



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:01 am GMT

PDB ID : 2GH5
Title : Crystal Structure of human Glutathione Reductase complexed with a Fluoro-Analogue of the Menadione Derivative M5
Authors : Fritz-Wolf, K.; Winzer, A.; Bauer, H.; Schirmer, H.; Davioud-Charvet, E.
Deposited on : 2006-03-25
Resolution : 1.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

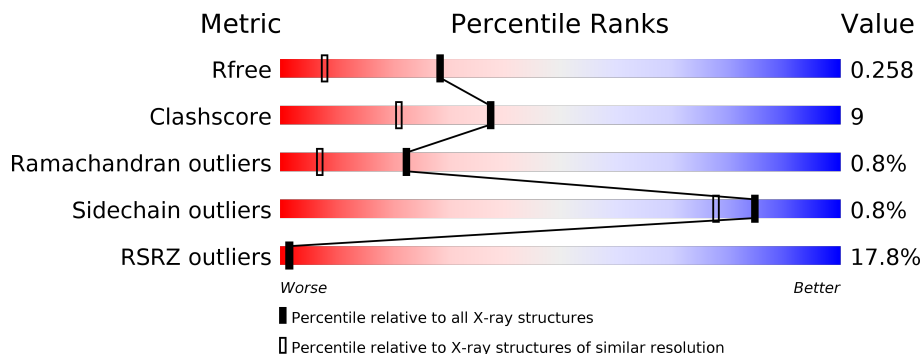
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	<div> <div>14%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	B	478	<div> <div>21%</div> <div>78%</div> <div>18%</div> <div>.</div> </div>

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	ELI	A	958	-	-	-	X
5	GOL	A	808	-	X	-	X
5	GOL	A	809	-	X	-	-
5	GOL	A	810	-	X	-	-
5	GOL	A	813	-	X	-	-
5	GOL	A	817	-	X	-	X
5	GOL	B	801	-	X	-	X
5	GOL	B	802	-	X	-	-
5	GOL	B	803	-	X	-	X
5	GOL	B	805	-	X	-	-
5	GOL	B	806	-	X	-	X
5	GOL	B	811	-	X	-	-
5	GOL	B	812	-	X	-	X

2 Entry composition [i](#)

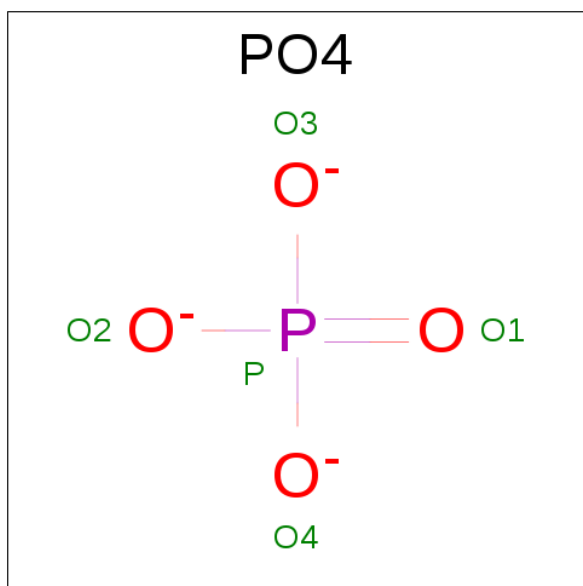
There are 6 unique types of molecules in this entry. The entry contains 7941 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glutathione reductase, mitochondrial.

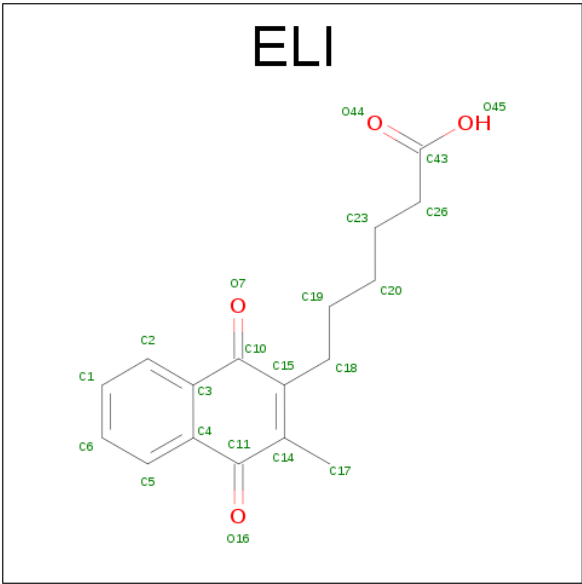
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3499	2212	603	660	24			
1	B	461	Total	C	N	O	S	0	0	0
			3499	2212	603	660	24			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



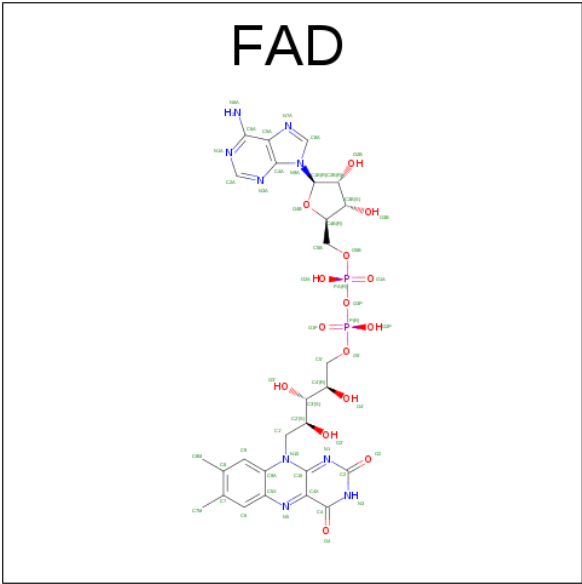
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 6-(3-METHYL-1,4-DIOXO-1,4-DIHYDRONAPHTHALEN-2-YL)HEXANOIC ACID (three-letter code: ELI) (formula: C₁₇H₁₈O₄).



