Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 05:06 am BST

PDB ID	:	1QFJ
Title	:	CRYSTAL STRUCTURE OF NAD(P)H:FLAVIN OXIDOREDUCTASE FROM ESCHERICHIA COLI
Authors	:	Ingelman, M.; Ramaswamy, S.; Niviere, V.; Fontecave, M.; Eklund, H.
Deposited on	:	1999-04-12
Resolution	:	2.20 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 (i) symbol.

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

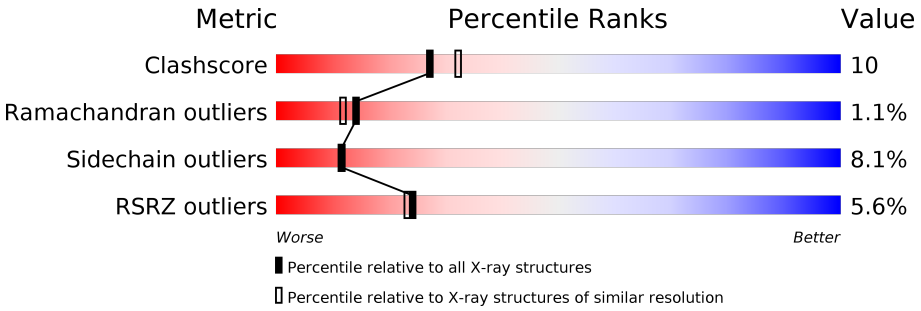
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	232	3% 73% 22%
1	B	232	9% 71% 22%
1	C	232	6% 72% 22%
1	D	232	4% 72% 20% 5%

2 Entry composition

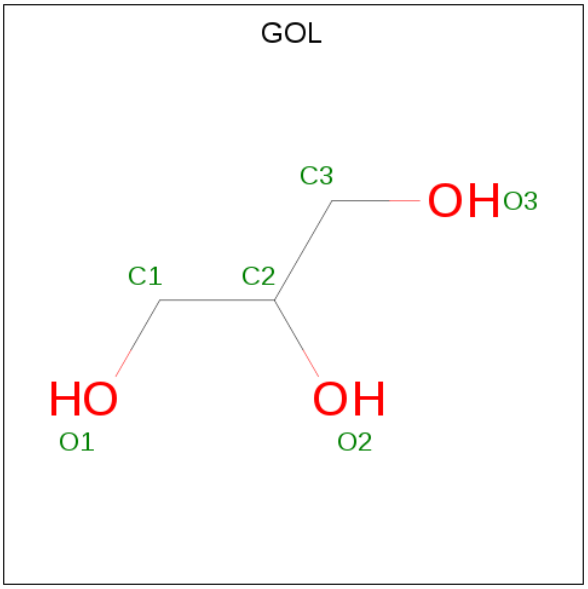
There are 3 unique types of molecules in this entry. The entry contains 7504 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (FLAVIN REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1794	1136	316	333	9			
1	B	226	Total	C	N	O	S	0	0	0
			1794	1136	316	333	9			
1	C	226	Total	C	N	O	S	0	0	0
			1794	1136	316	333	9			
1	D	226	Total	C	N	O	S	0	0	0
			1794	1136	316	333	9			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

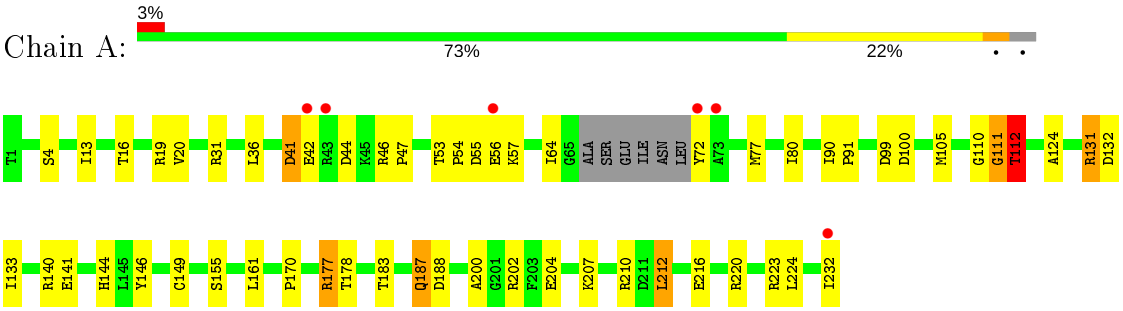
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	40	Total O 40 40	0	0
3	C	74	Total O 74 74	0	0
3	D	88	Total O 88 88	0	0

