Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 03:27 PM EDT

PDB ID	:	5O0W
Title	:	Crystal structure of the complex between Nb474 and Trypanosoma congolense fructose-1,6-bisphosphate aldolase
Authors	:	Pinto, J.; Magez, S.; Sterckx, Y.
Deposited on	:	2017-05-17
Resolution	:	2.57 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:

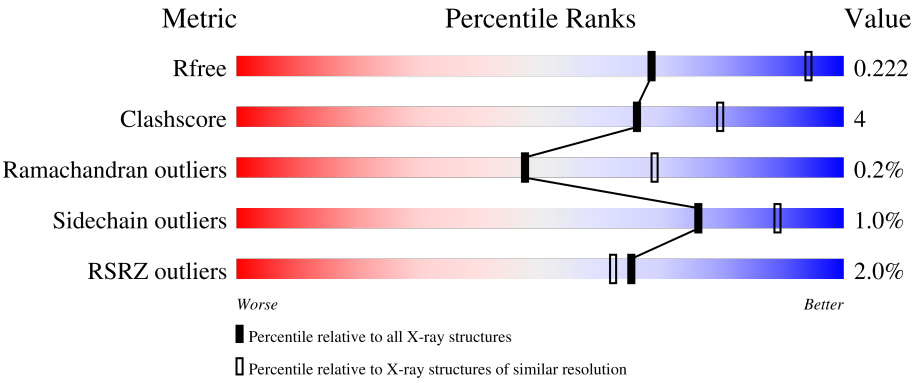
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.57 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 <=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	387	2% 82% 10% 7%
1	B	387	% 84% 9% 7%
1	C	387	% 83% 9% 7%
1	D	387	% 85% 7% 7%
2	E	143	2% 87% 9% .

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Mol	Chain	Length	Quality of chain
2	F	143	5% 85% 10%
2	G	143	6% 86% 10%
2	H	143	2% 81% 14% 5%

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	GOL	D	401	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15500 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2732	1719	484	512	17			
1	B	358	Total	C	N	O	S	0	0	0
			2728	1714	485	512	17			
1	C	360	Total	C	N	O	S	0	0	0
			2734	1718	485	514	17			
1	D	359	Total	C	N	O	S	0	0	0
			2714	1709	480	508	17			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLU	-	expression tag	UNP G0UWE7
A	374	ASN	-	expression tag	UNP G0UWE7
A	375	LEU	-	expression tag	UNP G0UWE7
A	376	TYR	-	expression tag	UNP G0UWE7
A	377	PHE	-	expression tag	UNP G0UWE7
A	378	GLN	-	expression tag	UNP G0UWE7
A	379	SER	-	expression tag	UNP G0UWE7
A	380	GLY	-	expression tag	UNP G0UWE7
A	381	GLY	-	expression tag	UNP G0UWE7
A	382	HIS	-	expression tag	UNP G0UWE7
A	383	HIS	-	expression tag	UNP G0UWE7
A	384	HIS	-	expression tag	UNP G0UWE7
A	385	HIS	-	expression tag	UNP G0UWE7
A	386	HIS	-	expression tag	UNP G0UWE7
A	387	HIS	-	expression tag	UNP G0UWE7
B	373	GLU	-	expression tag	UNP G0UWE7
B	374	ASN	-	expression tag	UNP G0UWE7
B	375	LEU	-	expression tag	UNP G0UWE7
B	376	TYR	-	expression tag	UNP G0UWE7
B	377	PHE	-	expression tag	UNP G0UWE7
B	378	GLN	-	expression tag	UNP G0UWE7