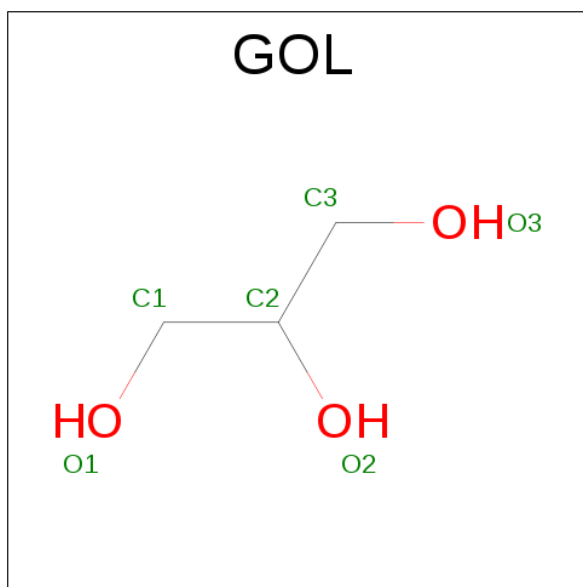
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	17	4		
3	B	1	Total	C	O	0	0
			21	17	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

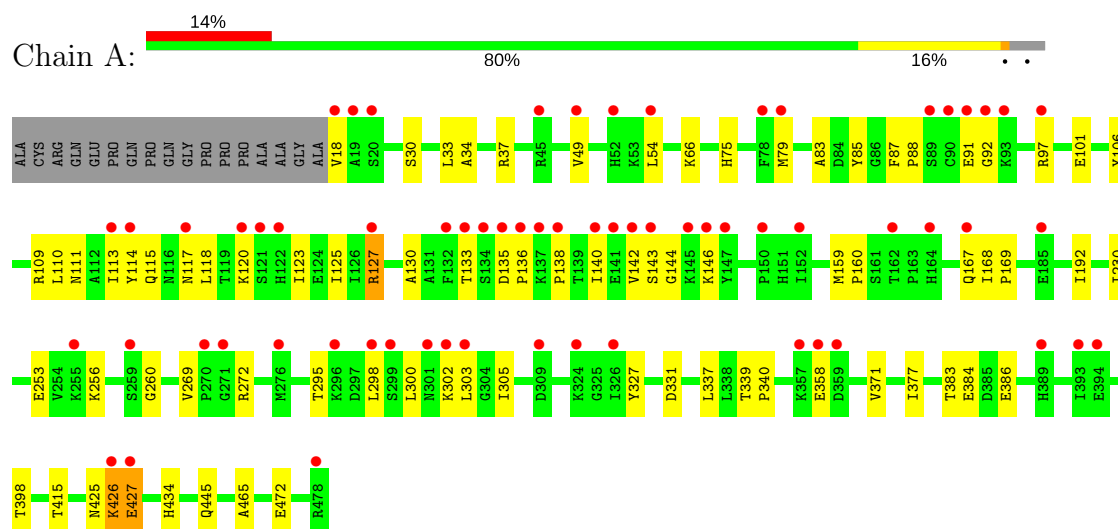
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	350	Total	O	0	0
			350	350		
6	B	353	Total	O	0	0
			353	353		

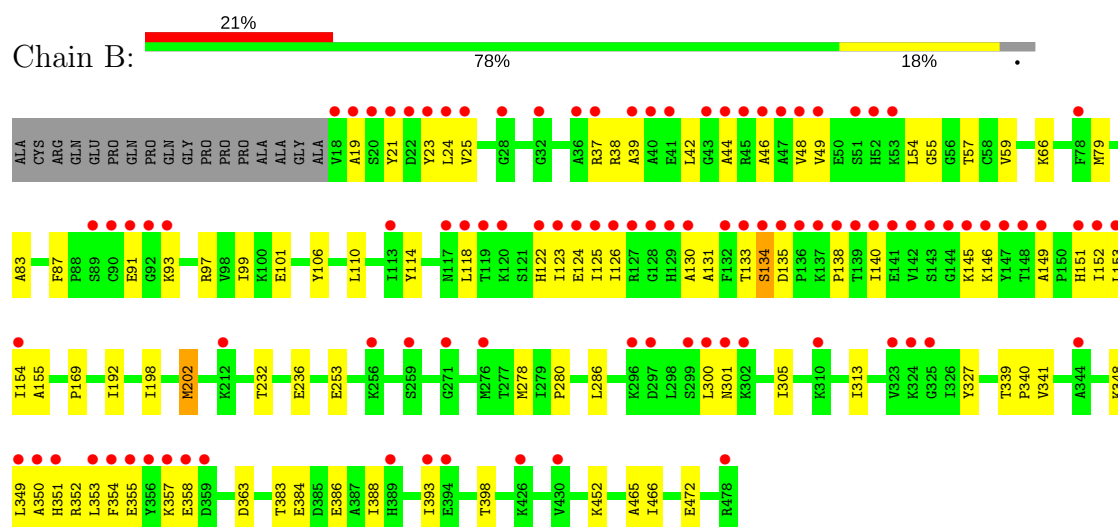
3 Residue-property plots [i](#)

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: glutathione reductase, mitochondrial



- Molecule 1: glutathione reductase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.70Å 63.60Å 103.99Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	19.74 – 1.70 19.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.74-1.70) 98.9 (19.74-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.256 0.225 , 0.258	Depositor DCC
R_{free} test set	5908 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7941	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.33 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.6982e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, ELI, FAD

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	0.29	0/3566	0.57	0/4824
1	B	0.29	0/3566	0.55	0/4824
All	All	0.29	0/7132	0.56	0/9648