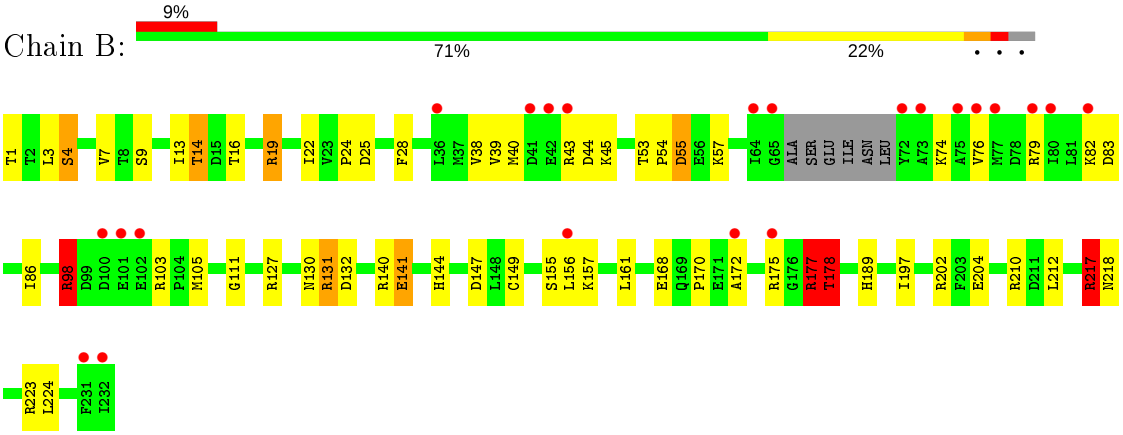
3 Residue-property plots (i)

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

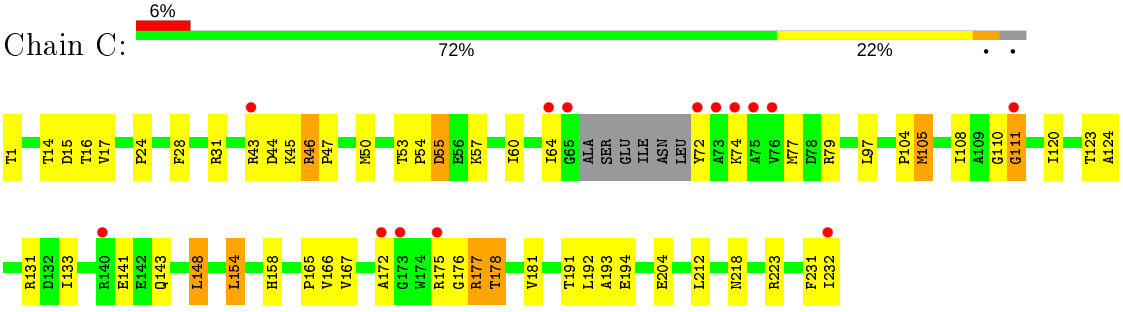
- Molecule 1: PROTEIN (FLAVIN REDUCTASE)



- Molecule 1: PROTEIN (FLAVIN REDUCTASE)

