



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 01:41 PM EDT

PDB ID : 2AAQ
Title : Crystal Structure Analysis of the human Glutathione Reductase, complexed with GoPI
Authors : Urig, S.; Fritz-Wolf, K.; Reau, R.; Herold-Mende, C.; Toth, K.; Davioud-Charvet, E.; Becker, K.
Deposited on : unknown
Resolution : 2.60 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 : rb-20030345
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) : rb-20030345

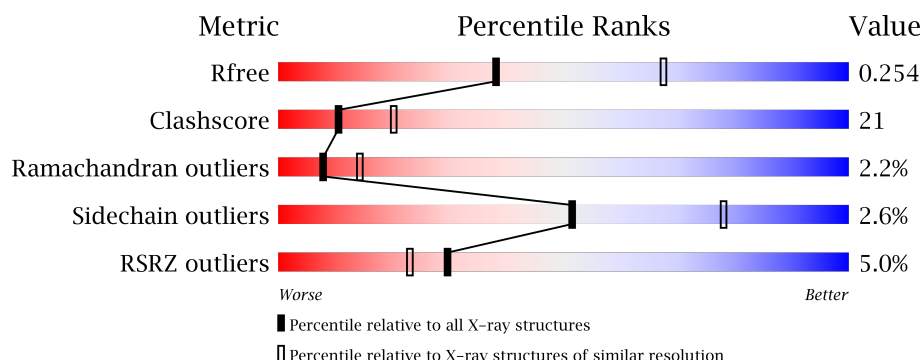
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	479	<div> <div>5%</div> <div>60%</div> <div>33%</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
2	PO4	A	502	-	-	X	-
2	PO4	A	504	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	700	-	-	X	-
8	GOL	A	804	-	X	-	X
8	GOL	A	805	-	X	X	-
8	GOL	A	806	-	X	-	X
8	GOL	A	807	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 3783 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3498	2212	603	659	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	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

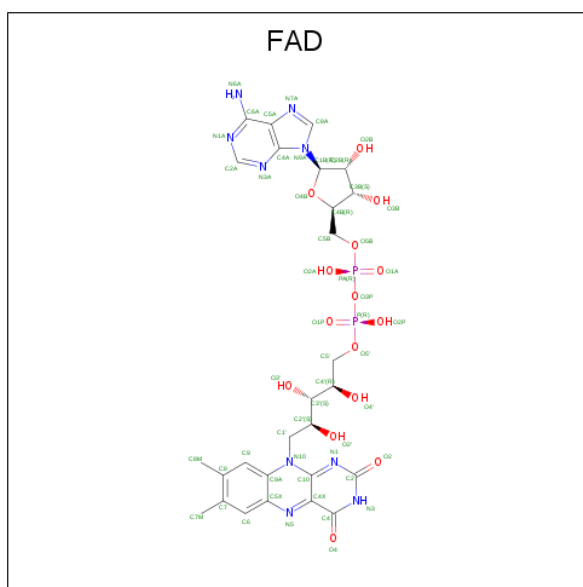
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

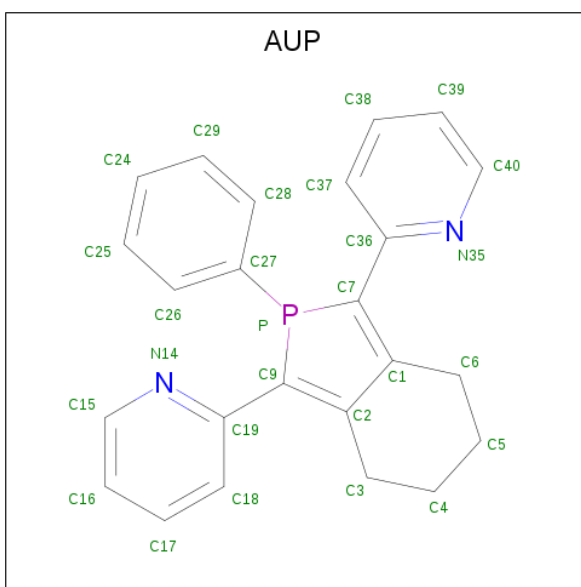
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 6 is 2-(2-PHENYL-3-PYRIDIN-2-YL-4,5,6,7-TETRAHYDRO-2H-ISOPHOSPHINDOL-1-YL)PYRIDINE (three-letter code: AUP) (formula: C₂₄H₂₁N₂P).