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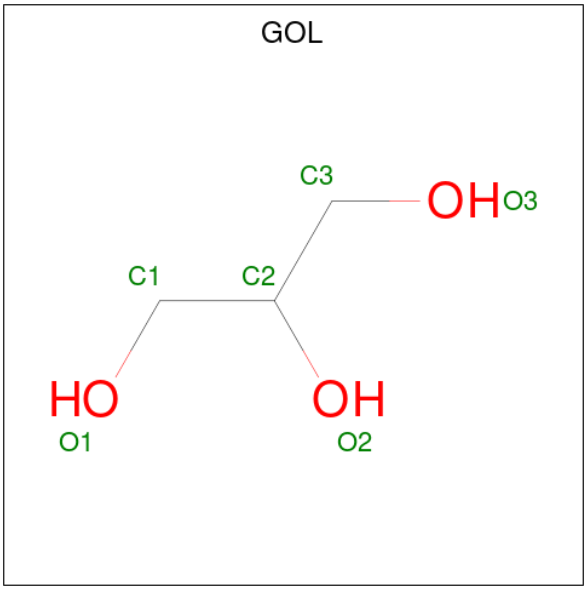
Chain	Residue	Modelled	Actual	Comment	Reference
B	379	SER	-	expression tag	UNP G0UWE7
B	380	GLY	-	expression tag	UNP G0UWE7
B	381	GLY	-	expression tag	UNP G0UWE7
B	382	HIS	-	expression tag	UNP G0UWE7
B	383	HIS	-	expression tag	UNP G0UWE7
B	384	HIS	-	expression tag	UNP G0UWE7
B	385	HIS	-	expression tag	UNP G0UWE7
B	386	HIS	-	expression tag	UNP G0UWE7
B	387	HIS	-	expression tag	UNP G0UWE7
C	373	GLU	-	expression tag	UNP G0UWE7
C	374	ASN	-	expression tag	UNP G0UWE7
C	375	LEU	-	expression tag	UNP G0UWE7
C	376	TYR	-	expression tag	UNP G0UWE7
C	377	PHE	-	expression tag	UNP G0UWE7
C	378	GLN	-	expression tag	UNP G0UWE7
C	379	SER	-	expression tag	UNP G0UWE7
C	380	GLY	-	expression tag	UNP G0UWE7
C	381	GLY	-	expression tag	UNP G0UWE7
C	382	HIS	-	expression tag	UNP G0UWE7
C	383	HIS	-	expression tag	UNP G0UWE7
C	384	HIS	-	expression tag	UNP G0UWE7
C	385	HIS	-	expression tag	UNP G0UWE7
C	386	HIS	-	expression tag	UNP G0UWE7
C	387	HIS	-	expression tag	UNP G0UWE7
D	373	GLU	-	expression tag	UNP G0UWE7
D	374	ASN	-	expression tag	UNP G0UWE7
D	375	LEU	-	expression tag	UNP G0UWE7
D	376	TYR	-	expression tag	UNP G0UWE7
D	377	PHE	-	expression tag	UNP G0UWE7
D	378	GLN	-	expression tag	UNP G0UWE7
D	379	SER	-	expression tag	UNP G0UWE7
D	380	GLY	-	expression tag	UNP G0UWE7
D	381	GLY	-	expression tag	UNP G0UWE7
D	382	HIS	-	expression tag	UNP G0UWE7
D	383	HIS	-	expression tag	UNP G0UWE7
D	384	HIS	-	expression tag	UNP G0UWE7
D	385	HIS	-	expression tag	UNP G0UWE7
D	386	HIS	-	expression tag	UNP G0UWE7
D	387	HIS	-	expression tag	UNP G0UWE7

- Molecule 2 is a protein called Nb474.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	137	Total	C	N	O	S	0	0	0
			1009	620	178	206	5			
2	F	137	Total	C	N	O	S	0	0	0
			1015	621	179	210	5			
2	G	138	Total	C	N	O	S	0	0	0
			1016	624	179	208	5			
2	H	136	Total	C	N	O	S	0	0	0
			1000	615	175	205	5			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