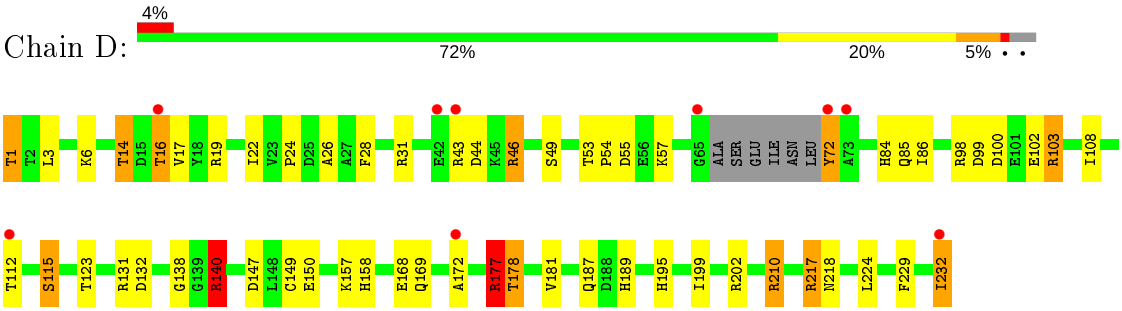


- Molecule 1: PROTEIN (FLAVIN REDUCTASE)



- Molecule 1: PROTEIN (FLAVIN REDUCTASE)

Chain D:


4%
72%
20%
5%
T1 T2 L3 K6 T14 D15 T16 V17 Y18 R19 I22 V23 P24 D25 A26 A27 F28 R31 E42 R43 D44 K45 R46 S49 T53 P54 D55 E56 K57 G65 ALA SER GLU ILE ASN LEU Y72 A73 H84 Q85 I86 R98 D99 D100 E101 E102 R103 I108
T112 S115 T123 R131 D132 G138 G139 R140 D147 L148 C149 E150 K157 H158 E168 Q169 A172 R177 T178 V181 Q187 D188 H189 H195 I199 R202 R210 R217 N218 L224 F229 I232

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.20Å 96.92Å 210.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.71 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.20) 93.3 (19.71-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.46 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.290 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7504	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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	0.48	0/1831	1.22	10/2477 (0.4%)
1	B	0.42	0/1831	1.27	16/2477 (0.6%)
1	C	0.44	0/1831	1.22	8/2477 (0.3%)
1	D	0.46	0/1831	1.25	18/2477 (0.7%)
All	All	0.45	0/7324	1.24	52/9908 (0.5%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	C	31	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	B	98	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	B	210	ARG	NE-CZ-NH1	-11.79	114.40	120.30
1	A	220	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	C	31	ARG	CD-NE-CZ	11.07	139.09	123.60
1	B	210	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	C	31	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	D	217	ARG	NE-CZ-NH2	9.28	124.94	120.30
1	D	217	ARG	NE-CZ-NH1	-9.23	115.68	120.30
1	A	220	ARG	CD-NE-CZ	8.46	135.44	123.60
1	D	177	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	A	210	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	D	210	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	D	210	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	D	19	ARG	CD-NE-CZ	7.08	133.51	123.60
1	D	140	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	220	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	223	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	B	98	ARG	CD-NE-CZ	6.75	133.05	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	131	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	217	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	31	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	D	98	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	D	177	ARG	CD-NE-CZ	6.17	132.23	123.60
1	B	55	ASP	CB-CG-OD1	6.15	123.84	118.30
1	B	127	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	223	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	D	178	THR	CA-C-N	5.98	128.15	116.20
1	B	177	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	140	ARG	CD-NE-CZ	5.95	131.94	123.60
1	A	56	GLU	N-CA-C	-5.95	94.94	111.00
1	D	31	ARG	CD-NE-CZ	5.92	131.90	123.60
1	B	178	THR	CA-C-N	5.81	127.82	116.20
1	B	223	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	D	46	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	C	55	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	72	TYR	CA-CB-CG	5.45	123.75	113.40
1	C	231	PHE	CB-CA-C	5.43	121.26	110.40
1	D	19	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	154	LEU	CB-CG-CD1	5.39	120.17	111.00
1	B	132	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	55	ASP	N-CA-CB	5.30	120.13	110.60
1	A	55	ASP	CA-CB-CG	-5.27	101.80	113.40
1	D	31	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	217	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	B	177	ARG	CB-CA-C	5.15	120.69	110.40
1	D	177	ARG	CB-CA-C	5.10	120.60	110.40
1	D	132	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	105	MET	CG-SD-CE	5.09	108.35	100.20
1	A	200	ALA	N-CA-CB	5.06	117.19	110.10
1	B	19	ARG	CD-NE-CZ	5.03	130.64	123.60