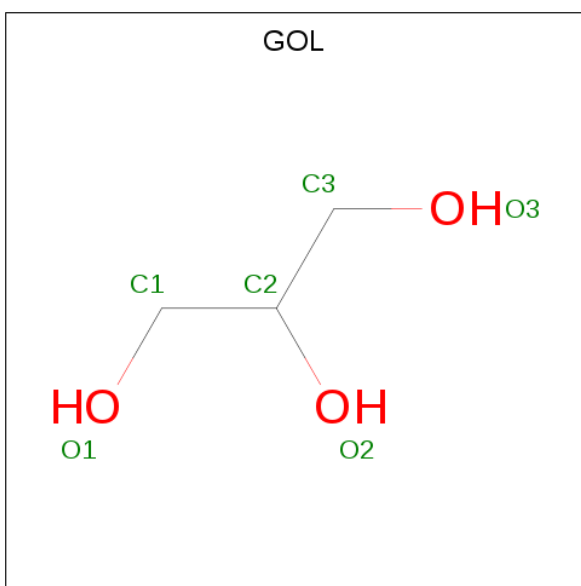


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	P	0	0
			27	24	2	1		

- Molecule 7 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Au	0	0
			2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

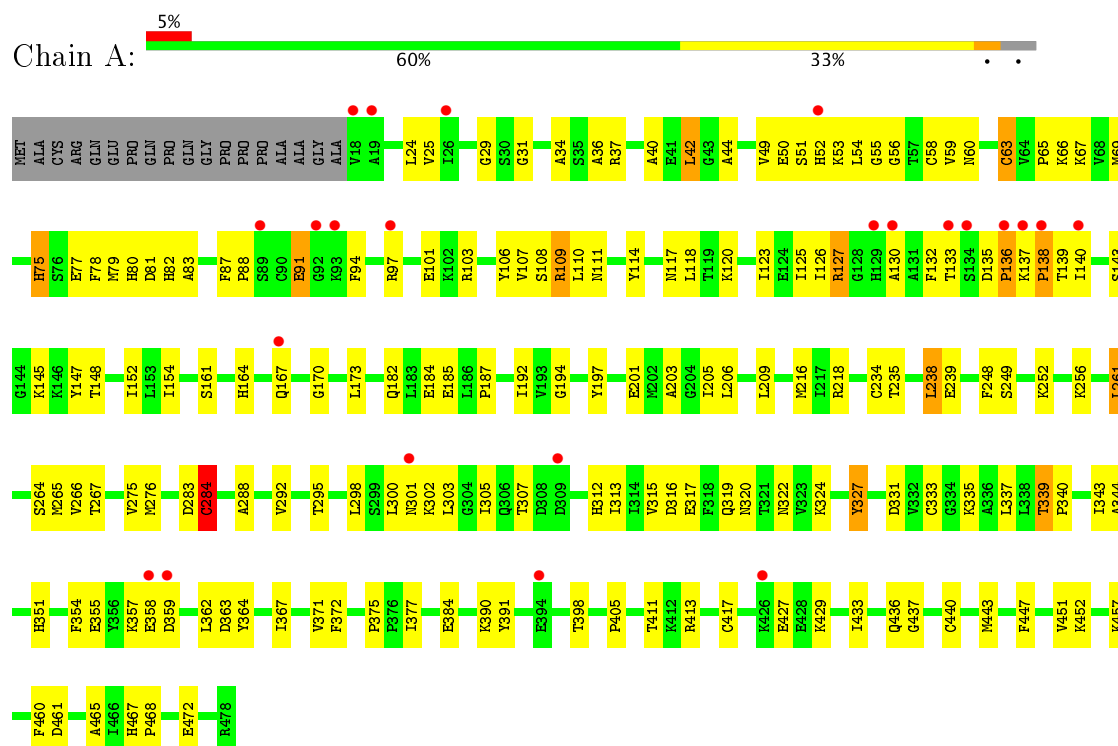
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	157	Total	O	0	0
			157	157		

