Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:50 PM 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

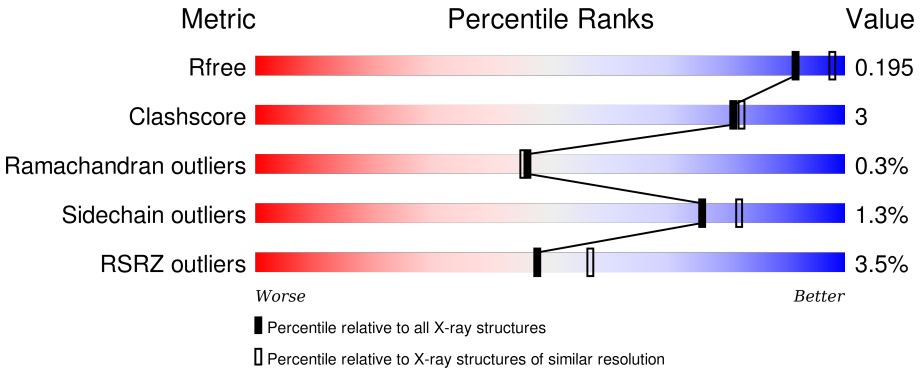
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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 <=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	306	2% 89% 6%
1	C	306	2% 89% 7%
1	E	306	% 88% 8%
1	G	306	5% 88% 9%
2	B	62	5% 63% 34%

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Mol	Chain	Length	Quality of chain
2	D	62	6% 52% 11% 37%
2	F	62	3% 56% 5% 37%
2	H	62	15% 60% 6% 31%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MN	A	401	-	-	-	X
3	MN	E	402	-	-	-	X
4	GOL	A	405	-	-	-	X
4	GOL	C	403	-	-	-	X
4	GOL	C	404	-	-	-	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 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	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 640 202 306 54 78	0	0	0
2	D	39	Total C H N O S 601 190 284 52 74 1	0	0	0
2	F	39	Total C H N O 614 194 295 52 73	0	0	0
2	H	43	Total C H N O S 669 210 322 57 79 1	0	0	0

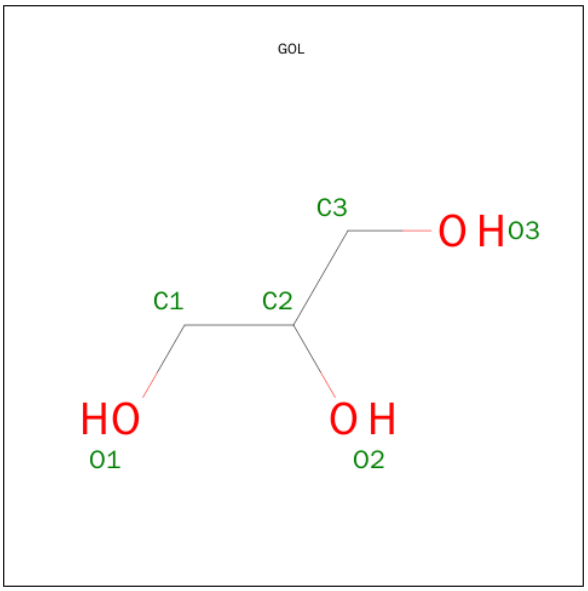
There are 12 discrepancies between the modelled and reference sequences:

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).

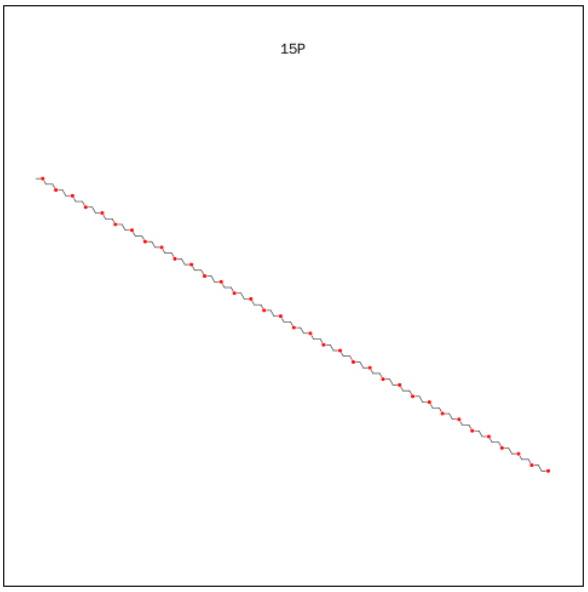
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Mn 2 2	0	0
3	A	2	Total Mn 2 2	0	0
3	C	2	Total Mn 2 2	0	0
3	E	2	Total Mn 2 2	0	0