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	1794	0	1773	39	0
1	B	1794	0	1773	31	0
1	C	1794	0	1773	35	0
1	D	1794	0	1773	43	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
2	C	6	0	8	1	0
2	D	6	0	8	0	0
3	A	102	0	0	1	0
3	B	40	0	0	0	0
3	C	74	0	0	3	0
3	D	88	0	0	7	0
All	All	7504	0	7124	143	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 10.

All (143) 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:A:105:MET:HE2	1:A:131:ARG:HG2	1.39	1.00
1:A:149:CYS:HG	1:D:149:CYS:HG	1.02	0.99
1:A:170:PRO:HG3	1:A:178:THR:HG22	1.45	0.95
1:C:204:GLU:HG3	1:D:202:ARG:HD2	1.54	0.89
1:A:77:MET:HE2	1:A:80:ILE:HD12	1.54	0.86
1:C:105:MET:CE	1:C:131:ARG:HG2	2.10	0.82
1:D:177:ARG:HH11	1:D:177:ARG:HG2	1.46	0.80
1:A:64:ILE:HD13	1:A:77:MET:HE1	1.65	0.79
1:D:53:THR:HG23	1:D:123:THR:OG1	1.81	0.79
1:C:105:MET:HE2	1:C:131:ARG:HG2	1.62	0.79
1:D:14:THR:HG22	1:D:17:VAL:H	1.44	0.78
1:D:53:THR:HG22	1:D:55:ASP:H	1.48	0.76
1:D:140:ARG:HH21	1:D:169:GLN:HE22	1.33	0.75
1:B:53:THR:HG22	1:B:55:ASP:H	1.52	0.73
1:C:47:PRO:HB2	2:C:603:GOL:H32	1.72	0.70
1:A:77:MET:CE	1:A:80:ILE:HD12	2.22	0.69
1:A:64:ILE:HG21	1:A:77:MET:HE3	1.75	0.69
1:B:141:GLU:H	1:B:144:HIS:CD2	2.11	0.69
1:B:105:MET:HE2	1:B:131:ARG:HG2	1.76	0.68
1:A:111:GLY:O	1:A:112:THR:HB	1.94	0.68
1:A:177:ARG:HH22	1:A:187:GLN:HG3	1.59	0.68
1:D:14:THR:HG22	1:D:17:VAL:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:MET:CE	1:B:131:ARG:HG2	2.24	0.67
1:C:14:THR:HG23	1:C:17:VAL:H	1.58	0.67
1:C:105:MET:HE3	1:C:133:ILE:HD11	1.77	0.66
1:B:39:VAL:HG22	1:B:45:LYS:HD2	1.78	0.64
1:A:105:MET:CE	1:A:131:ARG:HG2	2.20	0.64
1:A:64:ILE:CD1	1:A:77:MET:HE1	2.28	0.63
1:A:141:GLU:H	1:A:144:HIS:HD2	1.47	0.62
1:C:53:THR:HG22	1:C:54:PRO:HD2	1.82	0.62
1:A:183:THR:O	1:A:187:GLN:HG2	1.99	0.61
1:A:105:MET:HE3	1:A:124:ALA:HB1	1.82	0.61
1:A:178:THR:HG23	3:A:694:HOH:O	2.00	0.61
1:D:1:THR:HG22	3:D:663:HOH:O	2.00	0.61
1:D:46:ARG:NH1	1:D:72:TYR:HB2	2.15	0.61
1:D:229:PHE:HA	1:D:232:ILE:HG22	1.82	0.61
1:B:140:ARG:HA	1:B:168:GLU:HB2	1.83	0.60
1:B:53:THR:HG23	1:B:54:PRO:HD2	1.82	0.60
1:B:155:SER:HA	1:B:161:LEU:HD23	1.84	0.60
1:A:204:GLU:HG2	1:B:202:ARG:HD2	1.84	0.60
1:D:108:ILE:HG23	1:D:181:VAL:HG11	1.85	0.59
1:D:158:HIS:HB3	3:D:672:HOH:O	2.03	0.58
1:C:53:THR:HG23	1:C:123:THR:OG1	2.04	0.58
1:D:14:THR:HG23	1:D:16:THR:H	1.69	0.57