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.31Å 62.72Å 83.99Å 90.00° 122.47° 90.00°	Depositor
Resolution (Å)	14.98 – 2.60 19.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.98-2.60) 100.0 (19.91-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.259 0.199 , 0.254	Depositor DCC
R_{free} test set	816 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3783	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, K, AUP, AU, PO4, 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	0.36	0/3565	0.62	0/4824

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 [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	3498	0	3537	147	2
2	A	20	0	0	6	1
3	A	1	0	0	2	0
4	A	1	0	0	0	0
5	A	53	0	31	4	0
6	A	27	0	21	5	0
7	A	2	0	0	0	0
8	A	24	0	16	4	0
9	A	157	0	0	26	0
All	All	3783	0	3605	148	2

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 21.

All (148) 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:335:LYS:HB3	8:A:805:GOL:H12	1.34	1.02
1:A:29:GLY:HA3	5:A:499:FAD:H52A	1.62	0.82
1:A:405:PRO:HG3	9:A:827:HOH:O	1.83	0.78
1:A:59:VAL:HG23	1:A:60:ASN:H	1.49	0.77
1:A:335:LYS:HB3	8:A:805:GOL:C1	2.16	0.75
1:A:417:CYS:SG	9:A:928:HOH:O	2.35	0.74
1:A:139:THR:HG22	1:A:148:THR:HB	1.68	0.74
1:A:256:LYS:HA	1:A:261:LEU:HD12	1.70	0.73
1:A:440:CYS:SG	9:A:928:HOH:O	2.46	0.72
1:A:49:VAL:HG22	1:A:126:ILE:HB	1.69	0.72
1:A:339:THR:HG22	1:A:340:PRO:HD3	1.73	0.71
1:A:138:PRO:HB3	9:A:938:HOH:O	1.93	0.68
1:A:411:THR:HG22	1:A:413:ARG:N	2.09	0.67
1:A:91:GLU:H	1:A:91:GLU:CD	1.98	0.67
1:A:427:GLU:OE1	1:A:429:LYS:HE3	1.95	0.67
1:A:317:GLU:HG2	9:A:941:HOH:O	1.94	0.66
1:A:59:VAL:HG23	1:A:60:ASN:N	2.10	0.66
1:A:97:ARG:HG3	9:A:904:HOH:O	1.94	0.66
1:A:161:SER:HB2	1:A:292:VAL:HG23	1.78	0.66
1:A:182:GLN:CB	6:A:601:AUP:H39	2.26	0.65
1:A:192:ILE:HD11	1:A:206:LEU:HD12	1.78	0.65
3:A:700:CL:CL	9:A:946:HOH:O	2.49	0.65
1:A:182:GLN:HB2	6:A:601:AUP:H39	1.78	0.64
1:A:384:GLU:HG3	1:A:398:THR:HG21	1.80	0.64
1:A:34:ALA:HB3	9:A:823:HOH:O	1.99	0.63
1:A:24:LEU:HD21	1:A:140:ILE:HD11	1.82	0.62
1:A:300:LEU:HB3	1:A:305:ILE:HB	1.81	0.61
1:A:362:LEU:HB2	9:A:964:HOH:O	2.01	0.60
1:A:436:GLN:HG2	9:A:816:HOH:O	2.01	0.60
1:A:284:CYS:HB2	6:A:601:AUP:H18	1.82	0.60
1:A:75:HIS:HB3	2:A:502:PO4:O1	2.01	0.59
1:A:65:PRO:O	1:A:69:MET:HG2	2.02	0.59
1:A:77:GLU:HA	1:A:80:HIS:HD2	1.66	0.59
1:A:127:ARG:HH11	1:A:127:ARG:HG3	1.67	0.59
1:A:83:ALA:HA	1:A:87:PHE:O	2.02	0.59