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



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

- Molecule 5 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).



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

- Molecule 6 is water.

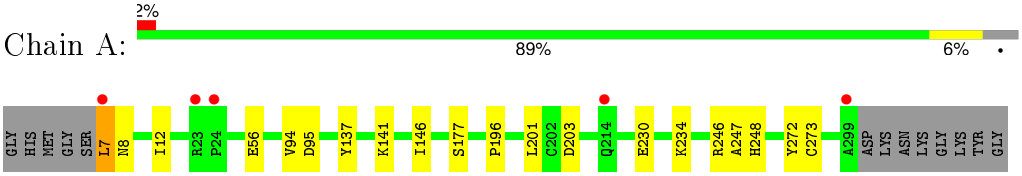
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	169	Total O 169 169	0	0
6	B	27	Total O 27 27	0	0
6	C	165	Total O 165 165	0	0
6	D	30	Total O 30 30	0	0
6	E	140	Total O 140 140	0	0
6	F	22	Total O 22 22	0	0
6	G	98	Total O 98 98	0	0
6	H	10	Total O 10 10	0	0

3 Residue-property plots (i)

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.

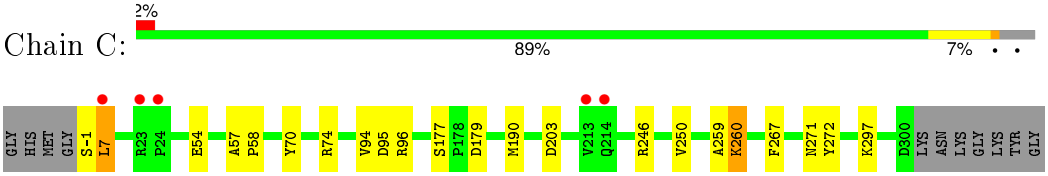
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

Chain A:



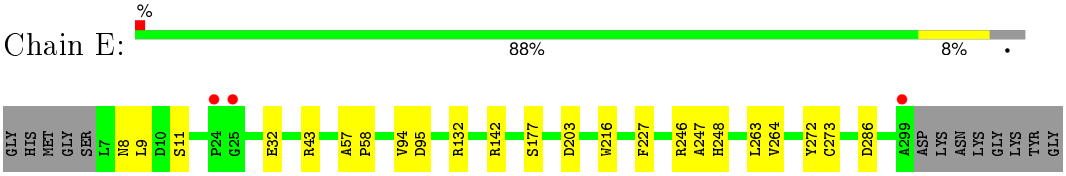
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

Chain C:



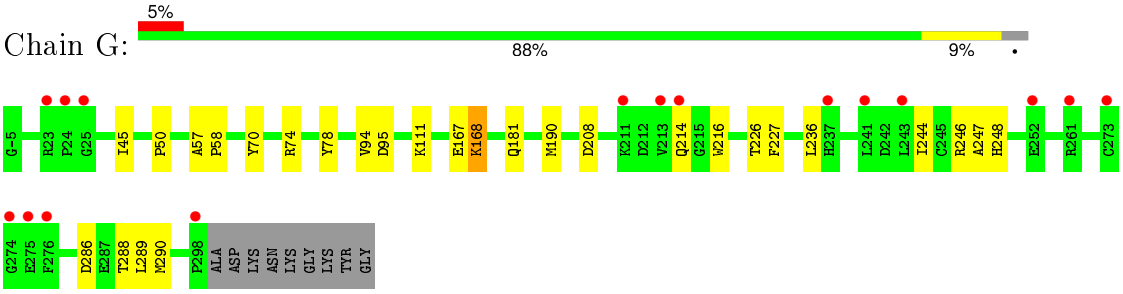
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