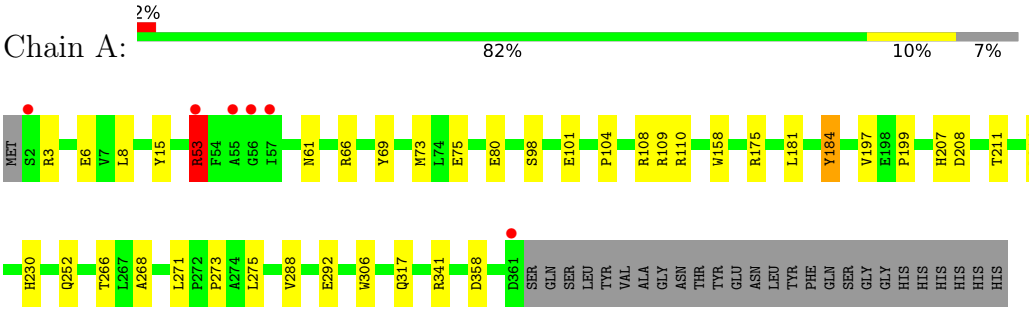
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	118	Total O 118 118	0	0
4	B	101	Total O 101 101	0	0
4	C	98	Total O 98 98	0	0
4	D	111	Total O 111 111	0	0
4	E	22	Total O 22 22	0	0
4	F	18	Total O 18 18	0	0
4	G	25	Total O 25 25	0	0
4	H	23	Total O 23 23	0	0

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.

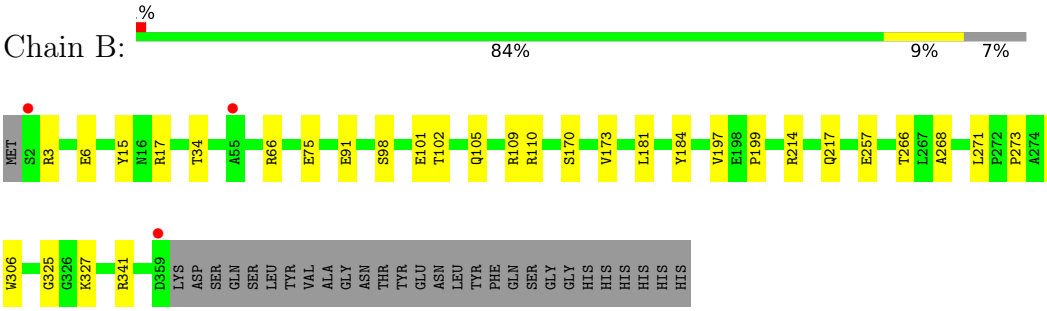
• Molecule 1: Fructose-bisphosphate aldolase

Chain A:



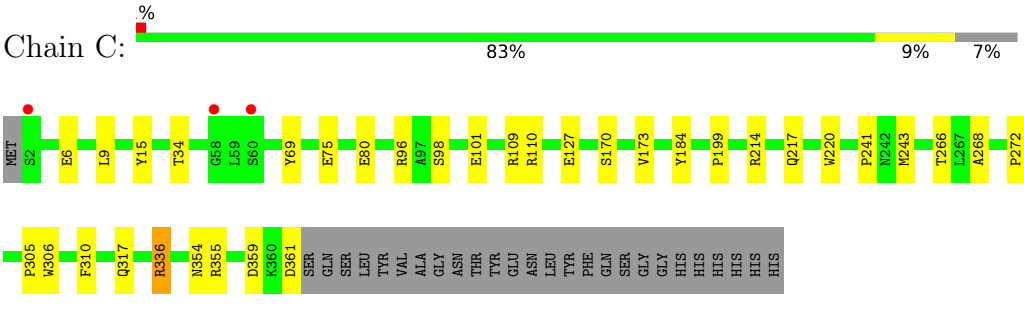
• Molecule 1: Fructose-bisphosphate aldolase

Chain B:



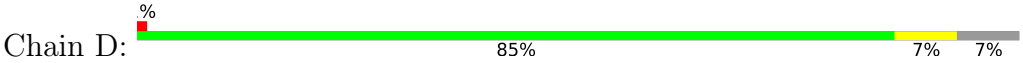
• Molecule 1: Fructose-bisphosphate aldolase