1:C:191:THR:HG22	1:C:193:ALA:H	1.69	0.57
1:C:64:ILE:HD12	1:C:77:MET:HE3	1.86	0.57
1:B:103:ARG:O	1:B:131:ARG:NH2	2.39	0.56
1:C:178:THR:HG22	3:C:653:HOH:O	2.05	0.56
1:C:158:HIS:HB3	3:C:642:HOH:O	2.05	0.55
1:B:7:VAL:HG22	1:B:22:ILE:HG22	1.88	0.54
1:C:204:GLU:HG3	1:D:202:ARG:CD	2.31	0.54
1:D:138:GLY:HA3	1:D:181:VAL:HG23	1.89	0.54
1:B:13:ILE:HD11	1:B:19:ARG:HB2	1.89	0.54
1:A:131:ARG:HG3	1:A:132:ASP:N	2.22	0.54
1:D:14:THR:HG21	3:D:678:HOH:O	2.07	0.54
1:D:46:ARG:HD3	1:D:72:TYR:HD1	1.72	0.54
1:B:38:VAL:HG11	1:B:76:VAL:HG13	1.90	0.54
1:B:14:THR:HG22	1:B:16:THR:H	1.72	0.53
1:D:24:PRO:HG2	1:D:28:PHE:CD1	2.45	0.52
1:D:189:HIS:O	1:D:217:ARG:NH1	2.42	0.52
1:D:177:ARG:HH22	1:D:187:GLN:HB2	1.74	0.52
1:A:64:ILE:HG21	1:A:77:MET:CE	2.39	0.52
1:C:44:ASP:OD1	1:C:46:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASP:HB2	1:A:44:ASP:HB3	1.92	0.51
1:D:102:GLU:O	1:D:103:ARG:HB2	2.10	0.51
1:C:14:THR:HG23	1:C:16:THR:H	1.75	0.51
1:A:105:MET:CE	1:A:124:ALA:HB1	2.41	0.50
1:A:141:GLU:H	1:A:144:HIS:CD2	2.26	0.50
1:C:14:THR:HG22	1:C:17:VAL:HB	1.93	0.50
1:A:202:ARG:HD2	1:B:204:GLU:HG3	1.94	0.50
1:B:40:MET:HB2	1:B:44:ASP:OD1	2.12	0.50
1:C:46:ARG:HH21	1:C:72:TYR:HB3	1.76	0.50
1:A:110:GLY:O	1:A:111:GLY:C	2.50	0.50
1:C:14:THR:CG2	1:C:17:VAL:H	2.25	0.49
1:D:22:ILE:HG21	1:D:86:ILE:HD11	1.93	0.49
1:B:189:HIS:O	1:B:217:ARG:NH1	2.45	0.49
1:B:98:ARG:N	1:B:98:ARG:HD2	2.26	0.49
1:B:177:ARG:HH11	1:B:177:ARG:CG	2.26	0.49
1:A:105:MET:HE3	1:A:133:ILE:HD11	1.94	0.49
1:B:24:PRO:HG2	1:B:28:PHE:CD1	2.48	0.49
1:C:104:PRO:HD2	1:C:194:GLU:O	2.13	0.49
1:C:175:ARG:HG2	1:C:176:GLY:H	1.77	0.49
1:A:53:THR:HG23	1:A:54:PRO:HD2	1.95	0.48
1:D:46:ARG:HD3	1:D:72:TYR:CD1	2.48	0.48
1:D:84:HIS:HD2	3:D:639:HOH:O	1.96	0.48
1:A:207:LYS:HB2	1:A:232:ILE:HD11	1.96	0.48
1:B:3:LEU:O	1:B:4:SER:CB	2.61	0.48
1:A:212:LEU:HD23	1:A:216:GLU:CG	2.45	0.47
1:D:46:ARG:HH12	1:D:72:TYR:HB2	1.80	0.47
1:A:20:VAL:HG11	1:A:80:ILE:HD13	1.97	0.47
1:D:131:ARG:HD3	3:D:627:HOH:O	2.15	0.47
1:B:177:ARG:HH11	1:B:177:ARG:HG2	1.78	0.47
1:B:170:PRO:HG3	1:B:178:THR:CG2	2.45	0.47
1:C:105:MET:HE3	1:C:124:ALA:HB1	1.97	0.47
1:A:13:ILE:HD11	1:A:19:ARG:HB2	1.96	0.47
1:C:105:MET:HE2	1:C:131:ARG:CG	2.40	0.46
1:A:177:ARG:NH2	1:A:188:ASP:OD1	2.43	0.46
1:A:212:LEU:HD23	1:A:216:GLU:HG2	1.98	0.46
1:C:166:VAL:HG13	1:C:177:ARG:HB2	1.97	0.46
