Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 06:22 PM JST

PDB ID	:	8GRJ
Title	:	Crystal structure of gamma-alpha subunit complex from Burkholderia cepacia FAD glucose dehydrogenase in complex with gluconolactone
Authors	:	Yoshida, H.; Kojima, K.; Tsugawa, W.; Okuda-Shimazaki, J.; Kerrigan, J.A.; Sode, K.
Deposited on	:	2022-09-01
Resolution	:	2.95 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:

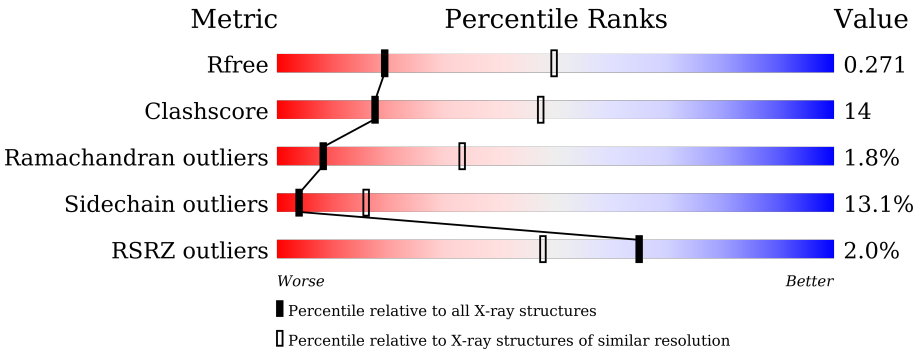
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

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

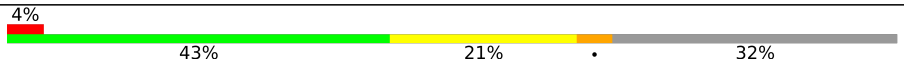
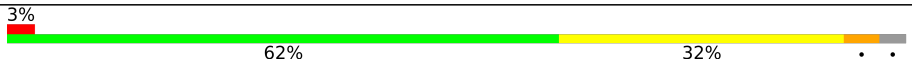
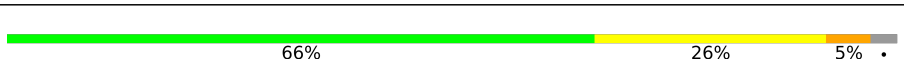
The reported resolution of this entry is 2.95 Å.

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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	168	
1	C	168	
2	B	545	
2	D	545	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10323 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 twin-arginine translocation pathway signal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			865	557	137	168	3			
1	C	114	Total	C	N	O	S	0	0	0
			865	557	137	168	3			

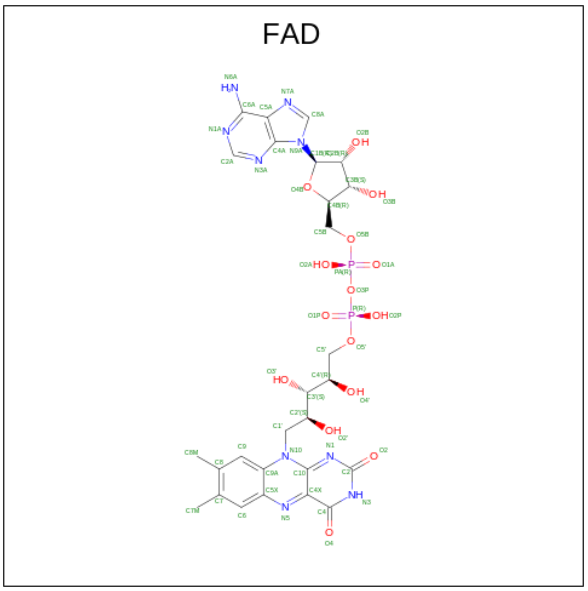
- Molecule 2 is a protein called Glucose dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	531	Total	C	N	O	S	0	0	0
			4150	2631	726	771	22			
2	D	531	Total	C	N	O	S	0	0	0
			4150	2631	726	771	22			

There are 12 discrepancies between the modelled and reference sequences:

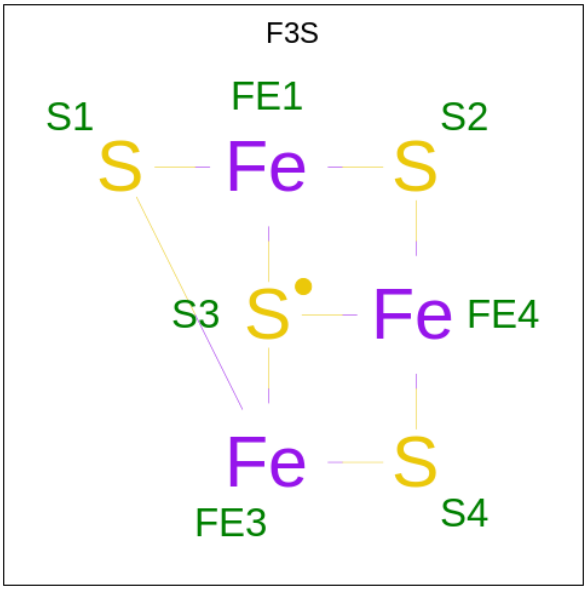
Chain	Residue	Modelled	Actual	Comment	Reference
B	540	HIS	-	expression tag	UNP Q8GQE7
B	541	HIS	-	expression tag	UNP Q8GQE7
B	542	HIS	-	expression tag	UNP Q8GQE7
B	543	HIS	-	expression tag	UNP Q8GQE7
B	544	HIS	-	expression tag	UNP Q8GQE7
B	545	HIS	-	expression tag	UNP Q8GQE7
D	540	HIS	-	expression tag	UNP Q8GQE7
D	541	HIS	-	expression tag	UNP Q8GQE7
D	542	HIS	-	expression tag	UNP Q8GQE7
D	543	HIS	-	expression tag	UNP Q8GQE7
D	544	HIS	-	expression tag	UNP Q8GQE7
D	545	HIS	-	expression tag	UNP Q8GQE7

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



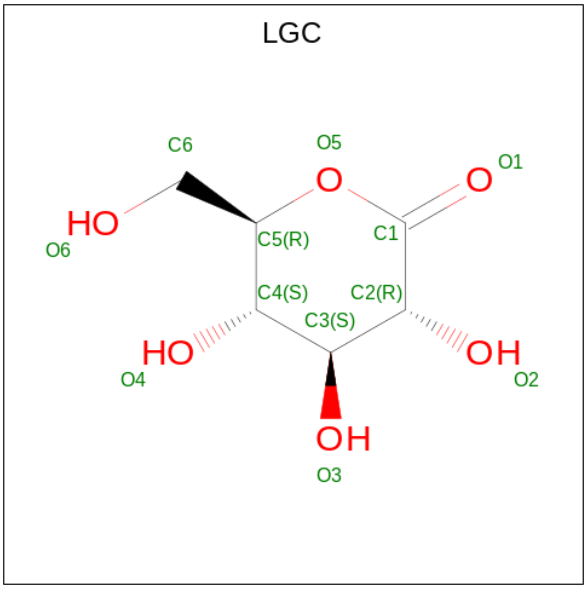
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	Fe	S		0	0
			7	3	4			
4	D	1	Total	Fe	S		0	0
			7	3	4			

- Molecule 5 is D-glucono-1,5-lactone (three-letter code: LGC) (formula: $C_6H_{10}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 12 6 6	0	0
5	D	1	Total C O 12 6 6	0	0

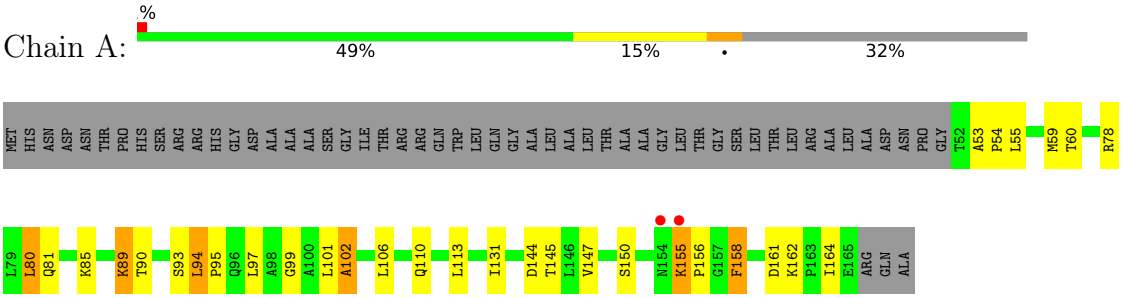
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	14	Total O 14 14	0	0
6	B	65	Total O 65 65	0	0
6	C	12	Total O 12 12	0	0
6	D	58	Total O 58 58	0	0

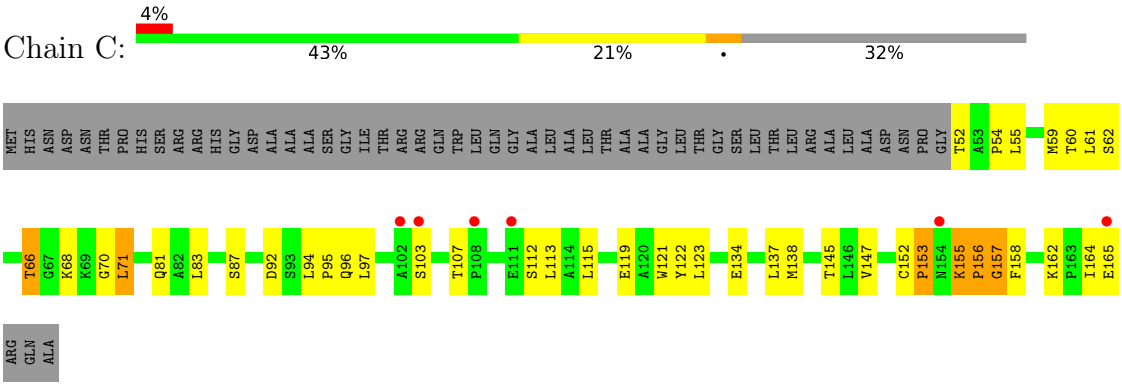
3 Residue-property plots (i)

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.