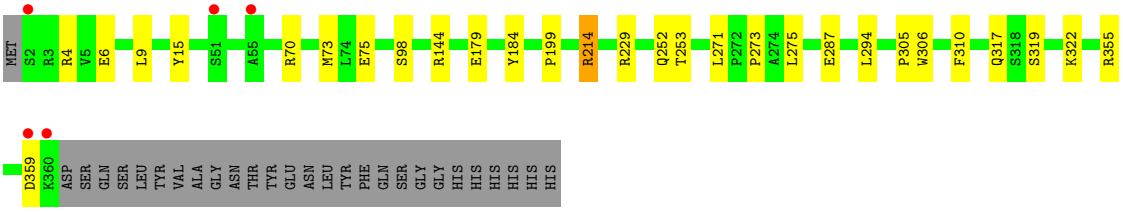
Chain C:



• Molecule 1: Fructose-bisphosphate aldolase

Chain D:



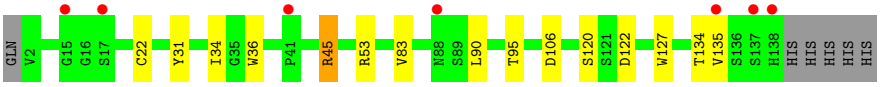


• Molecule 2: Nb474

Chain E:

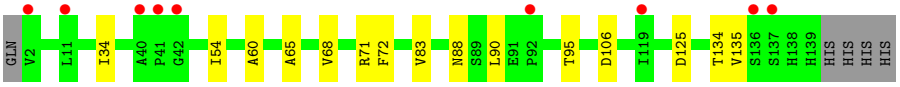
• Molecule 2: Nb474

Chain F:



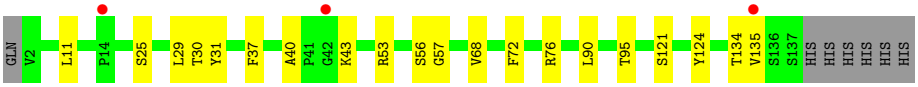
• Molecule 2: Nb474

Chain G:



• Molecule 2: Nb474

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.82Å 188.87Å 126.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 2.57 48.25 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.23-2.57) 99.0 (48.25-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.192 , 0.222 0.193 , 0.222	Depositor DCC
R_{free} test set	6839 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15500	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, 0.333 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: 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	0.27	0/2786	0.48	1/3780 (0.0%)
1	B	0.26	0/2782	0.46	0/3774
1	C	0.26	0/2788	0.46	0/3783
1	D	0.26	0/2768	0.45	0/3758
2	E	0.26	0/1027	0.52	0/1397
2	F	0.43	0/1033	0.60	0/1404
2	G	0.26	0/1034	0.49	0/1406
2	H	0.26	0/1018	0.53	0/1385
All	All	0.28	0/15236	0.49	1/20687 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	NE-CZ-NH2	5.95	123.28	120.30

