



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:21 AM UTC

PDB ID : 2IEG / pdb_00002ieg
Title : Crystal structure of rabbit muscle glycogen phosphorylase in complex with 3, 4-dihydro-2-quinolone
Authors : Birch, A.M.; Kenny, P.W.; Oikonomakos, N.G.; Otterbein, L.; Schofield, P.; Whittamore, P.R.O.; Whalley, D.P.; Rowsell, S.; Pauptit, R.; Pannifer, A.; Breed, J.; Minshull, C.
Deposited on : 2006-09-19
Resolution : 1.90 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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

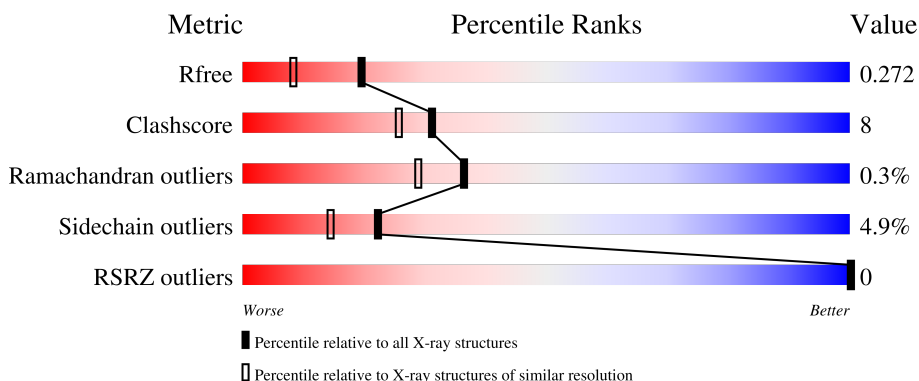
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	842	 80% 13% • 5%
1	B	842	 79% 14% • •

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	PLR	A	903	-	-	X	-
2	PLR	B	904	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13927 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.

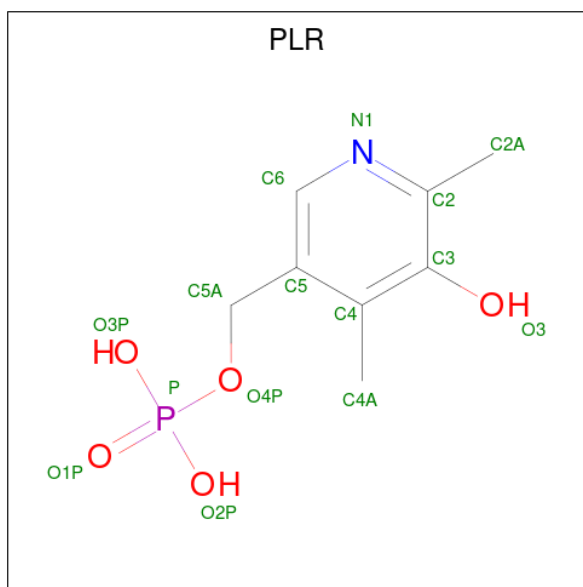
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	803	Total 6538	C 4174	N 1149	O 1186	S 29	0	7	0
1	B	805	Total 6562	C 4185	N 1159	O 1189	S 29	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (CCD ID: PLR) (formula: C₈H₁₂NO₅P).



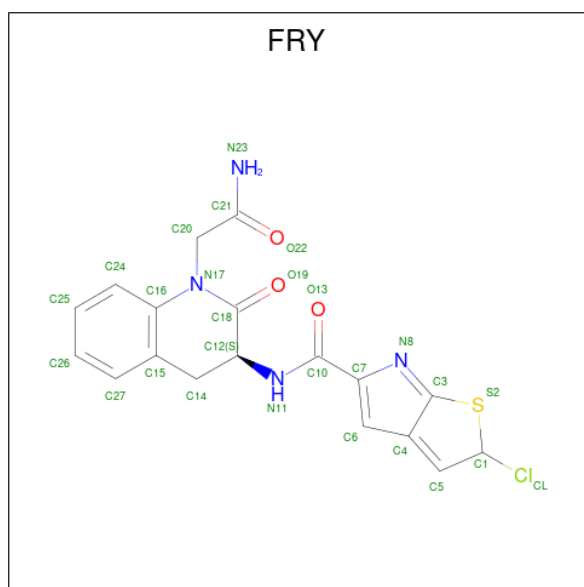
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	15	8	1	5	1	0	0