1:C:24:PRO:HG2	1:C:28:PHE:CD1	2.51	0.46
1:C:14:THR:OG1	1:C:15:ASP:N	2.48	0.46
1:D:3:LEU:HD22	1:D:26:ALA:HB3	1.98	0.46
1:B:217:ARG:HA	1:B:217:ARG:HD3	1.79	0.46
1:D:177:ARG:NH1	1:D:177:ARG:HG2	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:THR:HG22	1:B:55:ASP:N	2.27	0.46
1:C:141:GLU:OE1	1:C:143:GLN:NE2	2.49	0.46
1:D:195:HIS:HD2	3:D:610:HOH:O	1.98	0.46
1:C:110:GLY:O	1:C:111:GLY:C	2.53	0.45
1:D:157:LYS:HG2	1:D:158:HIS:NE2	2.31	0.45
1:B:79:ARG:O	1:B:83:ASP:HB2	2.16	0.45
1:A:155:SER:HA	1:A:161:LEU:HD23	1.98	0.45
1:B:105:MET:HE2	1:B:131:ARG:CG	2.46	0.45
1:A:47:PRO:HB2	2:A:601:GOL:H32	2.00	0.44
1:D:199:ILE:CD1	1:D:224:LEU:HD11	2.48	0.43
1:A:99:ASP:O	1:A:100:ASP:C	2.55	0.43
1:B:22:ILE:HG21	1:B:86:ILE:HD11	2.01	0.43
1:C:191:THR:HG22	1:C:192:LEU:N	2.34	0.43
1:A:90:ILE:HG13	1:A:91:PRO:HA	2.00	0.43
1:D:217:ARG:HA	1:D:217:ARG:HD3	1.89	0.43
1:D:44:ASP:OD2	1:D:46:ARG:NH2	2.50	0.43
1:B:217:ARG:O	1:B:218:ASN:HB2	2.18	0.43
1:D:210:ARG:HG3	1:D:224:LEU:CD2	2.49	0.42
1:D:55:ASP:O	1:D:57:LYS:HG2	2.19	0.42
1:C:97:LEU:HD13	1:C:120:ILE:HG23	2.01	0.42
1:D:157:LYS:HD3	3:D:643:HOH:O	2.18	0.42
1:B:141:GLU:H	1:B:144:HIS:HD2	1.65	0.42
1:C:167:VAL:O	1:C:178:THR:HA	2.19	0.42
1:D:140:ARG:HA	1:D:168:GLU:HB2	2.00	0.41
1:D:49:SER:HB2	1:D:115:SER:HB3	2.02	0.41
1:C:50:MET:HG3	1:C:60:ILE:HG23	2.01	0.41
1:D:99:ASP:O	1:D:100:ASP:C	2.57	0.41
1:A:53:THR:CG2	1:A:54:PRO:HD2	2.49	0.41
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.97	0.41
1:C:108:ILE:HG23	1:C:181:VAL:HG11	2.02	0.41
1:D:147:ASP:HA	1:D:150:GLU:OE1	2.21	0.41
1:A:90:ILE:HG13	1:A:91:PRO:CA	2.51	0.41
1:A:13:ILE:HG21	1:A:146:TYR:CD1	2.56	0.41
1:C:148:LEU:HD21	1:C:165:PRO:HB3	2.02	0.41
1:D:53:THR:CG2	1:D:54:PRO:HD2	2.50	0.41
1:D:199:ILE:HD11	1:D:224:LEU:HD11	2.03	0.40
1:A:36:LEU:C	1:A:36:LEU:HD12	2.42	0.40
1:B:197:ILE:HB	1:B:224:LEU:HD12	2.04	0.40
1:C:175:ARG:HD2	3:C:637:HOH:O	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	222/232 (96%)	211 (95%)	8 (4%)	3 (1%)	11 8
1	B	222/232 (96%)	212 (96%)	7 (3%)	3 (1%)	11 8
1	C	222/232 (96%)	214 (96%)	6 (3%)	2 (1%)	17 16
1	D	222/232 (96%)	213 (96%)	7 (3%)	2 (1%)	17 16
All	All	888/928 (96%)	850 (96%)	28 (3%)	10 (1%)	14 12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ALA
1	C	172	ALA
1	A	57	LYS
1	A	111	GLY
1	C	111	GLY
1	D	172	ALA
1	A	112	THR
1	B	4	SER
1	D	103	ARG
1	B	111	GLY