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	2732	0	2688	28	0
1	B	2728	0	2691	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2734	0	2691	24	0
1	D	2714	0	2664	21	0
2	E	1009	0	919	12	0
2	F	1015	0	923	11	0
2	G	1016	0	926	9	0
2	H	1000	0	913	11	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	12	0	16	1	0
3	D	12	0	16	0	0
4	A	118	0	0	2	0
4	B	101	0	0	0	0
4	C	98	0	0	0	0
4	D	111	0	0	2	0
4	E	22	0	0	0	0
4	F	18	0	0	0	0
4	G	25	0	0	0	0
4	H	23	0	0	0	0
All	All	15500	0	14463	118	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 (118) 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)
2:E:45:ARG:NH1	2:E:127:TRP:CZ2	2.40	0.90
2:E:45:ARG:NH1	2:E:127:TRP:CE2	2.45	0.84
1:A:101:GLU:OE2	1:A:109:ARG:NH1	2.14	0.80
2:E:45:ARG:NH1	2:E:127:TRP:CH2	2.53	0.77
1:C:336:ARG:NH1	2:G:125:ASP:OD2	2.23	0.72
1:A:53:ARG:HH11	1:A:53:ARG:HG2	1.56	0.71
1:C:75:GLU:OE1	1:C:98:SER:HB3	1.93	0.69
1:B:101:GLU:OE1	1:B:109:ARG:NH1	2.26	0.69
1:C:355:ARG:NH1	1:C:359:ASP:O	2.27	0.67
1:D:144:ARG:NH1	4:D:501:HOH:O	2.29	0.66
2:F:90:LEU:HB3	2:F:135:VAL:HG21	1.79	0.65
1:A:104:PRO:O	1:A:108:ARG:HG3	1.96	0.65
1:B:75:GLU:OE2	1:B:98:SER:OG	2.16	0.61
2:E:45:ARG:NH1	2:E:127:TRP:CD2	2.68	0.61
2:F:95:THR:HG23	2:F:134:THR:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:OE2	1:B:257:GLU:N	2.30	0.61
1:C:101:GLU:OE1	1:C:109:ARG:NH1	2.33	0.61
1:A:53:ARG:HG2	1:A:53:ARG:NH1	2.16	0.60
1:A:69:TYR:OH	1:A:317:GLN:OE1	2.19	0.60
1:A:61:ASN:OD1	1:A:66:ARG:NH1	2.33	0.59
2:F:45:ARG:NH1	2:F:127:TRP:CE2	2.72	0.58
2:E:34:ILE:HG13	2:E:83:VAL:HG21	1.85	0.57
1:C:69:TYR:OH	1:C:317:GLN:OE1	2.20	0.57
1:D:75:GLU:OE1	1:D:98:SER:OG	2.16	0.57
1:D:179:GLU:OE2	1:D:229:ARG:NH1	2.38	0.57
1:B:101:GLU:HB3	1:B:105:GLN:HE21	1.69	0.56
1:C:109:ARG:NH2	2:G:106:ASP:OD2	2.31	0.56
1:D:355:ARG:NH1	1:D:359:ASP:O	2.37	0.55
2:G:34:ILE:HG13	2:G:83:VAL:HG21	1.88	0.55
2:H:40:ALA:HB3	2:H:43:LYS:HD3	1.89	0.55
2:H:90:LEU:HB3	2:H:135:VAL:HG21	1.90	0.54
2:E:90:LEU:HB3	2:E:135:VAL:HG21	1.88	0.54
1:C:80:GLU:HG2	1:C:110:ARG:HB3	1.89	0.54
2:G:90:LEU:HB3	2:G:135:VAL:HG21	1.90	0.53