Chain E:



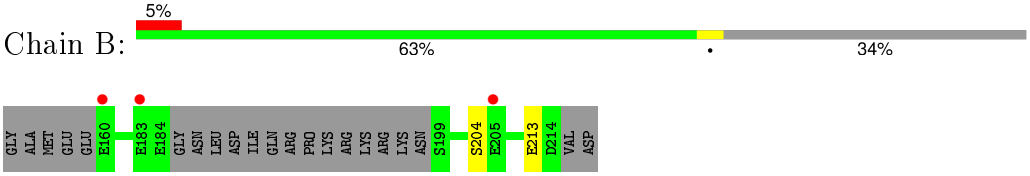
- Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit

Chain G:



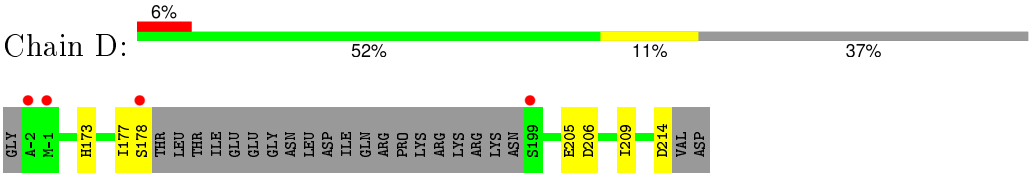
- Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain B:



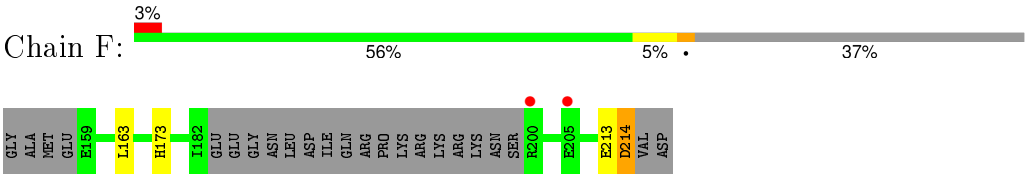
• Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain D:



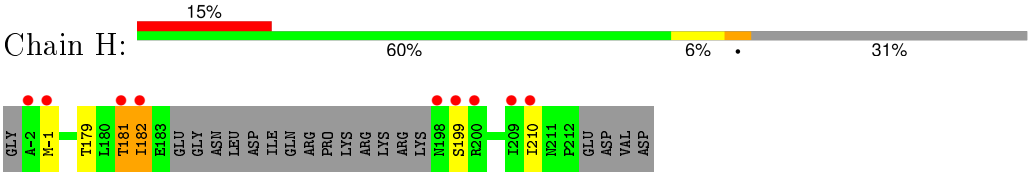
• Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain F:



• Molecule 2: Nuclear inhibitor of protein phosphatase 1

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	4.75 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.154 , 0.196 0.154 , 0.195	Depositor DCC
R_{free} test set	4409 reflections (5.49%)	DCC
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	2372	2348	2346	15	0
1	C	2376	2336	2336	15	0
1	E	2356	2321	2318	14	0
1	G	2388	2353	2352	16	0
2	B	334	306	305	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	317	284	286	6	0
2	F	319	295	294	3	0
2	H	347	322	324	9	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	24	1	0
4	C	18	24	24	1	0
4	E	18	24	24	0	0
4	G	6	8	8	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	2	0
All	All	11550	10645	10655	72	1

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.