- Molecule 3 is (2S)-N-[(3S)-1-(2-AMINO-2-OXOETHYL)-2-OXO-1,2,3,4-TETRAHYDRO QUINOLIN-3-YL]-2-CHLORO-2H-THIENO[2,3-B]PYRROLE-5-CARBOXAMIDE (CCD ID: FRY) (formula: C₁₈H₁₅ClN₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	27	18	1	4	3	1	0	0
3	B	1	27	18	1	4	3	1	0	0


- Molecule 4 is water.

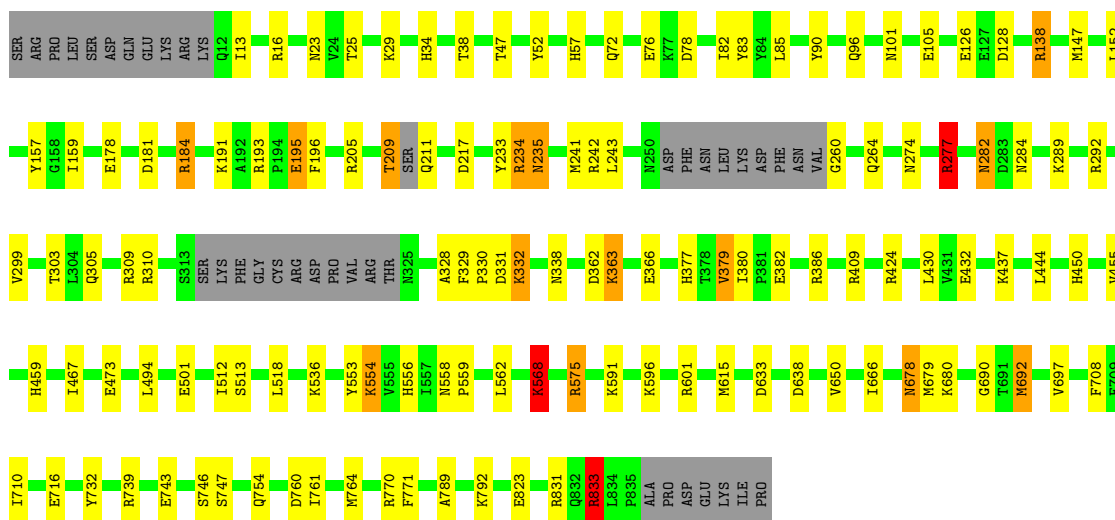
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	403	Total O 403 403	0	0
4	B	340	Total O 340 340	0	0

3 Residue-property plots


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.