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	3499	0	3537	60	0
1	B	3499	0	3537	70	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	21	0	14	5	0
3	B	21	0	14	2	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
5	A	30	0	20	1	0
5	B	42	0	28	0	0
6	A	350	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	353	0	0	11	0
All	All	7941	0	7212	127	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 9.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ALA:HB1	1:B:140:ILE:HD11	1.51	0.92
1:A:169:PRO:HG2	1:A:253:GLU:HG3	1.63	0.80
1:B:133:THR:HG22	1:B:134:SER:H	1.50	0.77
1:B:352:ARG:HA	6:B:6024:HOH:O	1.85	0.77
1:A:33:LEU:HD13	1:A:114:TYR:CE2	2.21	0.76
1:B:54:LEU:HD23	1:B:55:GLY:N	2.01	0.76
1:B:155:ALA:HB3	6:B:5818:HOH:O	1.85	0.75
1:B:169:PRO:HG2	1:B:253:GLU:HG3	1.71	0.72
1:B:130:ALA:HB1	1:B:140:ILE:CD1	2.19	0.71
1:B:23:TYR:HB3	1:B:46:ALA:HB2	1.72	0.71
1:B:466:ILE:HB	6:B:5707:HOH:O	1.90	0.71
1:A:79:MET:SD	1:A:92:GLY:HA2	2.30	0.70
1:B:145:LYS:HD3	1:B:146:LYS:N	2.07	0.70
1:A:30:SER:HA	3:A:958:ELI:H201	1.75	0.67
1:B:19:ALA:H	1:B:145:LYS:HE2	1.59	0.67
1:B:97:ARG:O	1:B:101:GLU:HG3	1.95	0.66
1:A:49:VAL:HG11	1:A:130:ALA:HB2	1.77	0.66
1:A:140:ILE:HB	6:A:5858:HOH:O	1.96	0.65
1:A:298:LEU:HD11	6:A:6049:HOH:O	1.95	0.65
1:A:33:LEU:HD22	1:A:118:LEU:HD21	1.78	0.65
1:B:351:HIS:O	1:B:355:GLU:HB2	1.96	0.65
1:A:97:ARG:O	1:A:101:GLU:HG3	1.96	0.65
1:A:18:VAL:HG12	1:A:146:LYS:HB2	1.79	0.63
1:A:230:ILE:HD11	1:A:434:HIS:HB3	1.80	0.63
1:A:383:THR:OG1	1:A:386:GLU:HG3	1.99	0.62
1:B:341:VAL:HG23	6:B:5709:HOH:O	1.99	0.62
1:B:202:MET:SD	1:B:286:LEU:HD11	2.40	0.62
1:A:117:ASN:HA	1:A:120:LYS:HZ2	1.64	0.62
1:B:152:ILE:N	1:B:152:ILE:HD12	2.16	0.61
1:B:133:THR:HG22	1:B:134:SER:N	2.16	0.60
1:A:295:THR:HA	1:A:298:LEU:HD13	1.83	0.60
1:B:126:ILE:HD12	1:B:126:ILE:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:HB2	1:B:305:ILE:HB	1.84	0.60
1:B:388:ILE:HG23	1:B:393:ILE:HG12	1.84	0.59
1:B:24:LEU:HD22	1:B:152:ILE:HG23	1.85	0.57
1:A:331:ASP:HA	1:A:337:LEU:HD22	1.86	0.57
1:A:358:GLU:HG2	6:A:5978:HOH:O	2.04	0.57
1:B:348:LYS:O	1:B:351:HIS:HB3	2.05	0.56
1:A:85:TYR:HA	1:B:99:ILE:HD11	1.87	0.56
1:A:120:LYS:HZ2	1:A:120:LYS:HB2	1.69	0.56
1:A:79:MET:HA	1:B:79:MET:HE1	1.88	0.56
1:A:465:ALA:HB1	1:A:472:GLU:HB2	1.87	0.56
1:B:57:THR:HG21	6:B:5879:HOH:O	2.05	0.55
1:A:120:LYS:NZ	1:A:120:LYS:HB2	2.21	0.55
1:A:88:PRO:HG2	1:B:91:GLU:OE2	2.06	0.55
1:A:384:GLU:HG3	1:A:398:THR:HG21	1.89	0.55
1:A:37:ARG:HD3	3:A:958:ELI:O44	2.07	0.55
1:B:37:ARG:HA	1:B:123:ILE:HD11	1.88	0.54
1:A:30:SER:HA	3:A:958:ELI:C20	2.37	0.54
1:B:49:VAL:HG22	1:B:126:ILE:HB	1.90	0.53
1:B:349:LEU:HG	6:B:5933:HOH:O	2.08	0.53
1:A:415:THR:HG21	5:A:817:GOL:H12	1.89	0.53
1:B:383:THR:OG1	1:B:386:GLU:HG3	2.09	0.52
1:B:340:PRO:HB2	6:B:5709:HOH:O	2.09	0.52
1:B:149:ALA:O	1:B:152:ILE:HD11	2.08	0.52
1:B:388:ILE:CG2	1:B:393:ILE:HG12	2.40	0.52
1:A:106:TYR:O	1:A:110:LEU:HG	2.10	0.52
1:B:39:ALA:O	1:B:44:ALA:HB3	2.10	0.51