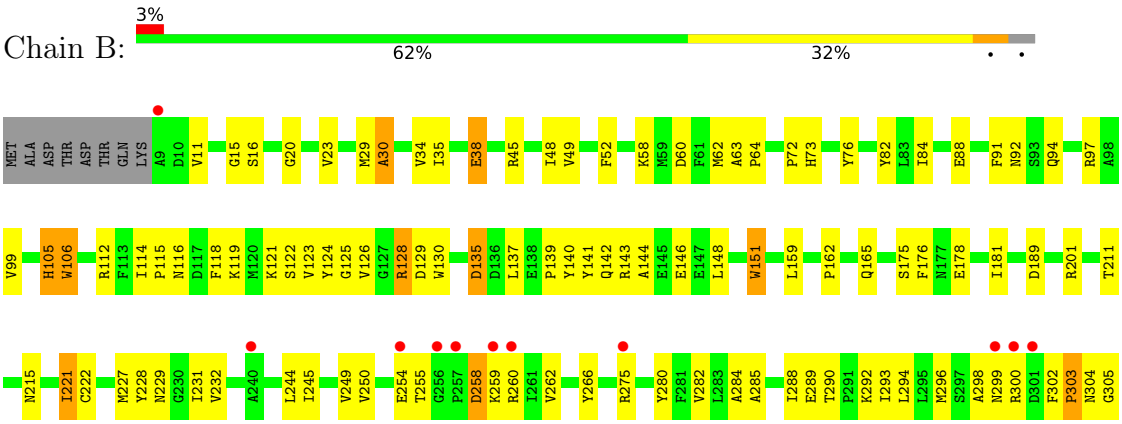
• Molecule 1: twin-arginine translocation pathway signal

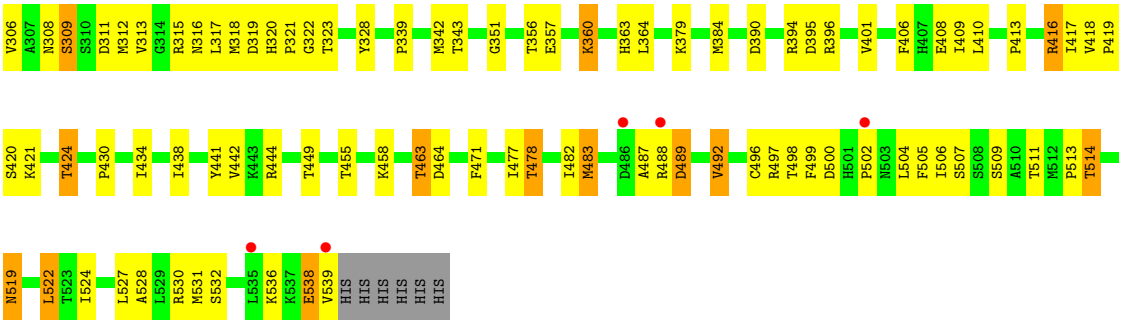


• Molecule 1: twin-arginine translocation pathway signal



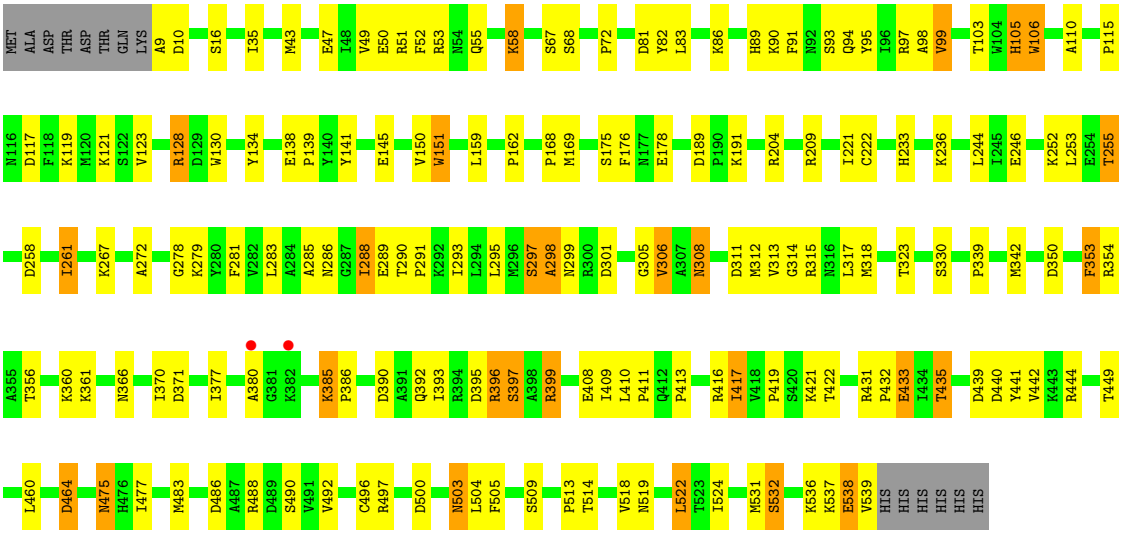
• Molecule 2: Glucose dehydrogenase





• Molecule 2: Glucose dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	111.23Å 111.23Å 527.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.04 – 2.95 50.04 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.04-2.95) 99.5 (50.04-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.02 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.198 , 0.270 0.203 , 0.271	Depositor DCC
R_{free} test set	2125 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.0	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	0.91	EDS
Total number of atoms	10323	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: F3S, FAD, LGC

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	0.69	0/881	0.85	0/1198
1	C	0.68	0/881	0.84	0/1198
2	B	0.70	0/4261	0.91	0/5795
2	D	0.69	0/4261	0.88	0/5795
All	All	0.70	0/10284	0.89	0/13986

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	865	0	881	19	0
1	C	865	0	881	27	0
2	B	4150	0	4072	129	0
2	D	4150	0	4072	108	0
3	B	53	0	30	6	0
3	D	53	0	30	6	0
4	B	7	0	0	1	0
4	D	7	0	0	1	0
5	B	12	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	12	0	10	2	0
6	A	14	0	0	0	0
6	B	65	0	0	6	0
6	C	12	0	0	1	0
6	D	58	0	0	3	0
All	All	10323	0	9986	277	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 14.