1:A:136:PRO:HG2	9:A:892:HOH:O	2.02	0.59
1:A:140:ILE:HB	9:A:866:HOH:O	2.03	0.58
1:A:197:TYR:O	1:A:201:GLU:HG3	2.03	0.58
1:A:125:ILE:HD12	1:A:125:ILE:N	2.19	0.58
1:A:132:PHE:HA	1:A:140:ILE:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:HD2	9:A:939:HOH:O	2.03	0.57
1:A:154:ILE:HG21	1:A:313:ILE:CD1	2.35	0.57
1:A:140:ILE:HD12	1:A:140:ILE:O	2.05	0.56
1:A:283:ASP:O	1:A:284:CYS:HB3	2.05	0.56
1:A:264:SER:HB3	1:A:276:MET:HE3	1.87	0.55
1:A:24:LEU:HD21	1:A:140:ILE:CG1	2.36	0.55
1:A:364:TYR:HA	1:A:367:ILE:HD11	1.88	0.54
1:A:467:HIS:CE1	1:A:468:PRO:HB3	2.43	0.54
1:A:411:THR:HG22	1:A:413:ARG:H	1.73	0.54
1:A:66:LYS:HD2	1:A:66:LYS:C	2.28	0.54
1:A:137:LYS:HB2	9:A:892:HOH:O	2.07	0.53
1:A:37:ARG:HA	1:A:123:ILE:HD11	1.89	0.53
1:A:63:CYS:HB2	2:A:504:PO4:O3	2.08	0.53
1:A:31:GLY:HA2	9:A:823:HOH:O	2.09	0.53
1:A:440:CYS:HA	1:A:443:MET:HE3	1.91	0.52
1:A:117:ASN:HA	1:A:120:LYS:HZ3	1.75	0.52
1:A:333:CYS:HB2	8:A:805:GOL:O1	2.09	0.52
1:A:56:GLY:HA2	5:A:499:FAD:O3B	2.10	0.51
1:A:59:VAL:HG23	1:A:60:ASN:CG	2.30	0.51
1:A:339:THR:N	1:A:340:PRO:HD2	2.26	0.51
1:A:82:HIS:NE2	1:A:87:PHE:HB3	2.25	0.51
1:A:339:THR:HG22	1:A:340:PRO:CD	2.39	0.51
1:A:117:ASN:HD22	1:A:120:LYS:HZ3	1.59	0.51
1:A:77:GLU:OE1	1:A:77:GLU:HA	2.11	0.50
1:A:108:SER:HA	1:A:111:ASN:HB3	1.94	0.50
1:A:25:VAL:HG21	1:A:36:ALA:HB2	1.94	0.50
1:A:249:SER:HA	1:A:266:VAL:O	2.12	0.50
1:A:465:ALA:HB1	1:A:472:GLU:HB2	1.94	0.50
1:A:75:HIS:CB	2:A:502:PO4:O1	2.60	0.50
1:A:138:PRO:HA	9:A:918:HOH:O	2.11	0.49
1:A:315:VAL:HA	1:A:320:ASN:O	2.12	0.49
1:A:78:PHE:O	1:A:81:ASP:HB2	2.12	0.49
1:A:182:GLN:HB3	6:A:601:AUP:H39	1.94	0.49
1:A:371:VAL:HB	1:A:377:ILE:HB	1.94	0.49
1:A:216:MET:HE1	1:A:265:MET:HB3	1.94	0.48
1:A:234:CYS:O	1:A:238:LEU:HD22	2.14	0.48
1:A:51:SER:C	1:A:52:HIS:ND1	2.67	0.48
1:A:333:CYS:HB3	8:A:805:GOL:H11	1.95	0.48
1:A:344:ALA:HB1	9:A:964:HOH:O	2.13	0.48
1:A:59:VAL:CG2	1:A:60:ASN:H	2.24	0.48
1:A:106:TYR:CE1	1:A:110:LEU:HD21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:O	1:A:239:GLU:HG3	2.12	0.48
1:A:267:THR:HB	1:A:275:VAL:CG2	2.44	0.48
1:A:75:HIS:ND1	2:A:502:PO4:O3	2.46	0.48
1:A:40:ALA:HA	1:A:44:ALA:O	2.13	0.48
1:A:340:PRO:HD2	5:A:499:FAD:O2	2.14	0.48
1:A:145:LYS:HB3	9:A:905:HOH:O	2.14	0.47
1:A:42:LEU:HD23	1:A:354:PHE:HB2	1.95	0.47
1:A:49:VAL:HG11	1:A:130:ALA:HB2	1.95	0.47
1:A:305:ILE:HA	1:A:322:ASN:OD1	2.14	0.47
1:A:447:PHE:O	1:A:451:VAL:HG23	2.14	0.47