1:B:49:VAL:HG12	4:B:479:FAD:H2A	1.93	0.51
1:A:135:ASP:OD1	1:A:136:PRO:HD2	2.10	0.51
1:B:49:VAL:HG11	1:B:130:ALA:HB2	1.90	0.51
1:A:109:ARG:O	1:A:113:ILE:HG22	2.11	0.51
1:A:117:ASN:HA	1:A:120:LYS:NZ	2.25	0.51
1:A:127:ARG:HH11	1:A:127:ARG:HG3	1.75	0.50
1:A:426:LYS:HB3	1:A:426:LYS:NZ	2.26	0.50
1:B:38:ARG:NH1	1:B:351:HIS:HB2	2.26	0.50
1:A:106:TYR:CE1	1:A:110:LEU:HD21	2.47	0.50
1:A:425:ASN:HB2	1:A:427:GLU:OE2	2.11	0.50
1:A:33:LEU:HB3	1:A:114:TYR:OH	2.11	0.50
1:A:302:LYS:C	1:A:303:LEU:HD22	2.32	0.49
1:A:192:ILE:HD12	1:A:192:ILE:N	2.28	0.49
1:A:54:LEU:HD11	1:A:125:ILE:HD13	1.94	0.49
1:A:167:GLN:HG2	1:A:168:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ALA:HB1	1:B:472:GLU:HB2	1.95	0.48
1:A:133:THR:HG21	1:A:146:LYS:HD2	1.95	0.48
1:B:118:LEU:CD2	1:B:125:ILE:HD11	2.43	0.48
1:A:37:ARG:HA	1:A:123:ILE:HD11	1.96	0.48
1:A:83:ALA:HA	1:A:87:PHE:O	2.14	0.48
1:B:384:GLU:HG3	1:B:398:THR:HG21	1.95	0.47
1:B:25:VAL:HB	1:B:48:VAL:HG12	1.95	0.47
1:B:355:GLU:HB2	6:B:5808:HOH:O	2.13	0.47
1:A:114:TYR:O	1:A:117:ASN:N	2.44	0.47
1:A:256:LYS:HD2	1:A:260:GLY:O	2.14	0.47
1:A:300:LEU:HB3	1:A:305:ILE:HB	1.96	0.47
1:A:445:GLN:HB2	6:B:5707:HOH:O	2.14	0.47
1:A:427:GLU:CD	1:A:427:GLU:H	2.18	0.46
1:B:21:TYR:HE2	1:B:124:GLU:OE2	1.98	0.46
1:B:192:ILE:N	1:B:192:ILE:HD12	2.31	0.46
1:B:42:LEU:HD22	1:B:355:GLU:OE1	2.16	0.46
1:A:111:ASN:O	1:A:115:GLN:HG3	2.16	0.46
1:B:351:HIS:HE1	1:B:357:LYS:HG3	1.80	0.46
1:B:37:ARG:HD3	3:B:958:ELI:O45	2.17	0.45
1:A:295:THR:CA	1:A:298:LEU:HD13	2.47	0.45
1:B:23:TYR:OH	1:B:153:LEU:HD22	2.17	0.45
1:A:426:LYS:HG2	6:A:6005:HOH:O	2.17	0.44
1:A:66:LYS:HD2	1:A:66:LYS:C	2.37	0.44
1:B:151:HIS:C	1:B:152:ILE:HD12	2.37	0.44
1:B:232:THR:O	1:B:236:GLU:HG3	2.18	0.44
1:B:114:TYR:HB2	3:B:958:ELI:H2	1.99	0.44
1:B:198:ILE:O	1:B:202:MET:HG3	2.18	0.44
1:A:339:THR:HB	1:A:340:PRO:HD3	1.99	0.44
1:B:278:MET:O	1:B:280:PRO:HD3	2.18	0.43
1:B:83:ALA:HA	1:B:87:PHE:O	2.19	0.43
1:A:142:VAL:O	1:A:143:SER:HB2	2.18	0.43
1:A:159:MET:HB2	1:A:160:PRO:HD2	2.01	0.43
1:B:118:LEU:HD21	1:B:125:ILE:HD11	2.00	0.43
1:B:38:ARG:HH12	1:B:351:HIS:CD2	2.36	0.43
1:B:339:THR:HB	1:B:340:PRO:HD3	2.01	0.42
1:A:114:TYR:HB2	3:A:958:ELI:H2	2.02	0.42
1:A:426:LYS:HD3	6:A:5983:HOH:O	2.19	0.41
1:B:106:TYR:O	1:B:110:LEU:HG	2.20	0.41
1:B:327:TYR:CD1	1:B:327:TYR:N	2.87	0.41
1:B:300:LEU:HD12	1:B:301:ASN:N	2.36	0.41
1:A:371:VAL:HB	1:A:377:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:THR:C	1:A:298:LEU:HD13	2.40	0.41
1:B:93:LYS:HG3	1:B:93:LYS:O	2.20	0.41
1:A:269:VAL:HB	1:A:272:ARG:HD2	2.02	0.41
1:B:131:ALA:O	1:B:140:ILE:HG13	2.21	0.41
1:B:363:ASP:OD2	1:B:452:LYS:HE3	2.21	0.41
1:B:66:LYS:C	1:B:66:LYS:HD2	2.40	0.41
1:B:350:ALA:O	1:B:354:PHE:HD1	2.04	0.41
1:A:34:ALA:HA	3:A:958:ELI:O45	2.20	0.41
1:B:24:LEU:C	1:B:24:LEU:HD23	2.41	0.40
1:B:353:LEU:HB2	1:B:354:PHE:CE1	2.56	0.40
1:B:154:ILE:HG21	1:B:313:ILE:CD1	2.52	0.40
1:B:59:VAL:HG22	6:B:5762:HOH:O	2.21	0.40
1:B:138:PRO:HB2	6:B:6035:HOH:O	2.20	0.40