All (277) 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:D:130:TRP:HE1	2:D:514:THR:HG22	1.10	1.10
2:D:130:TRP:NE1	2:D:514:THR:HG22	1.89	0.88
2:B:119:LYS:O	2:B:123:VAL:HG23	1.77	0.82
2:B:280:TYR:OH	2:B:538:GLU:HG2	1.84	0.77
2:B:478:THR:OG1	2:B:509:SER:HB2	1.83	0.77
2:B:15:GLY:HA3	2:B:284:ALA:O	1.86	0.75
1:C:162:LYS:HD2	2:D:176:PHE:CZ	2.23	0.74
2:D:89:HIS:HB3	6:D:854:HOH:O	1.89	0.73
2:D:279:LYS:O	2:D:503:ASN:ND2	2.21	0.73
2:B:72:PRO:HG2	2:B:82:TYR:CE1	2.23	0.72
2:B:293:ILE:HD11	3:B:701:FAD:N6A	2.05	0.72
2:D:297:SER:HB2	2:D:306:VAL:CG1	2.20	0.71
2:D:81:ASP:O	2:D:431:ARG:NH1	2.23	0.71
2:B:410:LEU:HD11	2:B:441:TYR:CZ	2.26	0.70
2:D:117:ASP:O	2:D:514:THR:HG21	1.92	0.69
2:D:519:ASN:ND2	5:D:703:LGC:O2	2.26	0.68
2:B:178:GLU:OE1	2:B:342:MET:HB2	1.94	0.67
2:B:222:CYS:SG	2:B:227:MET:HG2	2.35	0.67
2:D:52:PHE:CE1	2:D:58:LYS:HG2	2.30	0.67
2:B:408:GLU:OE1	2:B:514:THR:HG23	1.95	0.67
2:D:119:LYS:HG3	2:D:123:VAL:HG23	1.77	0.67
2:D:47:GLU:O	2:D:51:ARG:HG3	1.95	0.66
2:B:311:ASP:O	2:B:315:ARG:HD2	1.96	0.66
2:B:258:ASP:OD1	2:B:258:ASP:N	2.29	0.66
2:B:250:VAL:HG12	2:B:293:ILE:HD13	1.78	0.65
2:B:260:ARG:HG2	2:B:502:PRO:HG2	1.78	0.65
1:A:55:LEU:HD11	1:A:59:MET:CE	2.26	0.65
2:B:539:VAL:HG22	6:B:861:HOH:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:ASP:O	2:D:399:ARG:HG3	1.97	0.64
2:B:288:ILE:HG12	2:B:477:ILE:HG21	1.79	0.64
2:B:139:PRO:HB2	6:B:863:HOH:O	1.98	0.64
1:C:68:LYS:HB2	1:C:71:LEU:HD13	1.80	0.64
2:D:411:PRO:HG3	2:D:513:PRO:O	1.98	0.64
2:B:319:ASP:OD2	2:B:320:HIS:N	2.31	0.64
2:B:45:ARG:NH2	2:B:229:ASN:OD1	2.30	0.64
2:B:118:PHE:HA	2:B:130:TRP:CD1	2.32	0.64
2:D:110:ALA:HB1	2:D:522:LEU:HG	1.81	0.63
1:C:122:TYR:O	1:C:138:MET:HG2	1.99	0.62
2:D:308:ASN:HD21	2:D:312:MET:N	1.97	0.62
2:D:519:ASN:HB3	3:D:701:FAD:C2	2.29	0.62
2:D:289:GLU:O	2:D:293:ILE:HD12	2.01	0.61
2:B:390:ASP:O	2:B:394:ARG:HG3	2.00	0.61
2:B:105:HIS:CE1	3:B:701:FAD:HM71	2.36	0.61
2:D:52:PHE:CZ	2:D:58:LYS:HG2	2.35	0.60
2:B:309:SER:OG	2:B:500:ASP:OD2	2.20	0.60
1:C:55:LEU:HD11	1:C:59:MET:CE	2.32	0.60
2:D:86:LYS:O	2:D:435:THR:HA	2.02	0.60
2:B:121:LYS:HA	2:B:126:VAL:O	2.01	0.60
2:D:408:GLU:OE2	2:D:514:THR:OG1	2.20	0.60
2:B:483:MET:CE	2:B:496:CYS:SG	2.90	0.59
2:B:128:ARG:NH2	2:B:489:ASP:O	2.30	0.59
2:B:94:GLN:NE2	2:B:105:HIS:HE1	2.01	0.58
2:B:482:ILE:HG13	2:B:513:PRO:HA	1.86	0.58
2:B:121:LYS:O	2:B:125:GLY:N	2.37	0.58
2:D:95:TYR:CD2	2:D:286:ASN:ND2	2.72	0.57
2:D:255:THR:HB	2:D:299:ASN:HD21	1.70	0.57
2:B:498:THR:HG21	2:B:504:LEU:HD23	1.87	0.56
2:D:360:LYS:CE	2:D:449:THR:OG1	2.54	0.56
1:C:94:LEU:HB3	1:C:95:PRO:HD3	1.88	0.56
2:D:189:ASP:OD1	2:D:191:LYS:HG3	2.06	0.56
2:B:135:ASP:N	2:B:135:ASP:OD1	2.39	0.56
2:D:477:ILE:O	2:D:509:SER:OG	2.24	0.55
2:D:497:ARG:HH22	2:D:538:GLU:CD	2.10	0.55
2:B:506:ILE:O	2:B:511:THR:HG21	2.06	0.55
2:D:67:SER:HB3	6:D:838:HOH:O	2.06	0.55
2:B:487:ALA:HB2	2:B:499:PHE:CG	2.43	0.54
1:A:101:LEU:O	1:A:102:ALA:O	2.26	0.54
2:D:261:ILE:HG22	2:D:281:PHE:CD1	2.42	0.54
2:D:9:ALA:O	2:D:278:GLY:HA2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:TYR:O	2:D:145:GLU:HG3	2.07	0.53
2:B:483:MET:HA	2:B:492:VAL:HG23	1.90	0.53
2:D:537:LYS:C	2:D:539:VAL:H	2.11	0.53
1:A:106:LEU:HA	1:A:110:GLN:HE21	1.72	0.53
2:B:15:GLY:O	2:B:20:GLY:HA3	2.08	0.53
2:B:539:VAL:HG13	6:B:855:HOH:O	2.07	0.53
2:B:296:MET:CE	2:B:419:PRO:HB3	2.39	0.53
2:B:141:TYR:O	2:B:144:ALA:HB3	2.09	0.53
2:B:320:HIS:HB3	2:B:406:PHE:HB3	1.90	0.53
2:B:413:PRO:HD2	6:B:858:HOH:O	2.08	0.53
2:B:497:ARG:HB2	2:B:505:PHE:CE2	2.44	0.53
2:D:151:TRP:C	2:D:151:TRP:CD1	2.81	0.52
2:D:278:GLY:O	2:D:281:PHE:HE1	1.93	0.52
2:D:295:LEU:HD12	2:D:419:PRO:HD3	1.91	0.52
2:B:106:TRP:HA	3:B:701:FAD:C6	2.39	0.52
1:C:119:GLU:HG2	1:C:123:LEU:HD12	1.90	0.52
2:B:285:ALA:HB3	2:B:290:THR:OG1	2.09	0.52
2:D:91:PHE:CE2	2:D:288:ILE:HD11	2.44	0.52
1:A:106:LEU:HA	1:A:110:GLN:NE2	2.25	0.52
2:B:84:ILE:HD13	2:B:84:ILE:N	2.24	0.52
1:C:68:LYS:HB2	1:C:71:LEU:CD1	2.40	0.52
2:D:150:VAL:O	2:D:168:PRO:HG2	2.10	0.52
2:B:112:ARG:NE	2:B:141:TYR:HB3	2.25	0.51
2:B:112:ARG:HG2	2:B:141:TYR:CG	2.46	0.51
2:B:305:GLY:O	2:B:308:ASN:HB3	2.10	0.51
2:B:528:ALA:O	2:B:532:SER:OG	2.26	0.51
1:C:66:THR:HG21	1:C:71:LEU:HD21	1.93	0.51
1:A:53:ALA:HB1	1:A:54:PRO:CD	2.41	0.51
2:B:52:PHE:HB2	2:B:221:ILE:HD11	1.93	0.51
1:A:101:LEU:C	1:A:102:ALA:O	2.48	0.51
2:B:328:TYR:HB2	2:B:463:THR:HG22	1.92	0.51
2:B:289:GLU:O	2:B:293:ILE:HG13	2.11	0.51
1:C:92:ASP:OD1	1:C:96:GLN:NE2	2.43	0.51
2:B:16:SER:OG	2:B:99:VAL:HA	2.11	0.50
2:D:297:SER:HB2	2:D:306:VAL:HG12	1.93	0.50
2:D:315:ARG:HG2	2:D:413:PRO:O	2.10	0.50
2:B:527:LEU:O	2:B:531:MET:HG3	2.12	0.50
2:D:293:ILE:HD11	3:D:701:FAD:N6A	2.26	0.50
2:B:339:PRO:HA	4:B:702:F3S:S2	2.51	0.50
2:D:97:ARG:HA	3:D:701:FAD:O2B	2.11	0.50
2:D:317:LEU:HD22	2:D:417:ILE:HG22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD11	1:A:59:MET:HE1	1.94	0.49
2:B:487:ALA:HB2	2:B:499:PHE:CD2	2.47	0.49
2:D:47:GLU:OE2	2:D:51:ARG:NH1	2.46	0.49
2:D:283:LEU:HB3	2:D:290:THR:HG23	1.95	0.49
2:B:416:ARG:HH21	2:B:416:ARG:HB2	1.77	0.49
2:D:311:ASP:O	2:D:315:ARG:HD2	2.13	0.49
2:B:121:LYS:O	2:B:125:GLY:HA2	2.12	0.49
2:B:319:ASP:O	2:B:321:PRO:HD3	2.13	0.49
1:A:158:PHE:CZ	1:C:157:GLY:O	2.66	0.49
1:C:115:LEU:O	1:C:119:GLU:HB2	2.12	0.48
2:D:318:MET:HG2	2:D:409:ILE:HG23	1.95	0.48
2:D:308:ASN:HD21	2:D:311:ASP:C	2.16	0.48
2:B:30:ALA:HB2	2:B:536:LYS:HD3	1.94	0.48
2:B:52:PHE:CE1	2:B:58:LYS:HD2	2.48	0.48
2:B:121:LYS:O	2:B:125:GLY:CA	2.62	0.48
2:D:497:ARG:HB2	2:D:505:PHE:CE2	2.48	0.48
2:D:49:VAL:O	2:D:53:ARG:HG3	2.14	0.48
1:A:155:LYS:HB3	1:A:156:PRO:HD2	1.95	0.48
2:B:260:ARG:HG2	2:B:502:PRO:CG	2.42	0.48
2:D:509:SER:HB3	2:D:524:ILE:HD11	1.96	0.48
1:A:94:LEU:HB3	1:A:95:PRO:HD3	1.96	0.48
2:D:72:PRO:HG2	2:D:82:TYR:CE1	2.49	0.48
2:B:88:GLU:O	2:B:88:GLU:HG2	2.14	0.47
2:D:138:GLU:N	2:D:139:PRO:HD2	2.29	0.47
2:D:537:LYS:O	2:D:539:VAL:N	2.44	0.47
2:B:410:LEU:HD11	2:B:441:TYR:CE2	2.48	0.47
2:B:308:ASN:CG	2:B:308:ASN:O	2.51	0.47
2:B:539:VAL:CG2	6:B:861:HOH:O	2.58	0.47
2:D:178:GLU:OE1	2:D:342:MET:HG3	2.14	0.47
2:B:416:ARG:HH21	2:B:416:ARG:CG	2.28	0.47
2:B:16:SER:HB3	2:B:38:GLU:HG2	1.96	0.47
2:B:320:HIS:CB	2:B:406:PHE:HB3	2.45	0.47