All (72) 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:C:-1:SER:O	1:C:7:LEU:HB2	1.80	0.80
1:E:32:GLU:OE2	6:E:568:HOH:O	2.13	0.66
1:A:7:LEU:HD11	1:A:12:ILE:CD1	2.25	0.65
1:E:57:ALA:HB1	1:E:58:PRO:HA	1.81	0.62
2:H:179:THR:O	2:H:179:THR:HG22	2.02	0.60
1:A:56:GLU:H	4:A:403:GOL:H32	1.68	0.58
1:G:236:LEU:HD21	1:G:244:ILE:HG13	1.87	0.57
1:C:54:GLU:O	4:C:403:GOL:H31	2.04	0.56
1:G:286:ASP:OD2	1:G:290:MET:HB3	2.06	0.56
1:G:167:GLU:O	1:G:168:LYS:HD3	2.06	0.55
1:E:272:TYR:O	1:E:273:CYS:HB2	2.07	0.55
1:C:271:ASN:HB3	6:C:655:HOH:O	2.06	0.55
1:C:94:VAL:O	1:C:95:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLU:O	2:B:213:GLU:HG2	2.06	0.54
1:G:288:THR:O	1:G:289:LEU:HB2	2.08	0.54
1:A:137:TYR:CE2	1:A:146[A]:ILE:HD12	2.42	0.54
1:A:177:SER:HB2	1:A:203:ASP:HB2	1.90	0.53
2:H:179:THR:HG22	2:H:182:ILE:HG12	1.90	0.53
1:E:177:SER:HB2	1:E:203:ASP:HB2	1.91	0.53
1:A:7:LEU:HD11	1:A:12:ILE:HD11	1.89	0.52
1:G:181:GLN:CG	2:H:181:THR:HG21	2.40	0.52
1:G:57:ALA:HB1	1:G:58:PRO:HA	1.92	0.51
1:A:247:ALA:O	1:A:248:HIS:HB3	2.10	0.51
1:E:94:VAL:O	1:E:95:ASP:HB2	2.11	0.51
1:G:94:VAL:O	1:G:95:ASP:HB2	2.12	0.50
2:H:182:ILE:O	2:H:182:ILE:HG22	2.11	0.50
1:C:177:SER:HB2	1:C:203:ASP:HB2	1.94	0.49
1:C:190:MET:HE2	2:D:173:HIS:ND1	2.28	0.49
1:C:-1:SER:O	1:C:7:LEU:CB	2.59	0.49
6:C:656:HOH:O	2:D:173:HIS:HE1	1.96	0.48
1:G:78:TYR:CD1	2:H:210:ILE:HG12	2.49	0.48
1:A:94:VAL:O	1:A:95:ASP:HB2	2.12	0.48
2:H:179:THR:HG22	2:H:182:ILE:CG1	2.44	0.47
1:E:247:ALA:O	1:E:248:HIS:HB3	2.14	0.47
1:G:50:PRO:HD2	4:G:403:GOL:H12	1.95	0.47
1:A:141:LYS:HB2	1:A:146[A]:ILE:HD11	1.96	0.47
1:C:250:VAL:HG22	1:C:267:PHE:CZ	2.50	0.47
1:C:259:ALA:O	1:C:260:LYS:HB2	2.15	0.47
1:G:78:TYR:CG	2:H:210:ILE:HG12	2.50	0.46
1:E:263:LEU:HD23	1:E:263:LEU:C	2.36	0.46
1:C:179:ASP:OD2	2:D:177:ILE:HG23	2.16	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
2:H:179:THR:HB	6:H:305:HOH:O	2.16	0.45
1:A:272:TYR:O	1:A:273:CYS:HB2	2.16	0.45
1:A:177:SER:HB2	1:A:203:ASP:CB	2.46	0.45
5:A:406:15P:H28	5:A:406:15P:H16	1.59	0.45
1:A:7:LEU:HD11	1:A:12:ILE:HD12	1.98	0.45
1:C:190:MET:CE	2:D:173:HIS:CG	3.00	0.45
1:C:70:TYR:O	1:C:74:ARG:HG3	2.17	0.45
1:E:263:LEU:HD23	1:E:264:VAL:N	2.33	0.44
1:C:96:ARG:HG3	1:C:272:TYR:OH	2.18	0.44
2:H:179:THR:CG2	2:H:182:ILE:HG12	2.47	0.43
1:E:8:ASN:ND2	1:E:11:SER:CB	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:ASP:O	1:G:226:THR:HA	2.19	0.43
1:E:216:TRP:CZ3	1:E:227:PHE:HB3	2.54	0.43
1:G:70:TYR:O	1:G:74:ARG:HG3	2.19	0.43
1:C:57:ALA:HB1	1:C:58:PRO:HA	2.01	0.42
1:G:45:ILE:HG21	1:G:111:LYS:HE3	2.00	0.42
1:A:230:GLU:HG3	1:A:234:LYS:HE3	2.02	0.42
1:C:297:LYS:HE2	2:D:209:ILE:HD12	2.01	0.42
1:E:142:ARG:NH1	6:E:629:HOH:O	2.24	0.42
2:F:213:GLU:O	2:F:214:ASP:HB2	2.19	0.42
1:G:247:ALA:O	1:G:248:HIS:HB3	2.20	0.41
1:A:7:LEU:HD12	1:A:8:ASN:N	2.36	0.41
1:G:190[B]:MET:HE1	6:H:306:HOH:O	2.19	0.41
1:A:196:PRO:HD3	1:A:201:LEU:HD23	2.02	0.41
1:E:8:ASN:ND2	1:E:11:SER:HB3	2.36	0.41
2:D:177:ILE:O	2:D:178:SER:CB	2.69	0.41
1:E:286:ASP:OD1	1:E:286:ASP:C	2.60	0.41
1:A:7:LEU:CD1	1:A:12:ILE:HD11	2.51	0.40
1:E:43:ARG:NH2	2:F:163:LEU:HD11	2.36	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	Interatomic distance (Å)	Clash overlap (Å)
6:C:653:HOH:O	6:E:622:HOH:O[4_556]	2.04	0.16