2:F:45:ARG:NH1	2:F:127:TRP:CD2	2.77	0.53
2:H:37:PHE:CE2	2:H:121:SER:HB3	2.44	0.53
2:H:95:THR:HG23	2:H:134:THR:HA	1.90	0.52
2:E:31:TYR:C	2:E:53:ARG:HD3	2.29	0.52
1:D:73:MET:SD	1:D:317:GLN:HG2	2.49	0.52
2:F:31:TYR:C	2:F:53:ARG:HD3	2.30	0.52
1:A:75:GLU:OE1	1:A:98:SER:OG	2.17	0.51
2:E:61:ARG:HD2	2:E:114:ARG:HD3	1.93	0.51
1:A:208:ASP:HB2	1:A:252:GLN:HE22	1.74	0.51
2:H:121:SER:HA	2:H:124:TYR:CD1	2.46	0.51
1:A:8:LEU:HD23	1:D:4:ARG:HG3	1.94	0.50
1:A:175:ARG:NH1	4:A:502:HOH:O	2.42	0.50
1:D:287:GLU:OE1	1:D:319:SER:OG	2.26	0.50
1:A:273:PRO:HG2	1:B:268:ALA:HA	1.92	0.50
2:H:68:VAL:HG13	2:H:72:PHE:CG	2.47	0.50
1:A:268:ALA:HA	1:B:273:PRO:HG2	1.93	0.50
2:H:31:TYR:C	2:H:53:ARG:HD3	2.33	0.49
2:G:95:THR:HG23	2:G:134:THR:HA	1.94	0.49
2:E:95:THR:HG23	2:E:134:THR:HA	1.95	0.49
1:B:181:LEU:HD22	1:B:197:VAL:HG13	1.94	0.49
2:F:22:CYS:HB3	2:F:83:VAL:HB	1.95	0.49
2:F:34:ILE:HG13	2:F:83:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:SER:OG	2:F:122:ASP:OD1	2.31	0.48
1:A:214:ARG:HD2	1:B:15:TYR:CD2	2.48	0.48
1:B:109:ARG:NH2	2:F:106:ASP:OD2	2.32	0.48
1:C:214:ARG:HD2	1:D:15:TYR:CD2	2.48	0.48
1:A:73:MET:SD	1:A:317:GLN:HG2	2.53	0.48
1:A:230:HIS:ND1	1:C:127:GLU:OE2	2.47	0.48
1:B:34:THR:HG21	1:B:277:GLY:HA3	1.97	0.47
1:D:271:LEU:HD11	1:D:275:LEU:HD22	1.96	0.47
2:E:45:ARG:NH1	2:E:127:TRP:CZ3	2.74	0.47
2:E:45:ARG:NH1	2:E:127:TRP:CE3	2.83	0.47
1:C:217:GLN:HB2	1:C:266:THR:HG23	1.96	0.47
1:B:3:ARG:HB3	1:C:9:LEU:HD12	1.96	0.46
2:H:11:LEU:HG	2:H:134:THR:OG1	2.15	0.46
2:G:65:ALA:O	2:G:68:VAL:HG12	2.15	0.46
1:C:305:PRO:HG3	1:D:305:PRO:HG3	1.97	0.46
1:C:15:TYR:CD2	1:D:214:ARG:HD3	2.51	0.46
1:A:158:TRP:HB3	1:A:184:TYR:CE2	2.51	0.46
1:D:4:ARG:HG2	1:D:4:ARG:HH21	1.81	0.46
2:H:29:LEU:O	2:H:76:ARG:NH1	2.49	0.45
1:B:109:ARG:NH2	1:B:110:ARG:HD2	2.31	0.45
1:A:181:LEU:HD22	1:A:197:VAL:HG13	1.99	0.45
1:B:170:SER:O	1:B:173:VAL:HG12	2.17	0.45
1:C:294:LEU:HD22	1:C:310:PHE:HB3	1.99	0.44
1:D:322:LYS:HB3	1:D:322:LYS:HE3	1.75	0.44
1:A:15:TYR:CD2	1:B:214:ARG:HD2	2.53	0.44
1:A:80:GLU:HG2	1:A:110:ARG:HB3	2.00	0.44
1:A:341:ARG:HH22	1:A:358:ASP:CG	2.20	0.44
1:B:102:THR:H	1:B:105:GLN:NE2	2.15	0.44