2:B:408:GLU:O	2:B:442:VAL:HG22	2.14	0.47
2:D:16:SER:OG	2:D:99:VAL:HA	2.15	0.47
2:D:360:LYS:HE2	2:D:449:THR:OG1	2.14	0.47
2:B:60:ASP:CG	2:B:63:ALA:HB2	2.35	0.47
2:B:178:GLU:OE1	2:B:342:MET:CE	2.63	0.47
2:B:229:ASN:HB2	2:B:231:ILE:HG22	1.97	0.47
2:B:509:SER:HB3	2:B:524:ILE:HD11	1.96	0.47
1:C:55:LEU:CD1	1:C:59:MET:HE2	2.44	0.47
2:B:48:ILE:HG22	2:B:221:ILE:HG12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ALA:HA	2:B:507:SER:O	2.15	0.47
2:D:519:ASN:HB3	3:D:701:FAD:N3	2.30	0.46
2:D:50:GLU:HA	2:D:50:GLU:OE1	2.13	0.46
2:D:532:SER:O	2:D:536:LYS:HG3	2.16	0.46
2:B:229:ASN:O	2:B:232:VAL:HG23	2.15	0.46
2:B:23:VAL:HG11	2:B:282:VAL:HG21	1.96	0.46
2:B:72:PRO:CG	2:B:82:TYR:CE1	2.97	0.45
2:B:137:LEU:O	2:B:140:TYR:HB2	2.15	0.45
1:C:156:PRO:C	1:C:158:PHE:H	2.18	0.45
2:B:94:GLN:HE21	2:B:105:HIS:HE1	1.63	0.45
2:D:252:LYS:CG	2:D:297:SER:HA	2.46	0.45
1:C:153:PRO:HB2	1:C:155:LYS:HG2	1.98	0.45
2:D:72:PRO:O	2:D:97:ARG:HD3	2.17	0.45
2:D:314:GLY:O	2:D:416:ARG:HA	2.17	0.45
2:D:360:LYS:HE3	2:D:449:THR:OG1	2.16	0.45
2:D:128:ARG:NH2	2:D:490:SER:OG	2.37	0.45
2:D:298:ALA:HB2	2:D:305:GLY:HA2	1.98	0.45
1:C:66:THR:HG23	1:C:68:LYS:H	1.82	0.45
1:C:55:LEU:HD11	1:C:59:MET:HE1	1.99	0.45
1:A:55:LEU:CD1	1:A:59:MET:CE	2.94	0.45
2:B:311:ASP:O	2:B:315:ARG:CD	2.64	0.45
2:D:209:ARG:NH2	6:D:805:HOH:O	2.46	0.45
2:B:519:ASN:HB3	3:B:701:FAD:C2	2.47	0.45
2:D:98:ALA:O	2:D:99:VAL:C	2.56	0.45
2:D:285:ALA:O	2:D:289:GLU:HB2	2.17	0.44
2:D:285:ALA:O	2:D:286:ASN:CG	2.55	0.44
2:D:361:LYS:HD3	2:D:518:VAL:HG12	1.98	0.44
2:D:151:TRP:C	2:D:151:TRP:HD1	2.21	0.44
2:B:62:MET:CE	2:B:73:HIS:CD2	3.01	0.44
1:C:121:TRP:HB3	1:C:137:LEU:HD22	1.99	0.44
2:B:124:TYR:CE1	2:B:351:GLY:O	2.71	0.44
2:B:181:ILE:HG21	2:B:364:LEU:HD22	2.00	0.44
2:B:356:THR:HG22	2:B:357:GLU:HG3	2.00	0.44
1:C:54:PRO:HD2	6:C:207:HOH:O	2.18	0.44
2:B:140:TYR:CE1	2:B:530:ARG:HA	2.52	0.44
2:B:487:ALA:HB2	2:B:499:PHE:CB	2.47	0.44
2:D:115:PRO:HA	2:D:134:TYR:HB2	2.00	0.44
2:B:175:SER:H	2:B:342:MET:CE	2.31	0.44
2:B:487:ALA:HA	2:B:499:PHE:CD2	2.53	0.44
2:D:94:GLN:HE21	2:D:105:HIS:HE1	1.66	0.44
1:A:55:LEU:CD1	1:A:59:MET:HE1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:O	1:A:102:ALA:HB3	2.18	0.44
2:B:116:ASN:OD1	2:B:116:ASN:N	2.51	0.44
2:B:298:ALA:HB1	2:B:303:PRO:O	2.18	0.44
2:B:395:ASP:OD1	2:B:396:ARG:NH1	2.51	0.44
2:D:312:MET:O	2:D:315:ARG:HB2	2.16	0.44
2:B:16:SER:CB	2:B:38:GLU:HG2	2.48	0.43
2:B:360:LYS:HE3	2:B:449:THR:HA	1.99	0.43
1:C:60:THR:HG22	1:C:61:LEU:N	2.32	0.43
1:C:138:MET:HE3	2:D:371:ASP:N	2.33	0.43
2:B:308:ASN:HB2	2:B:313:VAL:HG21	2.01	0.43
2:D:288:ILE:HG13	2:D:477:ILE:HG21	1.99	0.43
2:B:288:ILE:HG12	2:B:477:ILE:CG2	2.48	0.43
1:C:62:SER:O	1:C:66:THR:HB	2.18	0.43
2:D:393:ILE:O	2:D:397:SER:OG	2.25	0.43
1:C:138:MET:HE3	2:D:370:ILE:C	2.38	0.43
2:D:83:LEU:HD22	2:D:432:PRO:HB2	1.99	0.43
2:D:119:LYS:HG3	2:D:123:VAL:CG2	2.45	0.43
2:D:222:CYS:HA	4:D:702:F3S:S4	2.58	0.43
2:D:339:PRO:O	2:D:366:ASN:ND2	2.44	0.43
2:B:142:GLN:O	2:B:146:GLU:HG3	2.19	0.43
2:D:353:PHE:CD1	2:D:353:PHE:C	2.92	0.43
2:D:204:ARG:HG3	2:D:204:ARG:HH11	1.84	0.43
2:D:483:MET:HA	2:D:492:VAL:HG23	2.00	0.43
1:A:89:LYS:HE3	1:A:89:LYS:HA	2.01	0.43
1:C:70:GLY:O	1:C:71:LEU:C	2.57	0.43
2:D:267:LYS:HA	2:D:272:ALA:O	2.18	0.43
2:B:255:THR:HG21	2:B:302:PHE:CD2	2.54	0.42
2:B:114:ILE:HB	2:B:115:PRO:CD	2.49	0.42
2:B:410:LEU:CD1	2:B:441:TYR:CE2	3.02	0.42
2:B:201:ARG:HA	2:B:227:MET:HA	2.01	0.42
2:B:424:THR:HG23	6:B:822:HOH:O	2.19	0.42
2:D:258:ASP:OD1	2:D:258:ASP:N	2.46	0.42
1:A:144:ASP:OD1	1:A:144:ASP:N	2.52	0.42
2:B:91:PHE:CB	2:B:434:ILE:HG21	2.50	0.42
2:B:122:SER:OG	2:B:129:ASP:OD2	2.36	0.42
2:D:233:HIS:HA	2:D:236:LYS:HB2	2.02	0.42
1:A:97:LEU:HD22	1:A:113:LEU:HD23	2.01	0.42
1:A:162:LYS:HD2	2:B:176:PHE:CZ	2.55	0.42
2:B:63:ALA:N	2:B:64:PRO:CD	2.83	0.42
2:B:151:TRP:CD1	2:B:151:TRP:C	2.93	0.42
2:B:189:ASP:OD1	2:B:189:ASP:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:410:LEU:HD11	2:D:441:TYR:CZ	2.55	0.42
1:A:54:PRO:HB2	1:A:80:LEU:HD11	2.00	0.42
1:C:68:LYS:NZ	2:D:390:ASP:OD2	2.37	0.42
2:D:385:LYS:O	2:D:386:PRO:C	2.58	0.42
2:B:522:LEU:HD23	2:B:522:LEU:HA	1.86	0.42
2:B:148:LEU:HD22	2:B:228:TYR:CE2	2.55	0.41
1:C:55:LEU:CD1	1:C:59:MET:CE	2.96	0.41
2:D:417:ILE:O	2:D:417:ILE:HG13	2.20	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.83	0.41
2:B:76:TYR:CE2	2:B:92:ASN:HB2	2.55	0.41
2:D:204:ARG:HG3	2:D:204:ARG:NH1	2.35	0.41
2:D:293:ILE:O	2:D:297:SER:OG	2.38	0.41
2:D:350:ASP:HA	2:D:354:ARG:HD2	2.02	0.41
2:D:377:ILE:O	2:D:380:ALA:HB3	2.20	0.41
2:D:440:ASP:O	2:D:444:ARG:HG3	2.20	0.41
2:B:266:TYR:CD1	2:B:266:TYR:C	2.94	0.41
2:B:318:MET:HG2	2:B:409:ILE:HG23	2.02	0.41
2:D:308:ASN:HD22	2:D:308:ASN:HA	1.56	0.41
2:B:308:ASN:HB2	2:B:313:VAL:CG2	2.50	0.41
2:B:137:LEU:O	2:B:140:TYR:N	2.50	0.41
2:D:91:PHE:HE2	2:D:288:ILE:HD11	1.85	0.41
2:D:106:TRP:HA	3:D:701:FAD:C6	2.51	0.41
2:D:105:HIS:CE1	3:D:701:FAD:HM71	2.56	0.41
2:D:392:GLN:O	2:D:396:ARG:HG2	2.20	0.41
2:B:49:VAL:O	2:B:52:PHE:HB3	2.21	0.41
2:B:416:ARG:HH21	2:B:416:ARG:CB	2.34	0.41
2:D:475:ASN:HD21	5:D:703:LGC:HC61	1.84	0.41
2:B:137:LEU:HD12	2:B:137:LEU:HA	1.93	0.41
1:C:83:LEU:O	1:C:87:SER:HB2	2.21	0.41
2:B:106:TRP:HB2	3:B:701:FAD:C4X	2.50	0.41
2:B:308:ASN:HD21	2:B:311:ASP:CA	2.34	0.41
2:D:103:THR:O	2:D:106:TRP:CD1	2.73	0.41
2:D:409:ILE:HG13	2:D:442:VAL:HG21	2.03	0.41
2:B:320:HIS:CG	2:B:406:PHE:HB3	2.56	0.40
2:B:322:GLY:O	2:B:471:PHE:HA	2.21	0.40
2:B:519:ASN:HB3	3:B:701:FAD:N3	2.36	0.40
2:B:175:SER:H	2:B:342:MET:HE3	1.86	0.40
2:B:483:MET:CA	2:B:492:VAL:HG23	2.51	0.40
2:B:487:ALA:HB2	2:B:499:PHE:HB3	2.03	0.40
2:D:261:ILE:CG2	2:D:281:PHE:CD1	3.04	0.40
2:D:290:THR:N	2:D:291:PRO:HD2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ASN:O	2:B:308:ASN:ND2	2.55	0.40
1:C:62:SER:O	1:C:66:THR:HG22	2.20	0.40
2:D:417:ILE:HA	2:D:433:GLU: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	112/168 (67%)	102 (91%)	7 (6%)	3 (3%)	5 23
1	C	112/168 (67%)	97 (87%)	11 (10%)	4 (4%)	3 16
2	B	529/545 (97%)	468 (88%)	53 (10%)	8 (2%)	10 38
2	D	529/545 (97%)	482 (91%)	39 (7%)	8 (2%)	10 38
All	All	1282/1426 (90%)	1149 (90%)	110 (9%)	23 (2%)	8 33