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	294/306 (96%)	284 (97%)	10 (3%)	0	100 100
1	C	294/306 (96%)	278 (95%)	14 (5%)	2 (1%)	26 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	2	0
All	All	1321/1472 (90%)	1258 (95%)	59 (4%)	4 (0%)	46	45

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 (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	261/267 (98%)	259 (99%)	2 (1%)	86	91
1	C	261/267 (98%)	260 (100%)	1 (0%)	93	96
1	E	258/267 (97%)	255 (99%)	3 (1%)	78	84
1	G	262/267 (98%)	259 (99%)	3 (1%)	80	85
2	B	40/58 (69%)	39 (98%)	1 (2%)	55	59
2	D	37/58 (64%)	34 (92%)	3 (8%)	15	10
2	F	38/58 (66%)	37 (97%)	1 (3%)	54	58
2	H	41/58 (71%)	39 (95%)	2 (5%)	31	28
All	All	1198/1300 (92%)	1182 (99%)	16 (1%)	76	82

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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	GLN
1	E	8	ASN
1	E	198	GLN
2	F	173	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	0.32	0	5,5,5	0.32	0
4	GOL	A	404	-	5,5,5	0.33	0	5,5,5	0.34	0
4	GOL	A	405	-	5,5,5	0.38	0	5,5,5	0.17	0
5	15P	A	406	-	11,11,103	0.63	0	10,10,102	1.37	0
4	GOL	C	403	-	5,5,5	0.38	0	5,5,5	0.33	0
4	GOL	C	404	-	5,5,5	0.34	0	5,5,5	0.23	0
4	GOL	C	405	-	5,5,5	0.40	0	5,5,5	0.32	0
4	GOL	E	403	-	5,5,5	0.36	0	5,5,5	0.42	0
4	GOL	E	404	-	5,5,5	0.29	0	5,5,5	0.34	0
4	GOL	E	405	-	5,5,5	0.41	0	5,5,5	0.13	0
4	GOL	G	403	-	5,5,5	0.26	0	5,5,5	0.33	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
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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	GOL	1	0
5	A	406	15P	1	0
4	C	403	GOL	1	0
4	G	403	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	293/306 (95%)	-0.04	5 (1%) 73 78	12, 23, 52, 113	0
1	C	295/306 (96%)	0.00	5 (1%) 73 78	11, 22, 55, 102	0
1	E	293/306 (95%)	-0.10	3 (1%) 84 87	14, 28, 56, 105	0
1	G	297/306 (97%)	0.30	16 (5%) 29 38	18, 38, 78, 119	0
2	B	41/62 (66%)	0.49	3 (7%) 18 24	14, 36, 78, 81	0
2	D	39/62 (62%)	0.43	4 (10%) 9 12	18, 36, 76, 96	0