2:H:56:SER:HA	2:H:57:GLY:HA2	1.68	0.44
1:A:288:VAL:O	1:A:292:GLU:HG2	2.18	0.44
1:D:70:ARG:NH1	4:D:503:HOH:O	2.44	0.44
2:F:34:ILE:HG21	2:F:83:VAL:HG21	2.00	0.44
1:B:66:ARG:NH1	1:B:91:GLU:OE2	2.51	0.43
1:A:6:GLU:HA	1:D:6:GLU:HA	1.99	0.43
2:G:68:VAL:HG21	2:G:72:PHE:CD2	2.54	0.43
1:C:34:THR:HG21	1:C:277:GLY:HA3	2.00	0.43
1:C:268:ALA:HA	1:D:273:PRO:HG2	2.00	0.43
1:A:214:ARG:HD2	1:B:15:TYR:CE2	2.54	0.43
1:A:273:PRO:HD3	1:B:273:PRO:HD3	2.00	0.43
1:B:325:GLY:O	1:B:327:LYS:HG3	2.19	0.42
1:A:207:HIS:HB2	1:A:211:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:MET:H	3:C:402:GOL:H12	1.85	0.42
1:A:3:ARG:HB3	1:D:9:LEU:HD12	2.01	0.42
1:B:6:GLU:HA	1:C:6:GLU:HA	2.01	0.42
1:C:170:SER:O	1:C:173:VAL:HG12	2.20	0.42
1:C:214:ARG:HD2	1:D:15:TYR:CE2	2.55	0.42
1:D:294:LEU:HD22	1:D:310:PHE:HB3	2.02	0.42
1:B:271:LEU:HD11	1:B:275:LEU:HD22	2.02	0.41
1:B:217:GLN:HB2	1:B:266:THR:HG23	2.01	0.41
1:A:217:GLN:HB2	1:A:266:THR:HG23	2.02	0.41
1:C:15:TYR:CE2	1:D:214:ARG:HD3	2.56	0.41
1:A:271:LEU:HD11	1:A:275:LEU:HD22	2.02	0.41
1:C:220:TRP:CZ2	1:C:241:PRO:HB2	2.56	0.41
1:C:272:PRO:HA	1:C:273:PRO:HD3	1.92	0.41
1:D:252:GLN:HG2	1:D:253:THR:N	2.36	0.41
2:E:3:GLN:HG3	2:E:127:TRP:O	2.21	0.40
2:F:36:TRP:HE1	2:F:83:VAL:HG12	1.87	0.40
4:A:598:HOH:O	1:B:17:ARG:HD2	2.22	0.40
2:G:54:ILE:HD13	2:G:60:ALA:HB2	2.03	0.40
1:C:96:ARG:HH11	1:C:96:ARG:HD3	1.76	0.40
2:G:71:ARG:HB3	2:G:88:ASN:O	2.22	0.40
2:H:30:THR:O	2:H:53:ARG:HD2	2.22	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	358/387 (92%)	352 (98%)	5 (1%)	1 (0%)	41	62
1	B	356/387 (92%)	349 (98%)	6 (2%)	1 (0%)	41	62
1	C	358/387 (92%)	352 (98%)	5 (1%)	1 (0%)	41	62
1	D	357/387 (92%)	350 (98%)	6 (2%)	1 (0%)	41	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	135/143 (94%)	130 (96%)	5 (4%)	0	100	100
2	F	135/143 (94%)	131 (97%)	4 (3%)	0	100	100
2	G	136/143 (95%)	133 (98%)	3 (2%)	0	100	100
2	H	134/143 (94%)	130 (97%)	4 (3%)	0	100	100
All	All	1969/2120 (93%)	1927 (98%)	38 (2%)	4 (0%)	47	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	PRO
1	A	199	PRO
1	C	199	PRO
1	D	199	PRO