1:A:50:GLU:HG2	1:A:54:LEU:HD23	1.96	0.47
1:A:261:LEU:HD13	6:A:601:AUP:C16	2.43	0.47
1:A:411:THR:HG22	1:A:413:ARG:O	2.14	0.47
1:A:24:LEU:HD21	1:A:140:ILE:CD1	2.44	0.47
1:A:457:LYS:HE2	1:A:461:ASP:OD2	2.15	0.47
1:A:357:LYS:C	1:A:359:ASP:H	2.17	0.46
1:A:114:TYR:O	1:A:118:LEU:HG	2.16	0.46
1:A:135:ASP:O	1:A:303:LEU:HD21	2.15	0.46
1:A:56:GLY:O	1:A:60:ASN:ND2	2.49	0.46
1:A:319:GLN:O	1:A:327:TYR:HB3	2.15	0.46
1:A:170:GLY:O	1:A:173:LEU:HD23	2.15	0.46
1:A:331:ASP:HA	1:A:337:LEU:HD22	1.98	0.46
1:A:192:ILE:HD12	1:A:203:ALA:HA	1.98	0.46
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.31	0.45
1:A:88:PRO:HG2	9:A:879:HOH:O	2.17	0.45
1:A:140:ILE:HD11	1:A:147:TYR:HB2	2.00	0.44
1:A:145:LYS:HB2	9:A:914:HOH:O	2.17	0.44
1:A:185:GLU:O	1:A:187:PRO:HD3	2.17	0.44
1:A:301:ASN:C	1:A:303:LEU:H	2.21	0.44
1:A:339:THR:O	1:A:343:ILE:HG12	2.17	0.44
1:A:283:ASP:O	1:A:284:CYS:CB	2.66	0.44
1:A:331:ASP:OD1	5:A:499:FAD:H5'2	2.18	0.44
1:A:452:LYS:HE3	9:A:851:HOH:O	2.16	0.43
1:A:63:CYS:CB	2:A:504:PO4:O3	2.66	0.43
1:A:91:GLU:N	1:A:91:GLU:CD	2.71	0.43
1:A:123:ILE:O	1:A:125:ILE:HD12	2.18	0.43
1:A:67:LYS:HE3	1:A:372:PHE:CE1	2.53	0.43
1:A:82:HIS:HD2	1:A:88:PRO:O	2.01	0.43
1:A:164:HIS:N	1:A:167:GLN:OE1	2.41	0.43
1:A:24:LEU:HB3	1:A:152:ILE:HG12	2.01	0.43
1:A:109:ARG:NH1	9:A:838:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LYS:HE3	1:A:391:TYR:CZ	2.54	0.42
1:A:154:ILE:HG21	1:A:313:ILE:HD12	2.01	0.42
1:A:324:LYS:HB3	1:A:324:LYS:HE2	1.76	0.42
1:A:351:HIS:ND1	1:A:355:GLU:OE2	2.47	0.42
1:A:97:ARG:O	1:A:101:GLU:HG3	2.18	0.42
1:A:316:ASP:OD2	1:A:320:ASN:HB2	2.20	0.42
1:A:55:GLY:O	1:A:59:VAL:HG22	2.20	0.42
1:A:248:PHE:O	1:A:267:THR:HA	2.20	0.42
1:A:433:ILE:HD11	1:A:460:PHE:CZ	2.54	0.42
1:A:53:LYS:HD3	3:A:700:CL:CL	2.57	0.42
1:A:205:ILE:O	1:A:209:LEU:HG	2.20	0.42
1:A:103:ARG:O	1:A:107:VAL:HG23	2.20	0.41
1:A:184:GLU:HB3	9:A:904:HOH:O	2.18	0.41
1:A:362:LEU:HD13	9:A:964:HOH:O	2.19	0.41
1:A:405:PRO:HG2	9:A:850:HOH:O	2.19	0.41
1:A:252:LYS:HD2	1:A:252:LYS:HA	1.97	0.41
1:A:138:PRO:O	1:A:148:THR:HA	2.20	0.41
1:A:295:THR:HA	1:A:298:LEU:HD12	2.02	0.41
1:A:307:THR:HA	1:A:312:HIS:O	2.21	0.41
1:A:117:ASN:HD22	1:A:120:LYS:NZ	2.18	0.41
1:A:194:GLY:HA3	1:A:288:ALA:O	2.21	0.41
1:A:362:LEU:HD12	1:A:363:ASP:H	1.86	0.40
1:A:218:ARG:HB2	2:A:503:PO4:O1	2.21	0.40
1:A:411:THR:HG23	9:A:826:HOH:O	2.21	0.40
1:A:197:TYR:HB2	1:A:371:VAL:HG13	2.04	0.40
1:A:375:PRO:HB2	1:A:437:GLY:C	2.41	0.40