There are no symmetry-related clashes.

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	459/478 (96%)	439 (96%)	17 (4%)	3 (1%)	25	9
1	B	459/478 (96%)	432 (94%)	23 (5%)	4 (1%)	20	5
All	All	918/956 (96%)	871 (95%)	40 (4%)	7 (1%)	22	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	SER
1	A	91	GLU
1	B	135	ASP
1	A	144	GLY
1	B	358	GLU

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Mol	Chain	Res	Type
1	B	122	HIS
1	A	138	PRO

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	382/393 (97%)	377 (99%)	5 (1%)	73	60
1	B	382/393 (97%)	381 (100%)	1 (0%)	94	91
All	All	764/786 (97%)	758 (99%)	6 (1%)	85	78

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	127	ARG
1	A	327	TYR
1	A	426	LYS
1	A	427	GLU
1	B	202	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	116	ASN
1	A	182	GLN
1	A	365	ASN
1	A	425	ASN
1	B	111	ASN
1	B	115	GLN
1	B	167	GLN
1	B	250	GLN
1	B	351	HIS

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Mol	Chain	Res	Type
1	B	425	ASN

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 ⓘ

20 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$
4	FAD	A	479	-	51,58,58	1.87	12 (23%)	54,89,89	2.29	11 (20%)
2	PO4	A	5703	-	4,4,4	1.38	0	6,6,6	0.39	0
2	PO4	A	5706	-	4,4,4	1.44	0	6,6,6	0.39	0
5	GOL	A	808	-	5,5,5	4.92	5 (100%)	5,5,5	5.48	3 (60%)
5	GOL	A	809	-	5,5,5	4.92	5 (100%)	5,5,5	5.48	3 (60%)
5	GOL	A	810	-	5,5,5	4.89	5 (100%)	5,5,5	5.49	3 (60%)
5	GOL	A	813	-	5,5,5	4.93	5 (100%)	5,5,5	5.48	3 (60%)
5	GOL	A	817	-	5,5,5	4.92	5 (100%)	5,5,5	5.48	3 (60%)
3	ELI	A	958	1	19,22,22	5.46	14 (73%)	23,30,30	3.19	4 (17%)
4	FAD	B	479	-	51,58,58	1.88	10 (19%)	54,89,89	2.25	13 (24%)
2	PO4	B	5704	-	4,4,4	1.38	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	5705	-	4,4,4	1.43	0	6,6,6	0.40	0
5	GOL	B	801	-	5,5,5	4.92	5 (100%)	5,5,5	5.46	3 (60%)
5	GOL	B	802	-	5,5,5	4.95	5 (100%)	5,5,5	5.49	3 (60%)
5	GOL	B	803	-	5,5,5	4.93	5 (100%)	5,5,5	5.49	3 (60%)
5	GOL	B	805	-	5,5,5	4.93	5 (100%)	5,5,5	5.45	3 (60%)
5	GOL	B	806	-	5,5,5	4.91	5 (100%)	5,5,5	5.48	3 (60%)
5	GOL	B	811	-	5,5,5	4.91	5 (100%)	5,5,5	5.50	3 (60%)
5	GOL	B	812	-	5,5,5	4.93	5 (100%)	5,5,5	5.48	3 (60%)
3	ELI	B	958	1	19,22,22	5.24	13 (68%)	23,30,30	3.75	3 (13%)

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	FAD	A	479	-	-	0/28/50/50	0/6/6/6
2	PO4	A	5703	-	-	0/0/0/0	0/0/0/0
2	PO4	A	5706	-	-	0/0/0/0	0/0/0/0
5	GOL	A	808	-	-	0/4/4/4	0/0/0/0
5	GOL	A	809	-	-	0/4/4/4	0/0/0/0
5	GOL	A	810	-	-	0/4/4/4	0/0/0/0
5	GOL	A	813	-	-	0/4/4/4	0/0/0/0
5	GOL	A	817	-	-	0/4/4/4	0/0/0/0
3	ELI	A	958	1	-	0/6/28/28	0/2/2/2
4	FAD	B	479	-	-	0/28/50/50	0/6/6/6
2	PO4	B	5704	-	-	0/0/0/0	0/0/0/0
2	PO4	B	5705	-	-	0/0/0/0	0/0/0/0
5	GOL	B	801	-	-	0/4/4/4	0/0/0/0
5	GOL	B	802	-	-	0/4/4/4	0/0/0/0
5	GOL	B	803	-	-	0/4/4/4	0/0/0/0
5	GOL	B	805	-	-	0/4/4/4	0/0/0/0
5	GOL	B	806	-	-	0/4/4/4	0/0/0/0
5	GOL	B	811	-	-	0/4/4/4	0/0/0/0
5	GOL	B	812	-	-	0/4/4/4	0/0/0/0
3	ELI	B	958	1	-	0/6/28/28	0/2/2/2