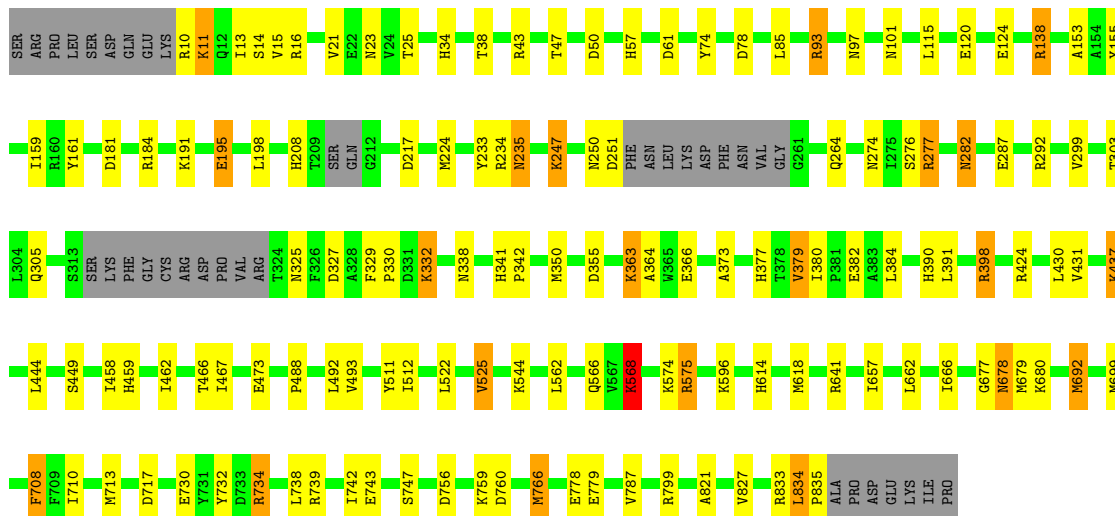
- Molecule 1: Glycogen phosphorylase, muscle form

Chain A: 



- Molecule 1: Glycogen phosphorylase, muscle form

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.12Å 125.16Å 128.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.97 – 1.90 32.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	81.3 (32.97-1.90) 77.2 (32.97-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.1.17	Depositor
R, R_{free}	0.228 , 0.269 0.236 , 0.272	Depositor DCC
R_{free} test set	5893 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.085 for -h,l,k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13927	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: FRY, PLR

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	0.75	0/6719	0.98	4/9092 (0.0%)
1	B	0.69	1/6754 (0.0%)	0.98	0/9139
All	All	0.72	1/13473 (0.0%)	0.98	4/18231 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	657	ILE	CA-C	5.23	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	690	GLY	N-CA-C	6.04	120.59	110.56
1	A	277	ARG	NE-CZ-NH2	5.63	124.26	119.20
1	A	277	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	A	833	ARG	NE-CZ-NH2	5.17	123.85	119.20

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	6538	0	6493	106	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6562	0	6508	109	0
2	A	15	0	10	10	0
2	B	15	0	10	8	0
3	A	27	0	14	7	0
3	B	27	0	14	1	0
4	A	403	0	0	11	1
4	B	340	0	0	12	1
All	All	13927	0	13049	214	1

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 8.