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	188/193 (97%)	175 (93%)	13 (7%)	15 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	188/193 (97%)	168 (89%)	20 (11%)	6 6
1	C	188/193 (97%)	173 (92%)	15 (8%)	12 12
1	D	188/193 (97%)	175 (93%)	13 (7%)	15 16
All	All	752/772 (97%)	691 (92%)	61 (8%)	11 12

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	16	THR
1	A	41	ASP
1	A	42	GLU
1	A	46	ARG
1	A	72	TYR
1	A	112	THR
1	A	131	ARG
1	A	140	ARG
1	A	177	ARG
1	A	187	GLN
1	A	212	LEU
1	A	224	LEU
1	B	1	THR
1	B	9	SER
1	B	14	THR
1	B	25	ASP
1	B	43	ARG
1	B	57	LYS
1	B	74	LYS
1	B	82	LYS
1	B	98	ARG
1	B	130	ASN
1	B	141	GLU
1	B	147	ASP
1	B	149	CYS
1	B	156	LEU
1	B	157	LYS
1	B	175	ARG
1	B	177	ARG
1	B	178	THR
1	B	212	LEU
1	B	217	ARG

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Mol	Chain	Res	Type
1	C	1	THR
1	C	43	ARG
1	C	45	LYS
1	C	46	ARG
1	C	55	ASP
1	C	57	LYS
1	C	74	LYS
1	C	79	ARG
1	C	148	LEU
1	C	154	LEU
1	C	177	ARG
1	C	178	THR
1	C	212	LEU
1	C	218	ASN
1	C	232	ILE
1	D	1	THR
1	D	6	LYS
1	D	14	THR
1	D	16	THR
1	D	43	ARG
1	D	85	GLN
1	D	112	THR
1	D	115	SER
1	D	140	ARG
1	D	177	ARG
1	D	178	THR
1	D	218	ASN
1	D	232	ILE

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

Mol	Chain	Res	Type
1	A	144	HIS
1	B	130	ASN
1	B	144	HIS
1	C	130	ASN
1	D	84	HIS
1	D	169	GLN
1	D	195	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