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	812	GOL	C3-C2	-8.47	1.20	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	813	GOL	C3-C2	-8.42	1.21	1.52
5	B	802	GOL	C3-C2	-8.42	1.21	1.52
5	B	803	GOL	C3-C2	-8.40	1.21	1.52
5	A	817	GOL	C3-C2	-8.39	1.21	1.52
5	A	808	GOL	C3-C2	-8.37	1.21	1.52
5	A	809	GOL	C3-C2	-8.36	1.21	1.52
5	B	805	GOL	C3-C2	-8.35	1.21	1.52
5	B	811	GOL	C3-C2	-8.34	1.21	1.52
5	A	810	GOL	C3-C2	-8.33	1.21	1.52
5	B	806	GOL	C3-C2	-8.33	1.21	1.52
5	B	801	GOL	C3-C2	-8.30	1.21	1.52
5	B	801	GOL	C1-C2	-3.39	1.39	1.52
5	B	803	GOL	C1-C2	-3.37	1.39	1.52
5	A	808	GOL	C1-C2	-3.37	1.39	1.52
5	A	817	GOL	C1-C2	-3.33	1.39	1.52
5	B	812	GOL	C1-C2	-3.31	1.40	1.52
5	A	810	GOL	C1-C2	-3.31	1.40	1.52
5	A	809	GOL	C1-C2	-3.31	1.40	1.52
5	B	802	GOL	C1-C2	-3.30	1.40	1.52
5	B	806	GOL	C1-C2	-3.30	1.40	1.52
5	A	813	GOL	C1-C2	-3.28	1.40	1.52
5	B	811	GOL	C1-C2	-3.25	1.40	1.52
5	B	805	GOL	C1-C2	-3.24	1.40	1.52
5	B	803	GOL	O2-C2	-2.93	1.34	1.43
5	A	813	GOL	O2-C2	-2.90	1.34	1.43
5	B	812	GOL	O2-C2	-2.89	1.34	1.43
5	B	802	GOL	O2-C2	-2.89	1.34	1.43
5	B	806	GOL	O2-C2	-2.86	1.35	1.43
5	B	801	GOL	O2-C2	-2.85	1.35	1.43
5	B	811	GOL	O2-C2	-2.84	1.35	1.43
5	A	809	GOL	O2-C2	-2.84	1.35	1.43
5	A	808	GOL	O2-C2	-2.83	1.35	1.43
5	B	805	GOL	O2-C2	-2.80	1.35	1.43
5	A	817	GOL	O2-C2	-2.80	1.35	1.43
5	A	810	GOL	O2-C2	-2.79	1.35	1.43
3	A	958	ELI	C17-C14	2.04	1.55	1.50
3	A	958	ELI	O7-C10	2.10	1.27	1.23
4	A	479	FAD	C10-N1	2.22	1.36	1.33
4	B	479	FAD	C4X-C10	2.22	1.44	1.41
4	A	479	FAD	C9-C8	2.26	1.43	1.37
4	A	479	FAD	C6-C5X	2.29	1.45	1.41
3	A	958	ELI	C19-C18	2.45	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	479	FAD	C4X-C10	2.64	1.45	1.41
3	B	958	ELI	O7-C10	2.69	1.29	1.23
4	B	479	FAD	C9A-C5X	2.74	1.48	1.42
4	A	479	FAD	C9A-C5X	2.79	1.48	1.42
4	B	479	FAD	C9-C8	2.80	1.45	1.37
4	A	479	FAD	C2A-N3A	2.83	1.36	1.32
4	B	479	FAD	C2A-N3A	2.92	1.37	1.32
4	A	479	FAD	C5X-N5	3.13	1.40	1.35
4	B	479	FAD	C5X-N5	3.17	1.40	1.35
4	A	479	FAD	C2A-N1A	3.31	1.40	1.33
5	B	812	GOL	O3-C3	3.32	1.56	1.42
5	A	813	GOL	O3-C3	3.32	1.56	1.42
4	B	479	FAD	C2A-N1A	3.33	1.40	1.33
5	B	803	GOL	O3-C3	3.36	1.56	1.42
5	A	808	GOL	O3-C3	3.38	1.56	1.42
5	A	809	GOL	O3-C3	3.39	1.56	1.42
5	A	817	GOL	O3-C3	3.39	1.56	1.42
5	B	806	GOL	O3-C3	3.39	1.56	1.42
5	B	802	GOL	O3-C3	3.43	1.56	1.42
5	A	810	GOL	O3-C3	3.43	1.56	1.42
5	B	811	GOL	O3-C3	3.43	1.56	1.42
5	B	805	GOL	O3-C3	3.45	1.56	1.42
3	B	958	ELI	C17-C14	3.47	1.58	1.50
5	B	801	GOL	O3-C3	3.48	1.57	1.42
4	B	479	FAD	C4A-N3A	3.93	1.41	1.35
4	B	479	FAD	C9A-N10	3.99	1.44	1.38
4	A	479	FAD	C4A-N3A	4.00	1.41	1.35
4	A	479	FAD	C4-N3	4.15	1.40	1.33
4	B	479	FAD	C4-N3	4.39	1.41	1.33
5	B	803	GOL	O1-C1	4.42	1.61	1.42
5	B	812	GOL	O1-C1	4.44	1.61	1.42
5	A	810	GOL	O1-C1	4.46	1.61	1.42
5	A	808	GOL	O1-C1	4.48	1.61	1.42
5	B	801	GOL	O1-C1	4.49	1.61	1.42
5	A	817	GOL	O1-C1	4.51	1.61	1.42
5	A	809	GOL	O1-C1	4.52	1.61	1.42
5	A	813	GOL	O1-C1	4.54	1.61	1.42
5	B	802	GOL	O1-C1	4.54	1.61	1.42
5	B	811	GOL	O1-C1	4.55	1.61	1.42
5	B	806	GOL	O1-C1	4.56	1.61	1.42
5	B	805	GOL	O1-C1	4.64	1.61	1.42
4	A	479	FAD	C9A-N10	4.76	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	958	ELI	C15-C14	5.02	1.46	1.35
3	B	958	ELI	C3-C10	5.05	1.58	1.48
3	A	958	ELI	C3-C10	5.54	1.59	1.48
3	B	958	ELI	C6-C5	5.78	1.49	1.38
3	B	958	ELI	C6-C1	5.85	1.52	1.38
3	A	958	ELI	C6-C5	5.86	1.50	1.38
3	B	958	ELI	C1-C2	5.88	1.50	1.38
3	A	958	ELI	C6-C1	5.99	1.52	1.38
4	A	479	FAD	C4X-N5	6.03	1.42	1.33
3	A	958	ELI	C4-C11	6.11	1.60	1.48
3	B	958	ELI	C4-C11	6.17	1.60	1.48
3	A	958	ELI	C2-C3	6.38	1.50	1.39
3	A	958	ELI	C1-C2	6.49	1.51	1.38
4	B	479	FAD	C4X-N5	6.65	1.42	1.33
3	A	958	ELI	C15-C10	6.69	1.64	1.47
3	B	958	ELI	C2-C3	6.84	1.50	1.39
3	A	958	ELI	C15-C14	6.90	1.50	1.35
3	B	958	ELI	C14-C11	6.97	1.63	1.48
3	A	958	ELI	C14-C11	6.97	1.63	1.48
3	A	958	ELI	C5-C4	7.25	1.51	1.39
3	B	958	ELI	C15-C10	7.59	1.66	1.47
3	B	958	ELI	C5-C4	7.83	1.52	1.39
3	B	958	ELI	C4-C3	9.63	1.57	1.40
3	A	958	ELI	C4-C3	11.47	1.60	1.40