All (2) 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)
1:A:79:MET:SD	1:A:79:MET:SD[2_557]	2.10	0.10
1:A:82:HIS:ND1	2:A:502:PO4:O4[2_557]	2.17	0.03

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	459/479 (96%)	410 (89%)	39 (8%)	10 (2%)	8	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLU
1	A	63	CYS
1	A	94	PHE
1	A	138	PRO
1	A	284	CYS
1	A	358	GLU
1	A	143	SER
1	A	302	LYS
1	A	58	CYS
1	A	136	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	382/394 (97%)	372 (97%)	10 (3%)	51	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	75	HIS
1	A	109	ARG
1	A	127	ARG
1	A	133	THR
1	A	238	LEU
1	A	261	LEU

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Mol	Chain	Res	Type
1	A	284	CYS
1	A	327	TYR
1	A	339	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	82	HIS
1	A	116	ASN
1	A	117	ASN
1	A	250	GLN
1	A	425	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
5	FAD	A	499	-	51,58,58	1.58	8 (15%)	54,89,89	2.36	9 (16%)
2	PO4	A	501	-	4,4,4	1.35	0	6,6,6	0.40	0
2	PO4	A	502	-	4,4,4	1.97	2 (50%)	6,6,6	0.41	0
2	PO4	A	503	-	4,4,4	1.39	0	6,6,6	0.40	0
2	PO4	A	504	4	4,4,4	1.54	1 (25%)	6,6,6	0.38	0
6	AUP	A	601	-	29,31,31	4.78	21 (72%)	31,43,43	6.52	23 (74%)
8	GOL	A	804	-	5,5,5	4.89	5 (100%)	5,5,5	5.47	3 (60%)
8	GOL	A	805	-	5,5,5	5.48	5 (100%)	5,5,5	5.44	3 (60%)
8	GOL	A	806	4	5,5,5	4.89	5 (100%)	5,5,5	5.43	3 (60%)
8	GOL	A	807	-	5,5,5	4.88	5 (100%)	5,5,5	5.50	3 (60%)

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
5	FAD	A	499	-	-	0/28/50/50	0/6/6/6
2	PO4	A	501	-	-	0/0/0/0	0/0/0/0
2	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	PO4	A	503	-	-	0/0/0/0	0/0/0/0
2	PO4	A	504	4	-	0/0/0/0	0/0/0/0
6	AUP	A	601	-	-	0/0/63/63	0/5/5/5
8	GOL	A	804	-	-	0/4/4/4	0/0/0/0
8	GOL	A	805	-	-	0/4/4/4	0/0/0/0
8	GOL	A	806	4	-	0/4/4/4	0/0/0/0
8	GOL	A	807	-	-	0/4/4/4	0/0/0/0