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
2	B	489	ASP
2	D	298	ALA
2	D	439	ASP
2	D	464	ASP
1	A	150	SER
1	A	158	PHE
2	B	30	ALA
2	B	304	ASN
1	C	157	GLY
2	D	538	GLU
2	B	162	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	430	PRO
1	C	156	PRO
2	D	99	VAL
2	B	128	ARG
2	D	162	PRO
2	B	306	VAL
2	B	303	PRO
1	C	71	LEU
1	C	153	PRO
2	D	313	VAL
2	D	221	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/133 (71%)	80 (84%)	15 (16%)	2	10
1	C	95/133 (71%)	80 (84%)	15 (16%)	2	10
2	B	441/454 (97%)	382 (87%)	59 (13%)	4	15
2	D	441/454 (97%)	390 (88%)	51 (12%)	5	20
All	All	1072/1174 (91%)	932 (87%)	140 (13%)	4	16

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	78	ARG
1	A	80	LEU
1	A	81	GLN
1	A	85	LYS
1	A	89	LYS
1	A	90	THR
1	A	93	SER
1	A	94	LEU
1	A	131	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	145	THR
1	A	147	VAL
1	A	155	LYS
1	A	161	ASP
1	A	164	ILE
2	B	11	VAL
2	B	29	MET
2	B	34	VAL
2	B	35	ILE
2	B	38	GLU
2	B	97	ARG
2	B	105	HIS
2	B	106	TRP
2	B	135	ASP
2	B	143	ARG
2	B	151	TRP
2	B	159	LEU
2	B	165	GLN
2	B	211	THR
2	B	215	ASN
2	B	221	ILE
2	B	244	LEU
2	B	245	ILE
2	B	249	VAL
2	B	254	GLU
2	B	258	ASP
2	B	259	LYS
2	B	262	VAL
2	B	275	ARG
2	B	292	LYS
2	B	294	LEU
2	B	299	ASN
2	B	300	ARG
2	B	309	SER
2	B	312	MET
2	B	316	ASN
2	B	317	LEU
2	B	323	THR
2	B	343	THR
2	B	360	LYS
2	B	363	HIS
2	B	379	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	384	MET
2	B	401	VAL
2	B	416	ARG
2	B	417	ILE
2	B	418	VAL
2	B	420	SER
2	B	421	LYS
2	B	424	THR
2	B	438	ILE
2	B	444	ARG
2	B	455	THR
2	B	458	LYS
2	B	463	THR
2	B	464	ASP
2	B	478	THR
2	B	483	MET
2	B	488	ARG
2	B	492	VAL
2	B	514	THR
2	B	519	ASN
2	B	522	LEU
2	B	538	GLU
1	C	52	THR
1	C	66	THR
1	C	81	GLN
1	C	97	LEU
1	C	103	SER
1	C	107	THR
1	C	112	SER
1	C	113	LEU
1	C	134	GLU
1	C	145	THR
1	C	147	VAL
1	C	152	CYS
1	C	155	LYS
1	C	164	ILE
1	C	165	GLU
2	D	10	ASP
2	D	35	ILE
2	D	43	MET
2	D	55	GLN
2	D	58	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	68	SER
2	D	90	LYS
2	D	93	SER
2	D	105	HIS
2	D	106	TRP
2	D	121	LYS
2	D	128	ARG
2	D	151	TRP
2	D	159	LEU
2	D	169	MET
2	D	175	SER
2	D	244	LEU
2	D	246	GLU
2	D	253	LEU
2	D	255	THR
2	D	261	ILE
2	D	288	ILE
2	D	297	SER
2	D	301	ASP
2	D	306	VAL
2	D	308	ASN
2	D	323	THR
2	D	330	SER
2	D	353	PHE
2	D	356	THR
2	D	385	LYS
2	D	396	ARG
2	D	397	SER
2	D	399	ARG
2	D	417	ILE
2	D	421	LYS
2	D	422	THR
2	D	433	GLU
2	D	435	THR
2	D	460	LEU
2	D	464	ASP
2	D	475	ASN
2	D	486	ASP
2	D	488	ARG
2	D	496	CYS
2	D	500	ASP
2	D	503	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	504	LEU
2	D	522	LEU
2	D	531	MET
2	D	532	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
2	B	25	HIS
2	B	94	GLN
2	B	215	ASN
2	B	299	ASN
2	B	308	ASN
1	C	96	GLN
1	C	110	GLN
2	D	25	HIS
2	D	89	HIS
2	D	94	GLN
2	D	215	ASN
2	D	299	ASN
2	D	304	ASN
2	D	308	ASN
2	D	475	ASN
2	D	519	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 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	$\#\|Z\| > 2$
4	F3S	D	702	2	0,9,9	-	-	-		
5	LGC	B	703	-	12,12,12	2.15	1 (8%)	15,17,17	1.30	2 (13%)
3	FAD	B	701	2	53,58,58	0.60	0	68,89,89	0.89	3 (4%)
5	LGC	D	703	-	12,12,12	2.67	1 (8%)	15,17,17	1.46	3 (20%)
3	FAD	D	701	2	53,58,58	0.69	0	68,89,89	0.84	1 (1%)
4	F3S	B	702	2	0,9,9	-	-	-		

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	F3S	D	702	2	-	-	0/3/3/3
5	LGC	B	703	-	-	2/2/22/22	0/1/1/1
3	FAD	B	701	2	-	1/30/50/50	0/6/6/6
5	LGC	D	703	-	-	1/2/22/22	0/1/1/1
3	FAD	D	701	2	-	7/30/50/50	0/6/6/6
4	F3S	B	702	2	-	-	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	703	LGC	O5-C1	8.72	1.47	1.34
5	B	703	LGC	O5-C1	6.84	1.44	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	703	LGC	O5-C5-C4	3.31	115.61	109.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	703	LGC	C4-C3-C2	-2.62	106.02	110.18
3	B	701	FAD	O2P-P-O1P	2.41	124.14	112.24
5	D	703	LGC	O5-C5-C4	2.40	113.99	109.73
3	D	701	FAD	O5'-P-O1P	2.32	118.13	109.07
3	B	701	FAD	C4-N3-C2	-2.13	121.72	125.64
3	B	701	FAD	C5A-C6A-N6A	2.04	123.45	120.35
5	B	703	LGC	C3-C4-C5	2.02	113.85	110.24
5	D	703	LGC	O2-C2-C3	2.01	114.69	110.53

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	701	FAD	C5B-O5B-PA-O2A
3	D	701	FAD	O4B-C4B-C5B-O5B
3	D	701	FAD	C3B-C4B-C5B-O5B
5	B	703	LGC	O5-C5-C6-O6
5	D	703	LGC	O5-C5-C6-O6
5	B	703	LGC	C4-C5-C6-O6
3	D	701	FAD	C5B-O5B-PA-O3P
3	D	701	FAD	C5'-O5'-P-O3P
3	D	701	FAD	C5B-O5B-PA-O1A
3	B	701	FAD	O4B-C4B-C5B-O5B
3	D	701	FAD	C1'-C2'-C3'-O3'

There are no ring outliers.