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	479	FAD	C4X-C10-N10	-6.48	116.02	120.52
4	B	479	FAD	N3A-C2A-N1A	-6.25	123.42	128.86
4	A	479	FAD	N3A-C2A-N1A	-6.10	123.55	128.86
3	B	958	ELI	C20-C23-C26	-6.09	89.50	113.70
4	B	479	FAD	C4X-C10-N10	-5.97	116.37	120.52
4	B	479	FAD	C4-C4X-C10	-4.95	115.95	119.96
4	A	479	FAD	C4-C4X-C10	-4.51	116.31	119.96
4	A	479	FAD	C4X-C4-N3	-4.30	117.36	123.48
3	A	958	ELI	C19-C18-C15	-4.29	100.36	113.06
3	A	958	ELI	C20-C23-C26	-4.24	96.84	113.70
3	A	958	ELI	C23-C20-C19	-4.02	93.74	114.45
4	B	479	FAD	C4X-C4-N3	-3.82	118.04	123.48
3	B	958	ELI	C23-C20-C19	-3.21	97.91	114.45
4	B	479	FAD	O5B-PA-O1A	-2.25	100.19	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	479	FAD	C1'-N10-C10	-2.21	116.24	118.50
4	A	479	FAD	C8M-C8-C9	-2.15	114.95	120.34
4	A	479	FAD	O5B-PA-O1A	-2.03	101.07	109.25
4	B	479	FAD	O2B-C2B-C3B	2.01	118.27	111.83
4	A	479	FAD	O2A-PA-O1A	2.03	122.79	112.28
4	B	479	FAD	C4-C4X-N5	2.39	121.30	118.68
4	A	479	FAD	C10-C4X-N5	2.45	123.41	120.59
4	B	479	FAD	C8M-C8-C7	2.53	126.03	120.72
4	B	479	FAD	O2A-PA-O1A	2.54	125.44	112.28
4	B	479	FAD	C1'-N10-C9A	2.71	120.83	118.35
4	A	479	FAD	C8M-C8-C7	2.80	126.60	120.72
4	A	479	FAD	C4X-N5-C5X	2.81	119.73	116.76
4	B	479	FAD	C4X-N5-C5X	3.01	119.94	116.76
5	B	803	GOL	O1-C1-C2	3.02	125.27	110.07
5	B	801	GOL	O1-C1-C2	3.03	125.36	110.07
5	A	808	GOL	O1-C1-C2	3.04	125.37	110.07
5	A	810	GOL	O1-C1-C2	3.08	125.58	110.07
5	A	817	GOL	O1-C1-C2	3.09	125.65	110.07
5	B	805	GOL	O1-C1-C2	3.09	125.66	110.07
5	A	809	GOL	O1-C1-C2	3.09	125.66	110.07
5	B	811	GOL	O1-C1-C2	3.12	125.79	110.07
5	B	802	GOL	O1-C1-C2	3.13	125.84	110.07
5	B	812	GOL	O1-C1-C2	3.14	125.88	110.07
5	A	813	GOL	O1-C1-C2	3.14	125.90	110.07
5	B	806	GOL	O1-C1-C2	3.18	126.11	110.07
5	B	805	GOL	O2-C2-C3	6.33	138.73	108.84
5	B	806	GOL	O2-C2-C3	6.35	138.85	108.84
5	A	813	GOL	O2-C2-C3	6.36	138.87	108.84
5	B	802	GOL	O2-C2-C3	6.38	138.96	108.84
5	A	809	GOL	O2-C2-C3	6.38	138.98	108.84
5	B	801	GOL	O2-C2-C3	6.38	138.99	108.84
5	A	808	GOL	O2-C2-C3	6.40	139.04	108.84
5	B	812	GOL	O2-C2-C3	6.40	139.05	108.84
5	B	811	GOL	O2-C2-C3	6.40	139.05	108.84
5	A	810	GOL	O2-C2-C3	6.40	139.09	108.84
5	B	803	GOL	O2-C2-C3	6.41	139.10	108.84
5	A	817	GOL	O2-C2-C3	6.41	139.11	108.84
4	B	479	FAD	C4-N3-C2	8.81	122.86	115.16
5	B	805	GOL	O3-C3-C2	9.92	160.06	110.07
5	B	812	GOL	O3-C3-C2	9.92	160.07	110.07
5	B	801	GOL	O3-C3-C2	9.93	160.10	110.07
4	A	479	FAD	C4-N3-C2	9.93	123.85	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	813	GOL	O3-C3-C2	9.96	160.22	110.07
5	A	817	GOL	O3-C3-C2	9.96	160.23	110.07
5	B	806	GOL	O3-C3-C2	9.96	160.24	110.07
5	A	808	GOL	O3-C3-C2	9.97	160.28	110.07
5	A	809	GOL	O3-C3-C2	9.97	160.29	110.07
5	A	810	GOL	O3-C3-C2	9.97	160.32	110.07
5	B	802	GOL	O3-C3-C2	9.99	160.38	110.07
5	B	811	GOL	O3-C3-C2	10.00	160.44	110.07
5	B	803	GOL	O3-C3-C2	10.00	160.47	110.07
3	A	958	ELI	C20-C19-C18	13.03	160.99	113.24
3	B	958	ELI	C20-C19-C18	16.19	172.57	113.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	817	GOL	1	0
3	A	958	ELI	5	0
4	B	479	FAD	1	0
3	B	958	ELI	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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(Å ²)	Q<0.9
1	A	461/478 (96%)	0.76	65 (14%) 3 4	12, 25, 45, 62	0
1	B	461/478 (96%)	1.05	99 (21%) 1 1	13, 26, 62, 75	0
All	All	922/956 (96%)	0.91	164 (17%) 2 1	12, 25, 56, 75	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	PRO	11.8
1	B	18	VAL	10.2
1	B	134	SER	9.6
1	A	136	PRO	9.4
1	B	92	GLY	8.4
1	B	144	GLY	7.9
1	B	91	GLU	7.6
1	B	358	GLU	7.0
1	B	21	TYR	6.9
1	A	478	ARG	6.8
1	A	91	GLU	6.8
1	B	19	ALA	6.4
1	B	138	PRO	6.4
1	B	351	HIS	6.2