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	AUP	C7-C1	-11.37	1.36	1.55
6	A	601	AUP	C9-C2	-11.32	1.36	1.55
8	A	805	GOL	C3-C2	-9.00	1.18	1.52
6	A	601	AUP	C36-N35	-8.55	1.39	1.47
8	A	806	GOL	C3-C2	-8.33	1.21	1.52
8	A	804	GOL	C3-C2	-8.31	1.21	1.52
8	A	807	GOL	C3-C2	-8.31	1.21	1.52
6	A	601	AUP	C19-N14	-7.72	1.39	1.47
6	A	601	AUP	C18-C19	-5.96	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	AUP	C37-C36	-5.65	1.43	1.53
6	A	601	AUP	C2-C1	-4.83	1.42	1.55
8	A	805	GOL	C1-C2	-4.55	1.35	1.52
6	A	601	AUP	C38-C37	-4.51	1.41	1.53
6	A	601	AUP	C28-C27	-4.27	1.42	1.53
6	A	601	AUP	C26-C27	-4.21	1.42	1.53
6	A	601	AUP	C40-N35	-4.07	1.37	1.47
6	A	601	AUP	C29-C28	-4.05	1.42	1.53
6	A	601	AUP	C17-C18	-4.02	1.42	1.53
6	A	601	AUP	C25-C26	-3.82	1.43	1.53
6	A	601	AUP	C15-N14	-3.73	1.38	1.47
8	A	805	GOL	O2-C2	-3.67	1.32	1.43
6	A	601	AUP	C7-C36	-3.37	1.48	1.53
8	A	806	GOL	C1-C2	-3.24	1.40	1.52
8	A	804	GOL	C1-C2	-3.14	1.40	1.52
8	A	807	GOL	C1-C2	-3.06	1.40	1.52
8	A	807	GOL	O2-C2	-2.77	1.35	1.43
8	A	804	GOL	O2-C2	-2.75	1.35	1.43
8	A	806	GOL	O2-C2	-2.72	1.35	1.43
6	A	601	AUP	C17-C16	-2.51	1.41	1.51
6	A	601	AUP	C39-C38	-2.37	1.42	1.51
6	A	601	AUP	P-C27	-2.21	1.83	1.86
2	A	502	PO4	P-O4	-2.18	1.46	1.54
6	A	601	AUP	C25-C24	-2.15	1.42	1.51
2	A	502	PO4	P-O3	-2.12	1.46	1.54
6	A	601	AUP	C29-C24	-2.12	1.43	1.51
2	A	504	PO4	P-O3	-2.03	1.47	1.54
5	A	499	FAD	C2A-N3A	2.06	1.35	1.32
5	A	499	FAD	C5X-N5	2.46	1.39	1.35
5	A	499	FAD	C2A-N1A	2.50	1.38	1.33
5	A	499	FAD	C9-C8	2.68	1.44	1.37
5	A	499	FAD	C4A-N3A	2.81	1.39	1.35
8	A	804	GOL	O3-C3	3.34	1.56	1.42
8	A	806	GOL	O3-C3	3.37	1.56	1.42
8	A	807	GOL	O3-C3	3.41	1.56	1.42
5	A	499	FAD	C4-N3	3.48	1.39	1.33
8	A	805	GOL	O3-C3	3.50	1.57	1.42
5	A	499	FAD	C9A-N10	4.05	1.44	1.38
8	A	806	GOL	O1-C1	4.56	1.61	1.42
8	A	807	GOL	O1-C1	4.65	1.62	1.42
8	A	804	GOL	O1-C1	4.70	1.62	1.42
8	A	805	GOL	O1-C1	4.77	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	499	FAD	C4X-N5	5.90	1.41	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	499	FAD	C4B-O4B-C1B	-8.50	100.72	109.77
5	A	499	FAD	C4X-C4-N3	-5.35	115.87	123.48
5	A	499	FAD	C4X-C10-N10	-4.54	117.37	120.52
5	A	499	FAD	C4-C4X-C10	-2.87	117.64	119.96
6	A	601	AUP	P-C27-C28	-2.59	101.83	113.52
5	A	499	FAD	N3A-C2A-N1A	-2.52	126.67	128.86
6	A	601	AUP	C39-C40-N35	2.56	117.94	110.87
5	A	499	FAD	C10-C4X-N5	2.58	123.56	120.59
6	A	601	AUP	C16-C15-N14	2.67	118.23	110.87
8	A	805	GOL	O1-C1-C2	2.71	123.74	110.07
6	A	601	AUP	C4-C3-C2	2.83	117.64	111.63
6	A	601	AUP	C29-C24-C25	2.85	120.15	111.21
6	A	601	AUP	C18-C19-N14	2.92	116.19	111.90
8	A	806	GOL	O1-C1-C2	3.03	125.31	110.07
8	A	804	GOL	O1-C1-C2	3.13	125.82	110.07
8	A	807	GOL	O1-C1-C2	3.22	126.28	110.07