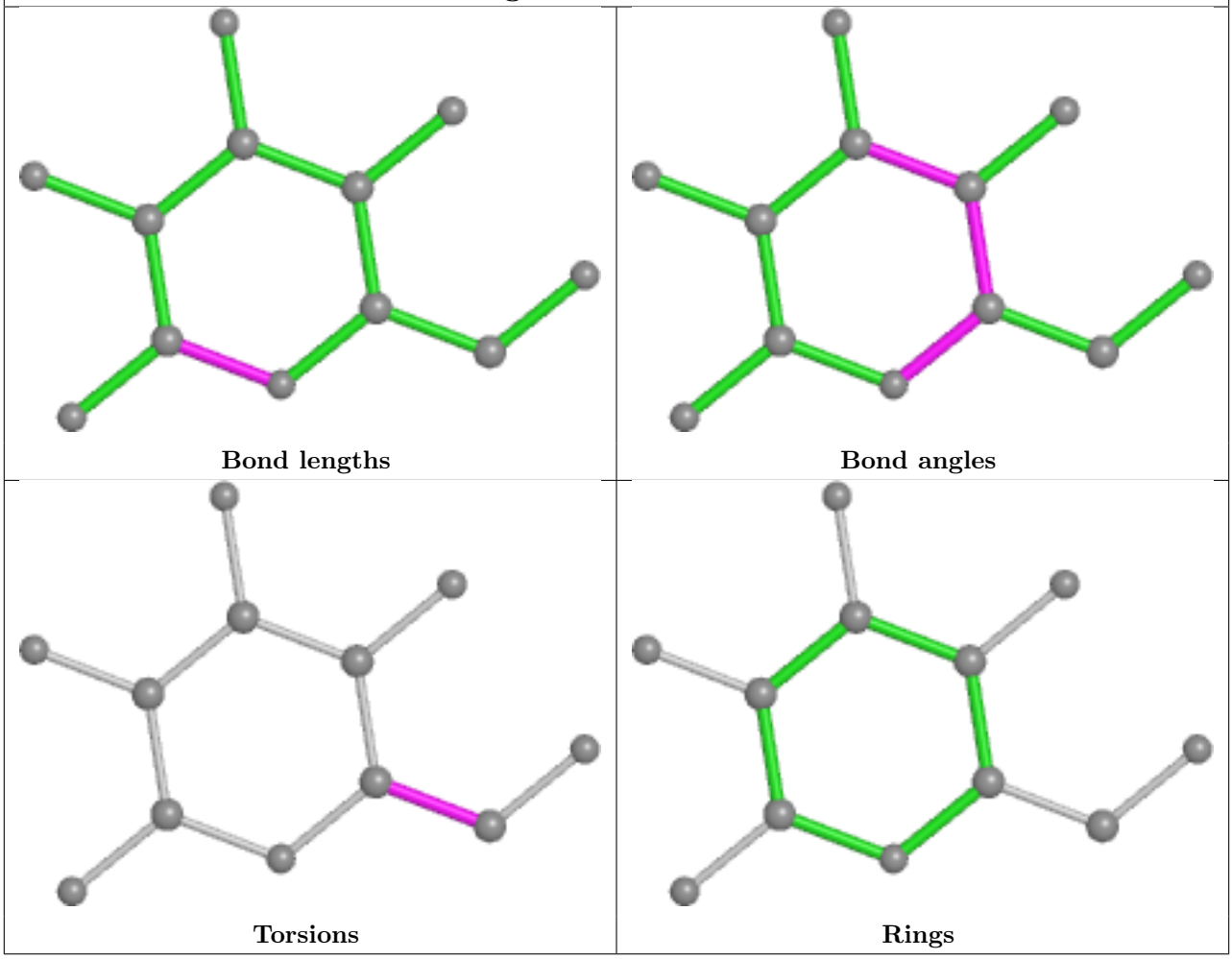
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	F3S	1	0
3	B	701	FAD	6	0
5	D	703	LGC	2	0
3	D	701	FAD	6	0
4	B	702	F3S	1	0

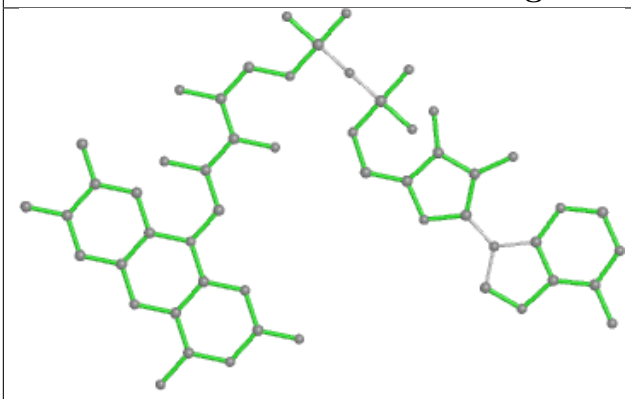
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