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	279/314 (89%)	276 (99%)	3 (1%)	73	88
1	B	281/314 (90%)	278 (99%)	3 (1%)	73	88
1	C	281/314 (90%)	276 (98%)	5 (2%)	59	78
1	D	276/314 (88%)	273 (99%)	3 (1%)	73	88
2	E	101/118 (86%)	101 (100%)	0	100	100
2	F	103/118 (87%)	102 (99%)	1 (1%)	76	89
2	G	102/118 (86%)	102 (100%)	0	100	100
2	H	101/118 (86%)	100 (99%)	1 (1%)	76	89
All	All	1524/1728 (88%)	1508 (99%)	16 (1%)	76	89

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

Mol	Chain	Res	Type
1	A	53	ARG
1	A	184	TYR
1	A	306	TRP
1	B	184	TYR
1	B	306	TRP
1	B	341	ARG
1	C	184	TYR
1	C	306	TRP
1	C	336	ARG
1	C	354	ASN
1	C	361	ASP
1	D	184	TYR
1	D	214	ARG
1	D	306	TRP
2	F	45	ARG
2	H	25	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	B	105	GLN
1	C	354	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands 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	GOL	A	401	-	5,5,5	0.35	0	5,5,5	0.36	0
3	GOL	D	401	-	5,5,5	0.37	0	5,5,5	0.22	0
3	GOL	D	402	-	5,5,5	0.35	0	5,5,5	0.30	0
3	GOL	C	402	-	5,5,5	0.35	0	5,5,5	0.34	0
3	GOL	B	401	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	C	401	-	5,5,5	0.36	0	5,5,5	0.28	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
3	GOL	A	401	-	-	4/4/4/4	-
3	GOL	D	401	-	-	2/4/4/4	-
3	GOL	D	402	-	-	4/4/4/4	-
3	GOL	C	402	-	-	2/4/4/4	-
3	GOL	B	401	-	-	4/4/4/4	-
3	GOL	C	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	O1-C1-C2-O2
3	A	401	GOL	O1-C1-C2-C3
3	A	401	GOL	C1-C2-C3-O3
3	C	402	GOL	O1-C1-C2-C3
3	D	401	GOL	O1-C1-C2-C3
3	D	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	402	GOL	C1-C2-C3-O3
3	B	401	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-O2
3	B	401	GOL	C1-C2-C3-O3
3	C	401	GOL	O1-C1-C2-C3
3	A	401	GOL	O2-C2-C3-O3
3	C	401	GOL	O1-C1-C2-O2
3	D	401	GOL	O1-C1-C2-O2
3	D	402	GOL	O1-C1-C2-O2
3	D	402	GOL	O2-C2-C3-O3
3	B	401	GOL	O1-C1-C2-C3
3	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	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	360/387 (93%)	-0.18	7 (1%)	66	64	35, 44, 64, 92	0
1	B	358/387 (92%)	-0.28	3 (0%)	86	85	35, 46, 72, 85	0
1	C	360/387 (93%)	-0.31	3 (0%)	86	85	35, 44, 68, 93	0
1	D	359/387 (92%)	-0.21	5 (1%)	75	73	34, 46, 67, 90	0
2	E	137/143 (95%)	-0.15	3 (2%)	62	58	48, 61, 81, 93	0
2	F	137/143 (95%)	0.14	7 (5%)	28	24	48, 68, 88, 99	0
2	G	138/143 (96%)	0.10	9 (6%)	18	16	47, 62, 85, 93	0
2	H	136/143 (95%)	-0.02	3 (2%)	62	58	43, 63, 82, 94	0
All	All	1985/2120 (93%)	-0.17	40 (2%)	65	62	34, 49, 77, 99	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	5.7
2	E	137	SER	4.9
1	C	2	SER	4.3
1	A	2	SER	4.0
2	G	42	GLY	3.4
1	A	56	GLY	3.3
2	E	136	SER	3.2
2	G	137	SER	3.2
2	G	2	VAL	3.1
1	B	55	ALA	3.1
2	H	14	PRO	3.1
2	G	11	LEU	3.0
2	G	41	PRO	3.0
2	E	42	GLY	3.0
2	F	41	PRO	3.0
2	F	137	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	135	VAL	2.9
1	B	359	ASP	2.7
1	A	55	ALA	2.7
1	D	55	ALA	2.7
2	G	40	ALA	2.7
2	G	136	SER	2.6
1	C	60	SER	2.5
1	A	225	SER	2.4
2	G	119	ILE	2.2
2	F	138	HIS	2.2
1	D	360	LYS	2.2
2	G	92	PRO	2.2
2	F	135	VAL	2.2
1	B	2	SER	2.1
1	A	361	ASP	2.1
1	A	57	ILE	2.1
2	H	42	GLY	2.1
1	D	359	ASP	2.1
2	F	88	ASN	2.1
2	F	15	GLY	2.1
1	C	58	GLY	2.0
1	D	51	SER	2.0
1	A	53	ARG	2.0
2	F	17	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
3	GOL	D	401	6/6	0.76	0.45	57,65,71,71	0
3	GOL	B	401	6/6	0.80	0.28	56,63,67,68	0
3	GOL	C	401	6/6	0.86	0.49	67,69,75,84	0
3	GOL	A	401	6/6	0.87	0.20	47,52,56,61	0
3	GOL	C	402	6/6	0.91	0.15	50,53,57,61	0
3	GOL	D	402	6/6	0.91	0.14	54,58,60,68	0

6.5 Other polymers (i)

There are no such residues in this entry.