5	A	499	FAD	O2A-PA-O1A	3.58	130.82	112.28
6	A	601	AUP	C38-C37-C36	4.01	117.38	111.46
5	A	499	FAD	C1'-N10-C9A	4.10	122.10	118.35
6	A	601	AUP	C24-C29-C28	4.11	119.91	111.42
6	A	601	AUP	C24-C25-C26	4.25	120.21	111.42
6	A	601	AUP	C6-C1-C2	4.52	120.27	113.13
6	A	601	AUP	C25-C26-C27	4.58	119.08	111.76
6	A	601	AUP	C39-C38-C37	4.80	121.34	111.42
6	A	601	AUP	C3-C2-C1	4.93	120.92	113.13
6	A	601	AUP	C29-C28-C27	4.95	119.67	111.76
6	A	601	AUP	C17-C18-C19	5.13	119.03	111.46
6	A	601	AUP	P-C27-C26	5.24	137.18	113.52
6	A	601	AUP	C16-C17-C18	5.28	122.34	111.42
6	A	601	AUP	C37-C36-N35	5.36	119.76	111.90
6	A	601	AUP	C9-C2-C1	6.33	114.21	105.26
8	A	806	GOL	O2-C2-C3	6.35	138.83	108.84
8	A	807	GOL	O2-C2-C3	6.35	138.84	108.84
8	A	804	GOL	O2-C2-C3	6.38	138.96	108.84
6	A	601	AUP	C7-C1-C2	6.40	114.31	105.26
6	A	601	AUP	C28-C27-C26	6.48	120.98	110.19
8	A	805	GOL	O2-C2-C3	6.54	139.71	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	499	FAD	C4-N3-C2	9.70	123.64	115.16
8	A	806	GOL	O3-C3-C2	9.87	159.79	110.07
8	A	805	GOL	O3-C3-C2	9.88	159.83	110.07
8	A	804	GOL	O3-C3-C2	9.93	160.12	110.07
8	A	807	GOL	O3-C3-C2	9.99	160.42	110.07
6	A	601	AUP	C40-N35-C36	18.79	123.56	111.62
6	A	601	AUP	C15-N14-C19	22.53	125.94	111.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	499	FAD	4	0
2	A	502	PO4	3	1
2	A	503	PO4	1	0
2	A	504	PO4	2	0
6	A	601	AUP	5	0
8	A	805	GOL	4	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	461/479 (96%)	-0.09	23 (4%) 30 23	11, 34, 63, 77	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	SER	3.8
1	A	18	VAL	3.7
1	A	92	GLY	3.6
1	A	19	ALA	3.6
1	A	136	PRO	3.2
1	A	138	PRO	2.5
1	A	89	SER	2.5
1	A	133	THR	2.5
1	A	140	ILE	2.4
1	A	394	GLU	2.4
1	A	93	LYS	2.3
1	A	359	ASP	2.3
1	A	130	ALA	2.3
1	A	129	HIS	2.2
1	A	309	ASP	2.2
1	A	167	GLN	2.2
1	A	358	GLU	2.2
1	A	137	LYS	2.1
1	A	26	ILE	2.1
1	A	52	HIS	2.1
1	A	97	ARG	2.0
1	A	301	ASN	2.0
1	A	426	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 [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
8	GOL	A	806	6/6	0.66	0.38	4.66	53,57,57,58	0
8	GOL	A	804	6/6	0.78	0.21	3.58	47,50,51,51	0
6	AUP	A	601	27/27	0.92	0.23	1.95	49,51,54,55	0
8	GOL	A	805	6/6	0.88	0.25	1.52	9,12,25,27	0
2	PO4	A	502	5/5	0.97	0.20	0.57	14,18,28,29	0
5	FAD	A	499	53/53	0.95	0.17	-0.12	32,39,44,45	0
2	PO4	A	504	5/5	0.94	0.17	-0.26	37,38,39,42	0
2	PO4	A	503	5/5	0.99	0.12	-0.45	39,40,40,43	0
2	PO4	A	501	5/5	0.98	0.10	-1.29	54,55,55,56	0
3	CL	A	700	1/1	0.94	0.08	-	51,51,51,51	0
7	AU	A	602	1/1	1.00	0.04	-	47,47,47,47	0
4	K	A	701	1/1	0.95	0.20	-	37,37,37,37	0
8	GOL	A	807	6/6	0.89	0.19	-	49,50,50,51	0
7	AU	A	603	1/1	1.00	0.04	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.