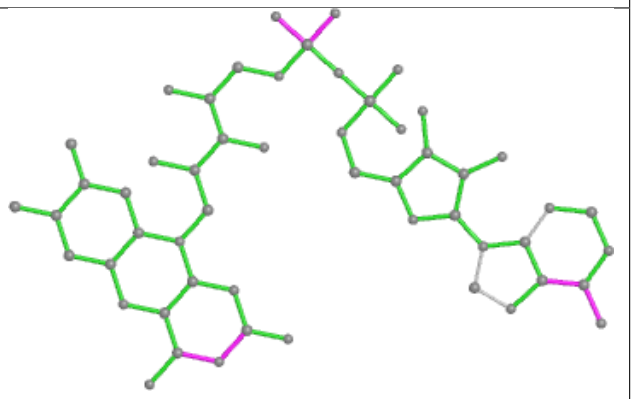
Ligand LGC B 703



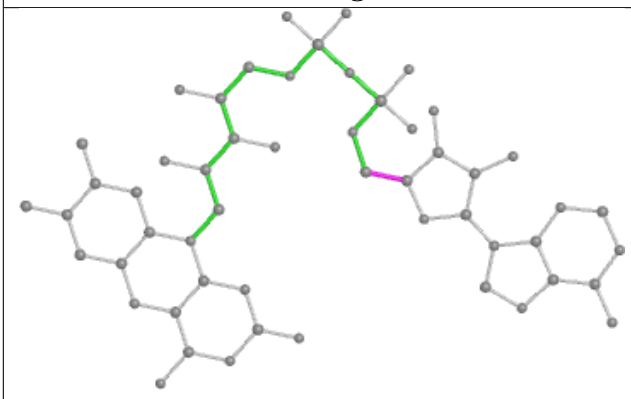
Ligand FAD B 701



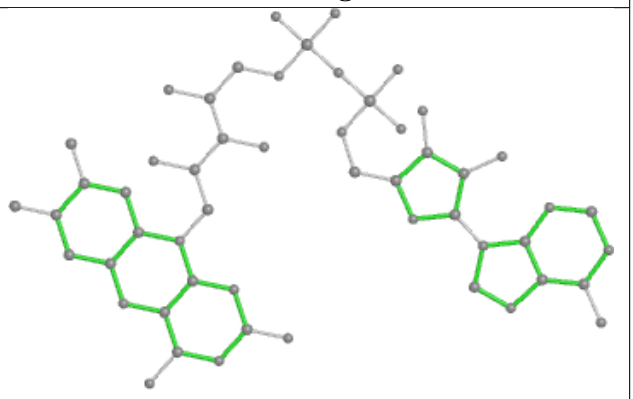
Bond lengths



Bond angles

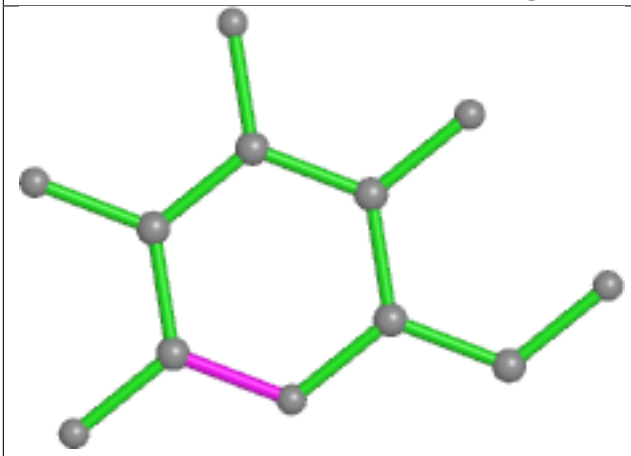


Torsions

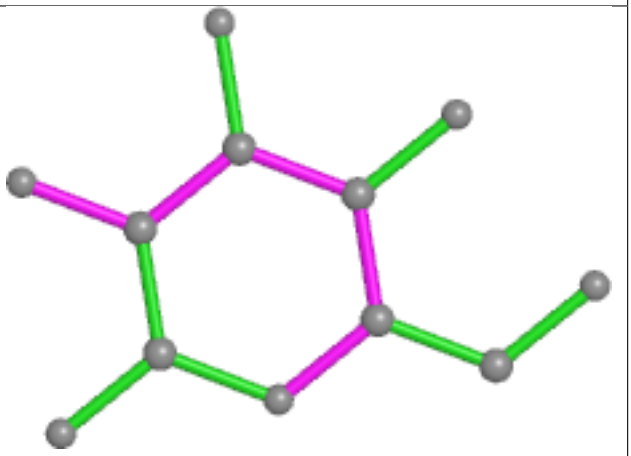


Rings

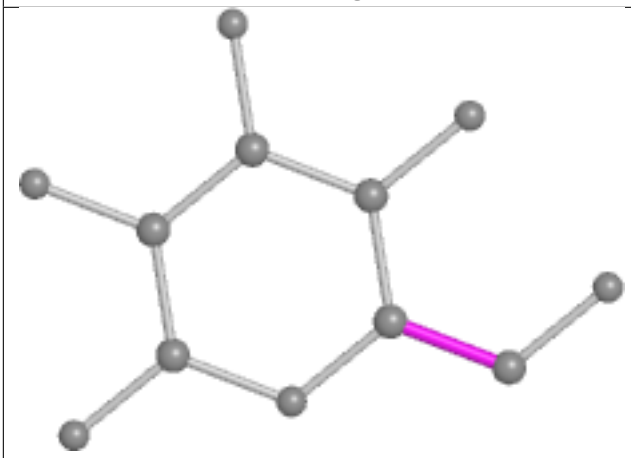
Ligand LGC D 703



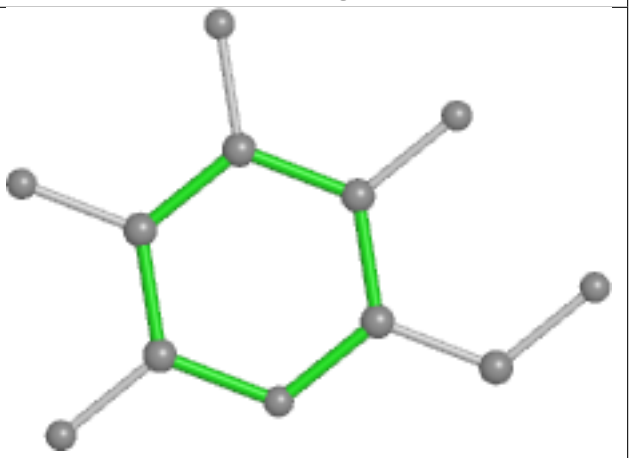
Bond lengths



Bond angles

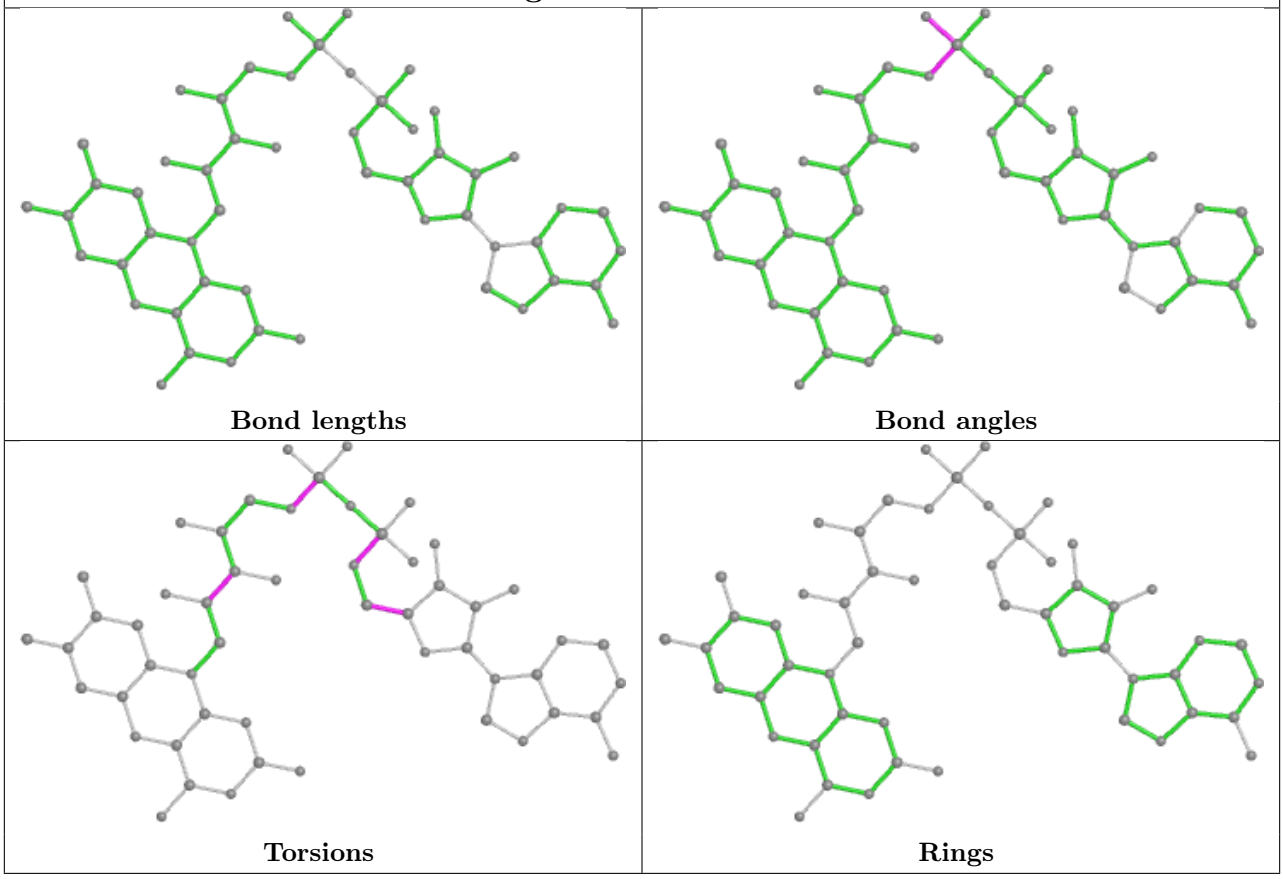


Torsions



Rings

Ligand FAD D 701



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	114/168 (67%)	-0.20	2 (1%) 68 51	17, 33, 75, 112	0
1	C	114/168 (67%)	0.02	6 (5%) 26 16	18, 39, 83, 94	0
2	B	531/545 (97%)	-0.10	16 (3%) 50 34	16, 39, 74, 90	0
2	D	531/545 (97%)	-0.21	2 (0%) 92 84	16, 37, 63, 87	0
All	All	1290/1426 (90%)	-0.14	26 (2%) 65 48	16, 38, 71, 112	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	ASN	4.9
1	C	165	GLU	3.6
1	A	154	ASN	3.3
2	B	260	ARG	3.0
2	B	240	ALA	2.9
2	B	256	GLY	2.9
2	B	257	PRO	2.8
2	B	486	ASP	2.7
2	B	301	ASP	2.6
2	B	254	GLU	2.6
1	C	103	SER	2.6
2	B	9	ALA	2.5
1	A	155	LYS	2.5
1	C	111	GLU	2.5
2	D	380	ALA	2.4
2	B	275	ARG	2.3
2	B	300	ARG	2.3
2	B	535	LEU	2.3
2	B	539	VAL	2.3
2	D	382	LYS	2.3
2	B	299	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	108	PRO	2.2
2	B	488	ARG	2.2
2	B	259	LYS	2.1
2	B	502	PRO	2.1
1	C	102	ALA	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)

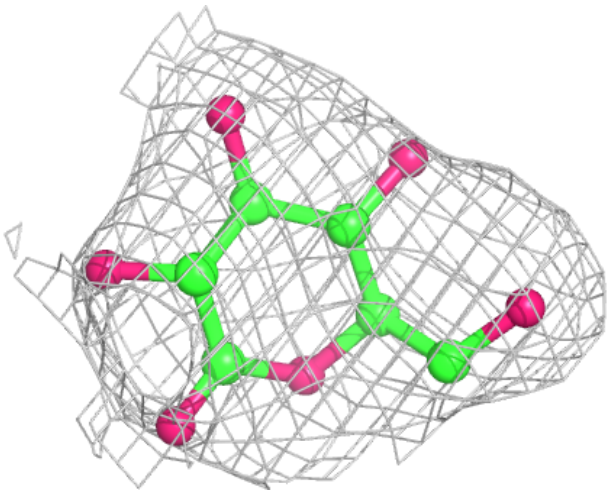
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

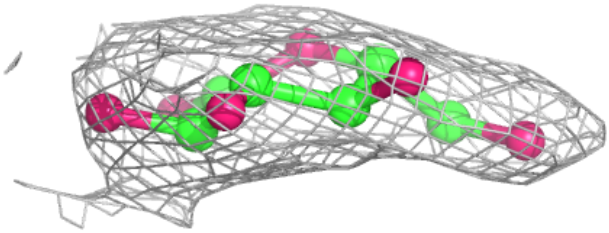
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LGC	D	703	12/12	0.95	0.15	35,40,43,43	0
3	FAD	B	701	53/53	0.96	0.15	23,33,38,40	0
5	LGC	B	703	12/12	0.97	0.13	35,42,46,50	0
3	FAD	D	701	53/53	0.97	0.13	16,21,35,36	0
4	F3S	B	702	7/7	0.98	0.08	26,30,30,36	0
4	F3S	D	702	7/7	0.99	0.07	23,26,28,29	0