1	B	45	ARG	5.9
1	B	143	SER	5.8
1	A	78	PHE	5.8
1	B	140	ILE	5.7
1	B	24	LEU	5.4
1	B	133	THR	5.4
1	A	137	LYS	5.3
1	A	92	GLY	5.3
1	A	138	PRO	5.3
1	B	354	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	125	ILE	5.2
1	A	303	LEU	5.0
1	B	357	LYS	4.9
1	B	90	CYS	4.7
1	A	134	SER	4.6
1	A	143	SER	4.5
1	B	139	THR	4.5
1	B	41	GLU	4.5
1	B	300	LEU	4.4
1	B	323	VAL	4.4
1	A	52	HIS	4.4
1	A	142	VAL	4.3
1	A	135	ASP	4.3
1	A	18	VAL	4.3
1	B	132	PHE	4.2
1	B	350	ALA	4.2
1	B	356	TYR	4.1
1	B	478	ARG	4.0
1	B	22	ASP	4.0
1	B	78	PHE	4.0
1	B	40	ALA	4.0
1	B	48	VAL	3.9
1	B	137	LYS	3.9
1	B	359	ASP	3.9
1	B	353	LEU	3.8
1	B	135	ASP	3.8
1	B	301	ASN	3.8
1	A	296	LYS	3.8
1	B	52	HIS	3.7
1	A	120	LYS	3.7
1	A	426	LYS	3.6
1	B	271	GLY	3.6
1	A	358	GLU	3.6
1	A	167	GLN	3.6
1	B	324	LYS	3.5
1	B	394	GLU	3.5
1	A	299	SER	3.5
1	A	298	LEU	3.5
1	B	44	ALA	3.5
1	B	127	ARG	3.4
1	B	20	SER	3.4
1	B	299	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	LYS	3.4
1	A	90	CYS	3.3
1	A	146	LYS	3.3
1	B	117	ASN	3.3
1	B	113	ILE	3.3
1	B	51	SER	3.2
1	B	128	GLY	3.1
1	B	349	LEU	3.1
1	A	394	GLU	3.1
1	B	23	TYR	3.0
1	B	146	LYS	3.0
1	B	259	SER	3.0
1	B	129	HIS	3.0
1	B	355	GLU	3.0
1	B	142	VAL	3.0
1	A	117	ASN	2.9
1	B	124	GLU	2.9
1	B	93	LYS	2.9
1	A	113	ILE	2.9
1	A	357	LYS	2.9
1	B	28	GLY	2.9
1	B	89	SER	2.9
1	B	297	ASP	2.9
1	A	54	LEU	2.8
1	B	126	ILE	2.8
1	A	93	LYS	2.7
1	A	150	PRO	2.7
1	B	141	GLU	2.7
1	B	256	LYS	2.7
1	B	130	ALA	2.7
1	B	151	HIS	2.7
1	B	393	ILE	2.7
1	B	302	LYS	2.6
1	B	25	VAL	2.6
1	B	145	LYS	2.6
1	B	325	GLY	2.6
1	B	148	THR	2.6
1	B	389	HIS	2.6
1	B	39	ALA	2.5
1	A	114	TYR	2.5
1	A	127	ARG	2.5
1	A	141	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	324	LYS	2.5
1	A	132	PHE	2.5
1	B	123	ILE	2.5
1	A	301	ASN	2.4
1	B	120	LYS	2.4
1	A	121	SER	2.4
1	A	276	MET	2.4
1	A	185	GLU	2.4
1	A	145	LYS	2.4
1	B	122	HIS	2.4
1	A	89	SER	2.4
1	A	259	SER	2.4
1	B	53	LYS	2.4
1	A	359	ASP	2.3
1	A	140	ILE	2.3
1	A	122	HIS	2.3
1	B	147	TYR	2.3
1	A	162	THR	2.3
1	B	118	LEU	2.3
1	B	430	VAL	2.3
1	A	302	LYS	2.3
1	B	344	ALA	2.3
1	A	309	ASP	2.3
1	B	296	LYS	2.3
1	A	49	VAL	2.2
1	B	49	VAL	2.2
1	A	270	PRO	2.2
1	A	271	GLY	2.2
1	A	79	MET	2.2
1	A	427	GLU	2.2
1	A	389	HIS	2.2
1	A	326	ILE	2.2
1	B	37	ARG	2.2
1	B	32	GLY	2.2
1	B	43	GLY	2.2
1	A	19	ALA	2.2
1	A	20	SER	2.1
1	B	36	ALA	2.1
1	B	46	ALA	2.1
1	B	47	ALA	2.1
1	B	149	ALA	2.1
1	B	212	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	426	LYS	2.1
1	A	45	ARG	2.1
1	B	154	ILE	2.1
1	B	119	THR	2.1
1	B	276	MET	2.1
1	B	153	LEU	2.1
1	A	152	ILE	2.1
1	A	164	HIS	2.1
1	A	133	THR	2.0
1	A	393	ILE	2.0
1	B	152	ILE	2.0
1	A	97	ARG	2.0
1	B	310	LYS	2.0
1	A	147	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	A	808	6/6	0.80	0.20	14.34	40,42,44,48	0
5	GOL	B	801	6/6	0.50	0.26	8.63	50,51,52,52	0
5	GOL	B	803	6/6	0.89	0.18	5.71	28,38,40,44	0
5	GOL	B	806	6/6	0.84	0.17	4.15	27,39,41,43	0
5	GOL	A	817	6/6	0.59	0.26	2.97	57,60,60,60	0
3	ELI	A	958	21/21	0.68	0.21	2.60	31,38,46,49	0
5	GOL	B	812	6/6	0.73	0.23	2.57	55,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ELI	B	958	21/21	0.78	0.19	1.33	33,40,43,45	0
2	PO4	B	5705	5/5	0.94	0.11	1.09	33,33,36,37	0
5	GOL	B	802	6/6	0.79	0.26	0.65	67,67,67,68	0
4	FAD	A	479	53/53	0.93	0.11	-0.25	13,18,32,34	0
4	FAD	B	479	53/53	0.94	0.11	-0.50	15,20,38,39	0
2	PO4	B	5704	5/5	0.97	0.07	-0.87	27,27,28,28	0
2	PO4	A	5703	5/5	0.97	0.09	-0.99	34,36,36,37	0
2	PO4	A	5706	5/5	0.98	0.09	-1.39	29,33,34,34	0
5	GOL	A	810	6/6	0.56	0.21	-	37,46,48,49	0
5	GOL	B	811	6/6	0.54	0.19	-	62,63,63,63	0
5	GOL	B	805	6/6	0.56	0.19	-	38,42,43,45	0
5	GOL	A	809	6/6	0.66	0.24	-	67,68,68,68	0
5	GOL	A	813	6/6	0.65	0.20	-	55,57,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.