5.4
2	H	201	VAL	5.3
2	H	209	ILE	5.0
2	H	181	THR	4.9
1	C	213	VAL	4.9
1	G	213	VAL	4.7
1	G	24	PRO	4.6
1	G	250	VAL	4.6
1	G	264	VAL	4.4
2	H	210	ILE	4.4
1	G	232	VAL	4.2
1	G	19	VAL	4.1
1	G	61	ILE	4.1
1	A	23	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	244	ILE	4.0
1	G	169	ILE	3.8
1	A	24	PRO	3.8
1	G	165	VAL	3.7
2	B	182	ILE	3.6
1	E	223	VAL	3.5
2	H	199	SER	3.5
1	C	232	VAL	3.4
1	G	276	PHE	3.3
1	E	213	VAL	3.3
1	C	7	LEU	3.3
2	H	198	ASN	3.2
1	E	285	VAL	3.2
2	B	209	ILE	3.2
1	A	214	GLN	3.1
2	B	160	GLU	3.1
2	F	210	ILE	3.0
1	E	161	ILE	2.9
2	D	177	ILE	2.9
1	E	146	ILE	2.9
1	G	243	LEU	2.9
1	A	19	VAL	2.8
1	G	251	VAL	2.8
1	C	24	PRO	2.8
1	C	23	ARG	2.8
2	F	200	ARG	2.8
2	D	-1	MET	2.7
1	C	231	VAL	2.7
1	G	285	VAL	2.7
2	D	178	SER	2.7
1	A	213	VAL	2.7
2	H	202	THR	2.6
1	C	250	VAL	2.6
2	F	209	ILE	2.6
1	G	295	ILE	2.5
2	F	201	VAL	2.5
2	D	201	VAL	2.5
2	D	-2	ALA	2.4
1	G	237	HIS	2.4
1	G	274	GLY	2.4
1	E	25	GLY	2.3
1	G	65	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	182	ILE	2.3
1	E	214	GLN	2.3
1	G	23	ARG	2.3
1	C	251	VAL	2.3
1	G	28	VAL	2.3
1	A	250	VAL	2.3
1	G	25	GLY	2.3
1	G	252	GLU	2.2
1	G	265	THR	2.2
2	B	210	ILE	2.2
1	G	266	LEU	2.2
2	B	183	GLU	2.2
1	E	288	THR	2.2
1	G	241	LEU	2.1
1	G	161	ILE	2.1
2	D	209	ILE	2.1
2	D	199	SER	2.1
1	G	235	PHE	2.1
1	E	65	ILE	2.0
1	G	186	ILE	2.0
1	A	28	VAL	2.0
1	E	19	VAL	2.0
1	A	299	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	C	403	6/6	0.27	6.28	31,52,60,63	4
4	GOL	E	404	6/6	0.23	4.14	42,50,60,60	3
4	GOL	E	405	6/6	0.21	3.82	45,55,64,69	1
4	GOL	A	405	6/6	0.28	3.82	47,57,66,67	2
4	GOL	C	405	6/6	0.31	3.54	49,59,70,78	2
4	GOL	G	403	6/6	0.17	3.22	41,51,66,73	1
3	MN	E	402	1/1	0.13	1.45	16,16,16,16	1
4	GOL	E	403	6/6	0.23	1.22	45,57,67,68	1
3	MN	A	401	1/1	0.11	1.09	20,20,20,20	1
5	15P	A	406	12/104	0.20	1.06	40,53,58,60	0
4	GOL	A	404	6/6	0.19	0.99	25,51,63,66	3
4	GOL	A	403	6/6	0.14	0.94	36,51,62,62	2
4	GOL	C	404	6/6	0.15	0.72	24,34,57,57	2
3	MN	C	402	1/1	0.09	-1.23	17,17,17,17	1
3	MN	G	401	1/1	0.06	-2.01	50,50,50,50	1
3	MN	G	402	1/1	0.09	-2.49	29,29,29,29	0
3	MN	C	401	1/1	0.04	-4.02	38,38,38,38	0
3	MN	E	401	1/1	0.04	-5.42	37,37,37,37	0
3	MN	A	402	1/1	0.04	-6.41	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.