4 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	$\#\|Z\| > 2$
2	GOL	C	603	-	5,5,5	0.69	0	5,5,5	1.09	1 (20%)
2	GOL	A	601	-	5,5,5	0.99	0	5,5,5	1.17	0
2	GOL	D	604	-	5,5,5	0.83	0	5,5,5	1.27	0
2	GOL	B	602	-	5,5,5	0.85	0	5,5,5	1.05	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
2	GOL	C	603	-	-	4/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
2	GOL	D	604	-	-	2/4/4/4	-
2	GOL	B	602	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	603	GOL	O2-C2-C1	-2.32	98.90	109.12

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	603	GOL	O1-C1-C2-C3
2	D	604	GOL	C1-C2-C3-O3
2	A	601	GOL	O1-C1-C2-C3
2	B	602	GOL	C1-C2-C3-O3
2	A	601	GOL	C1-C2-C3-O3
2	C	603	GOL	O1-C1-C2-O2
2	C	603	GOL	O2-C2-C3-O3
2	A	601	GOL	O1-C1-C2-O2
2	D	604	GOL	O2-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
2	B	602	GOL	O2-C2-C3-O3
2	C	603	GOL	C1-C2-C3-O3
2	B	602	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	603	GOL	1	0
2	A	601	GOL	1	0

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, 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	226/232 (97%)	-0.29	6 (2%) 54 52	10, 21, 48, 175	0
1	B	226/232 (97%)	0.22	22 (9%) 7 6	17, 33, 108, 237	0
1	C	226/232 (97%)	0.01	14 (6%) 20 19	12, 27, 67, 221	0
1	D	226/232 (97%)	-0.24	9 (3%) 38 36	13, 24, 51, 169	0
All	All	904/928 (97%)	-0.08	51 (5%) 24 23	10, 26, 75, 237	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	TYR	10.0
1	B	72	TYR	9.1
1	C	232	ILE	7.8
1	A	72	TYR	6.7
1	C	73	ALA	6.6
1	C	72	TYR	6.4
1	B	76	VAL	6.3
1	B	175	ARG	6.2
1	B	77	MET	5.7
1	B	65	GLY	5.3
1	D	73	ALA	5.2
1	B	80	ILE	4.9
1	C	76	VAL	4.3
1	B	73	ALA	4.2
1	A	232	ILE	4.2
1	B	75	ALA	4.1
1	B	172	ALA	4.1
1	D	172	ALA	4.0
1	C	43	ARG	3.5
1	B	232	ILE	3.5
1	C	173	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	82	LYS	3.4
1	C	175	ARG	3.4
1	C	75	ALA	3.3
1	B	101	GLU	3.2
1	D	42	GLU	3.1
1	C	64	ILE	3.1
1	D	65	GLY	3.1
1	A	43	ARG	3.0
1	D	43	ARG	3.0
1	C	65	GLY	2.8
1	B	64	ILE	2.8
1	B	156	LEU	2.7
1	B	102	GLU	2.7
1	B	231	PHE	2.7
1	A	73	ALA	2.6
1	B	43	ARG	2.5
1	B	100	ASP	2.3
1	B	42	GLU	2.3
1	D	232	ILE	2.3
1	C	111	GLY	2.3
1	A	56	GLU	2.3
1	B	79	ARG	2.3
1	C	74	LYS	2.3
1	C	172	ALA	2.2
1	D	16	THR	2.2
1	A	42	GLU	2.0
1	B	36	LEU	2.0
1	B	41	ASP	2.0
1	C	140	ARG	2.0
1	D	112	THR	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. 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
2	GOL	B	602	6/6	0.71	0.25	56,59,60,62	0
2	GOL	A	601	6/6	0.80	0.21	35,36,36,42	0
2	GOL	C	603	6/6	0.82	0.22	45,51,51,55	0
2	GOL	D	604	6/6	0.86	0.17	35,38,39,42	0

6.5 Other polymers

There are no such residues in this entry.