2	F	39/62 (62%)	0.38	2 (5%) 32 40	22, 43, 73, 91	0
2	H	43/62 (69%)	1.15	9 (20%) 1 1	26, 61, 98, 108	0
All	All	1340/1472 (91%)	0.11	47 (3%) 48 57	11, 28, 68, 119	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	6.5
2	H	182	ILE	5.9
1	G	24	PRO	5.3
2	H	200	ARG	5.2
2	H	181	THR	4.8
1	C	24	PRO	4.3
1	G	274	GLY	4.3
1	A	23	ARG	4.1
1	G	276	PHE	4.1
1	A	24	PRO	3.7
1	A	214	GLN	3.7
1	C	23	ARG	3.5
1	G	25	GLY	3.5
1	G	213	VAL	3.4
1	C	7	LEU	3.4
1	G	23	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	273	CYS	3.3
2	F	200	ARG	3.3
2	B	160	GLU	3.2
2	D	-1	MET	3.1
2	H	198	ASN	3.0
1	G	275	GLU	2.9
2	H	209	ILE	2.9
2	D	-2	ALA	2.7
2	F	205	GLU	2.7
1	E	24	PRO	2.7
1	E	25	GLY	2.7
2	H	-1	MET	2.6
2	H	199	SER	2.6
1	G	214	GLN	2.5
2	D	178	SER	2.5
1	G	252	GLU	2.4
2	B	183	GLU	2.4
1	G	261	ARG	2.3
1	G	243	LEU	2.3
1	G	237	HIS	2.3
1	G	241	LEU	2.2
2	H	-2	ALA	2.2
2	H	210	ILE	2.2
1	G	298	PRO	2.2
1	C	214	GLN	2.1
1	C	213	VAL	2.1
1	E	299	ALA	2.1
2	B	205	GLU	2.1
1	A	299	ALA	2.0
2	D	199	SER	2.0
1	G	211	LYS	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 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	405	6/6	0.87	0.27	13.25	47,57,66,67	2
4	GOL	C	405	6/6	0.86	0.34	10.05	49,59,70,78	2
4	GOL	C	403	6/6	0.88	0.26	6.85	31,52,60,63	4
4	GOL	E	405	6/6	0.79	0.20	4.98	45,55,64,69	1
4	GOL	G	403	6/6	0.89	0.19	4.96	41,51,66,73	1
3	MN	E	402	1/1	0.99	0.14	4.12	16,16,16,16	1
4	GOL	E	404	6/6	0.90	0.20	3.78	42,50,60,60	3
3	MN	A	401	1/1	0.99	0.12	2.28	20,20,20,20	1
4	GOL	C	404	6/6	0.97	0.15	2.19	24,34,57,57	2
5	15P	A	406	12/104	0.83	0.18	1.78	40,53,58,60	0
4	GOL	E	403	6/6	0.89	0.15	1.01	45,57,67,68	1
4	GOL	A	404	6/6	0.84	0.19	1.01	25,51,63,66	3
3	MN	C	402	1/1	0.99	0.11	0.64	17,17,17,17	1
4	GOL	A	403	6/6	0.90	0.14	0.59	36,51,62,62	2
3	MN	G	402	1/1	0.99	0.10	-0.32	29,29,29,29	0
3	MN	G	401	1/1	0.97	0.07	-1.45	50,50,50,50	1
3	MN	E	401	1/1	0.99	0.05	-4.59	37,37,37,37	0
3	MN	C	401	1/1	0.99	0.05	-4.87	38,38,38,38	0
3	MN	A	402	1/1	0.99	0.04	-6.56	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.