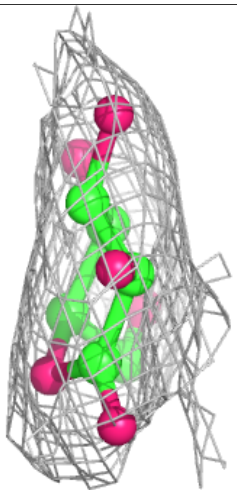
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LGC D 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

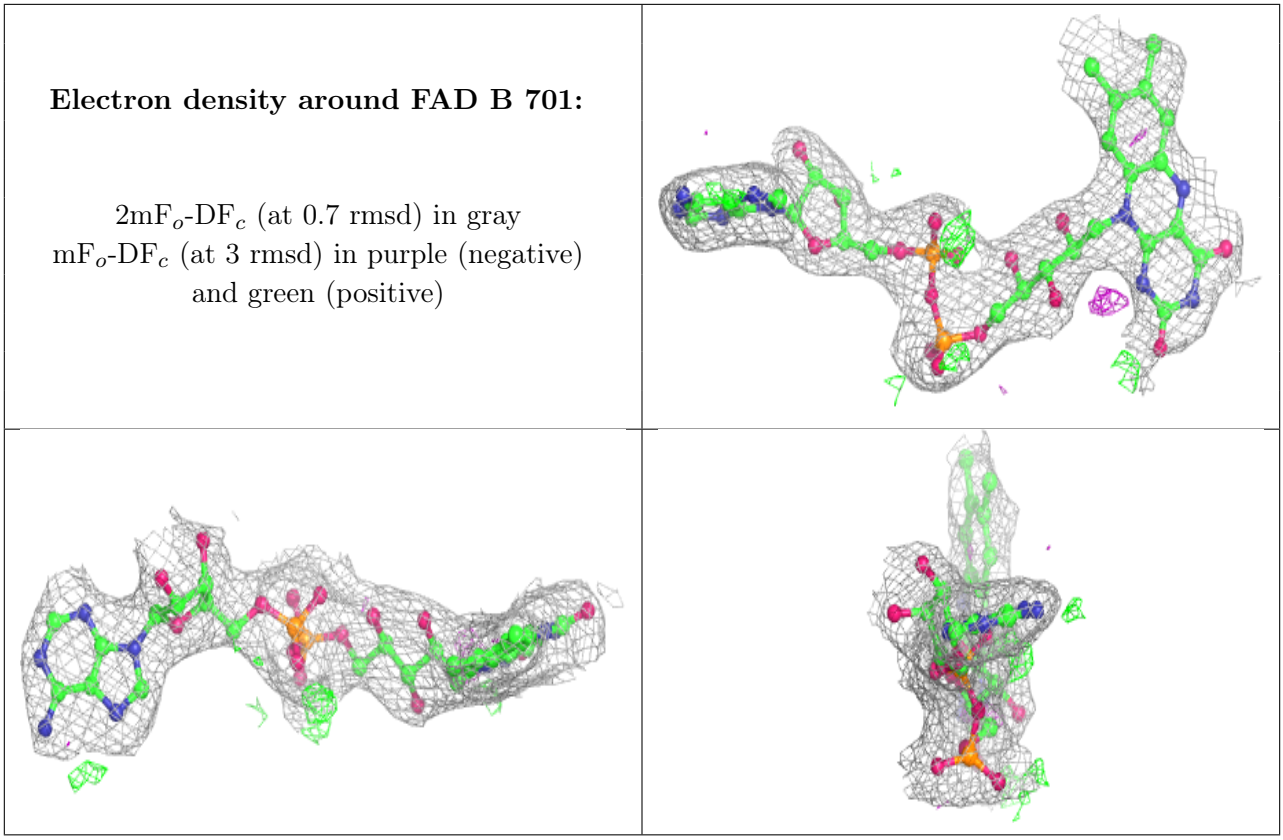






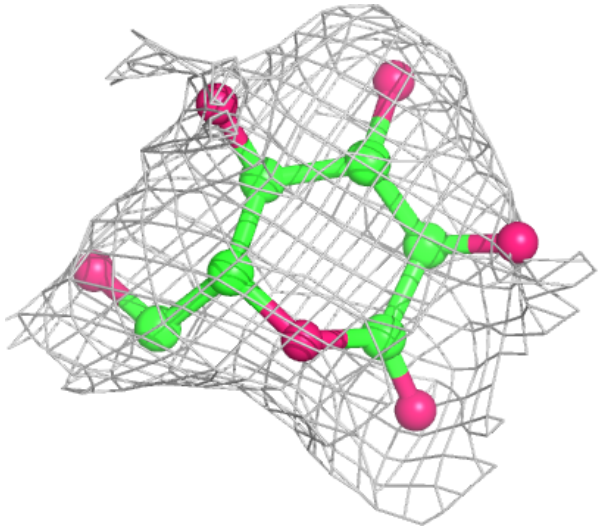
Electron density around FAD B 701:

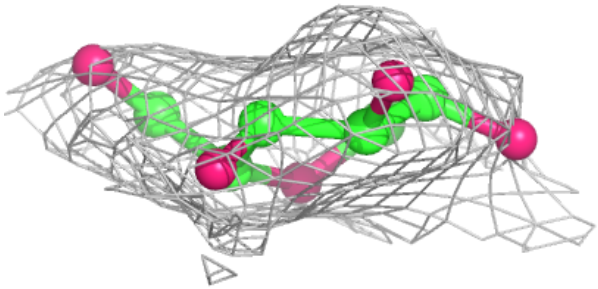
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

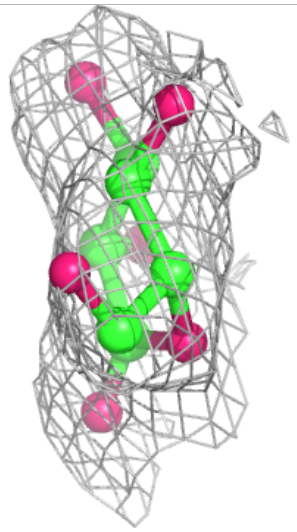


Electron density around LGC B 703:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

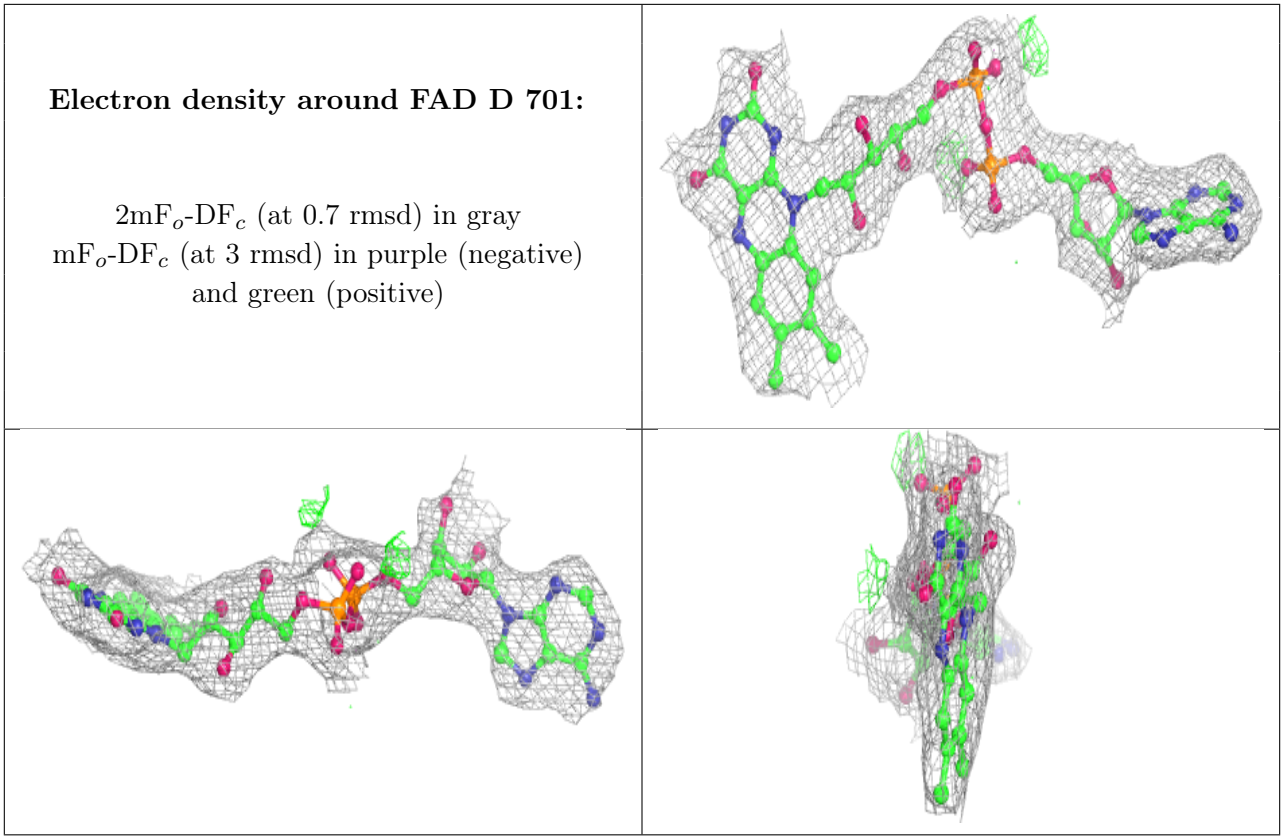






Electron density around FAD D 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.