All (214) 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:680:LYS:NZ	2:B:904:PLR:H4A3	1.16	1.43
1:A:680:LYS:NZ	2:A:903:PLR:H4A3	1.22	1.42
1:B:680:LYS:HZ1	2:B:904:PLR:C4A	1.43	1.29
1:A:680:LYS:HZ1	2:A:903:PLR:C4A	1.50	1.19
1:B:10:ARG:HA	1:B:11:LYS:CB	1.86	1.05
1:A:191:LYS:NZ	3:A:901:FRY:H231	1.56	1.03
1:A:191:LYS:NZ	3:A:901:FRY:N23	2.09	1.00
1:A:379:VAL:HG22	1:A:467:ILE:HG13	1.48	0.94
1:A:191:LYS:NZ	3:A:901:FRY:O19	2.01	0.92
1:B:680:LYS:HZ2	2:B:904:PLR:H4A3	1.19	0.91
1:A:680:LYS:HZ2	2:A:903:PLR:H4A3	1.13	0.89
1:A:90:TYR:HE1	4:A:1146:HOH:O	1.55	0.89
1:A:833:ARG:HH21	1:A:833:ARG:HG3	1.37	0.88
1:A:85:LEU:HD21	1:A:303:THR:HG21	1.60	0.83
1:B:766:MET:HE3	1:B:766:MET:HA	1.63	0.81
1:B:10:ARG:CA	1:B:11:LYS:CB	2.58	0.81
1:A:235:ASN:HA	1:A:833:ARG:HG2	1.61	0.79
1:A:101:ASN:HD22	1:A:233:TYR:HA	1.48	0.79
1:B:138:ARG:O	1:B:138:ARG:HD3	1.83	0.78
1:B:779[B]:GLU:OE2	4:B:1178:HOH:O	2.02	0.78
1:A:191:LYS:HZ2	3:A:901:FRY:H231	1.27	0.77
1:A:680:LYS:HZ2	2:A:903:PLR:C4A	1.75	0.76
1:A:181:ASP:OD2	1:B:247:LYS:HE3	1.86	0.76
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.68	0.75
1:A:591:LYS:NZ	1:A:633:ASP:OD2	2.21	0.74
1:A:209:THR:HG1	1:A:211:GLN:N	1.85	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:VAL:CG2	1:A:467:ILE:HG13	2.18	0.71
1:A:680:LYS:HZ1	2:A:903:PLR:H4A3	0.90	0.71
1:A:138:ARG:O	1:A:138:ARG:HD3	1.91	0.70
1:B:743:GLU:O	1:B:747:SER:OG	2.05	0.69
1:A:90:TYR:CE1	4:A:1146:HOH:O	2.35	0.69
1:A:47:THR:HG21	1:B:195:GLU:HG2	1.76	0.68
1:A:78:ASP:OD2	1:A:332:LYS:HE2	1.95	0.67
1:A:536[B]:LYS:HZ2	1:A:536[B]:LYS:HB2	1.60	0.67
1:A:209:THR:OG1	1:A:211:GLN:N	2.27	0.67
1:A:184:ARG:NH2	1:A:184:ARG:HB2	2.10	0.66
1:A:601:ARG:HD2	4:A:996:HOH:O	1.96	0.66
1:B:566:GLN:HG2	1:B:568:LYS:HD3	1.78	0.65
1:A:181:ASP:O	1:A:184:ARG:NH2	2.30	0.65
1:B:235:ASN:H	1:B:235:ASN:HD22	1.44	0.65
1:B:437:LYS:HZ3	1:B:437:LYS:HB3	1.61	0.64
1:A:615:MET:SD	1:A:761[A]:ILE:HD13	2.37	0.64
1:A:363:LYS:HE3	1:A:366:GLU:OE2	1.97	0.63
1:B:101:ASN:HD22	1:B:233:TYR:HA	1.64	0.63
1:A:83:TYR:HE1	1:A:310:ARG:HH21	1.46	0.63
1:A:282:ASN:HD22	1:A:282:ASN:H	1.47	0.63
1:B:355:ASP:OD2	1:B:398:ARG:HD3	1.99	0.62
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.82	0.62
1:A:282:ASN:HD22	1:A:282:ASN:N	1.98	0.62
1:B:680:LYS:HZ1	2:B:904:PLR:H4A3	0.76	0.62
1:B:493:VAL:CG2	1:B:512:ILE:HD12	2.31	0.61
1:B:766:MET:HA	1:B:766:MET:CE	2.29	0.61
1:A:680:LYS:NZ	2:A:903:PLR:H4A2	2.08	0.59
1:B:38:THR:HG21	1:B:57:HIS:CD2	2.37	0.59
1:B:21:VAL:O	1:B:25:THR:HG23	2.01	0.59
1:A:680:LYS:CE	2:A:903:PLR:C4A	2.78	0.59
1:B:834:LEU:HD12	1:B:835:PRO:HD2	1.85	0.59
1:A:235:ASN:H	1:A:235:ASN:HD22	1.51	0.59
1:A:196:PHE:HD2	1:A:242:ARG:HH12	1.49	0.59
1:A:692:MET:HE1	1:A:710:ILE:HD13	1.85	0.58
1:B:47:THR:HG23	1:B:50:ASP:OD2	2.02	0.58
1:A:568:LYS:NZ	2:A:903:PLR:O1P	2.33	0.58
1:A:536[B]:LYS:HB2	1:A:536[B]:LYS:NZ	2.18	0.58
1:B:159:ILE:HG13	1:B:299:VAL:CG2	2.33	0.58
1:B:678:ASN:HD22	1:B:679:MET:H	1.50	0.58
1:A:159:ILE:HG13	1:A:299:VAL:CG2	2.34	0.57
1:B:282:ASN:HD22	1:B:282:ASN:N	2.02	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:CG1	1:B:299:VAL:CG2	2.82	0.57
1:B:511:TYR:CE1	1:B:512:ILE:HD13	2.39	0.57
1:B:363:LYS:CE	1:B:363:LYS:HA	2.35	0.57
1:B:493:VAL:HG21	1:B:512:ILE:HD12	1.87	0.56
1:B:282:ASN:HD22	1:B:282:ASN:H	1.54	0.56
1:B:85[A]:LEU:HD21	1:B:303:THR:HG21	1.88	0.55
1:A:178:GLU:OE2	1:B:251:ASP:OD1	2.25	0.55
1:B:43:ARG:HH22	1:B:115:LEU:HB3	1.71	0.55
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.89	0.55
1:A:96:GLN:CD	1:A:494:LEU:HG	2.32	0.55
1:B:13:ILE:HG12	1:B:16:ARG:CD	2.36	0.55
1:B:13:ILE:HG12	1:B:16:ARG:HD3	1.89	0.55
3:A:901:FRY:N23	3:A:901:FRY:O19	2.32	0.54
1:B:614:HIS:CE1	1:B:618:MET:HG2	2.43	0.54
1:B:208:HIS:CE1	4:B:974:HOH:O	2.60	0.54
1:A:678:ASN:HD22	1:A:678:ASN:N	2.06	0.54
1:A:455:VAL:H	1:A:459:HIS:HD2	1.57	0.53
4:A:1262:HOH:O	1:B:195:GLU:HG3	2.08	0.53
1:A:159:ILE:CG1	1:A:299:VAL:CG2	2.86	0.53
1:B:424:ARG:NH2	1:B:473:GLU:OE1	2.41	0.53
1:B:34:HIS:CE1	1:B:61:ASP:OD2	2.63	0.52
1:B:678:ASN:ND2	1:B:679:MET:H	2.07	0.52
1:B:363:LYS:HE2	1:B:366:GLU:HB3	1.92	0.52
1:B:373:ALA:HA	1:B:449:SER:HB3	1.92	0.52
1:A:680:LYS:HZ1	2:A:903:PLR:H4A1	1.62	0.51
1:B:568:LYS:NZ	2:B:904:PLR:O1P	2.44	0.51
1:A:386[B]:ARG:HD2	1:A:432:GLU:OE1	2.10	0.51
1:B:680:LYS:HZ2	2:B:904:PLR:C4A	1.90	0.51
1:A:833:ARG:HG3	1:A:833:ARG:NH2	2.13	0.50
1:B:341:HIS:N	1:B:342:PRO:CD	2.74	0.50
1:B:93:ARG:HD3	4:B:948:HOH:O	2.11	0.50
1:B:120:GLU:HG3	4:B:1158:HOH:O	2.12	0.50
1:B:562:LEU:C	1:B:562:LEU:HD23	2.37	0.50
1:B:680:LYS:CE	2:B:904:PLR:C4A	2.88	0.50
1:A:191:LYS:HD2	1:A:193:ARG:HD3	1.92	0.50
1:A:241:MET:HE3	1:A:243:LEU:HD11	1.94	0.49
1:B:459:HIS:O	1:B:462:ILE:HG22	2.12	0.49
1:B:85[B]:LEU:HD11	1:B:303:THR:HG21	1.93	0.49
1:B:159:ILE:HG13	1:B:299:VAL:HG21	1.94	0.49
1:B:522:LEU:O	1:B:525:VAL:HG22	2.13	0.49
1:A:362:ASP:OD1	1:A:409:ARG:NH1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:ARG:CZ	4:B:1171:HOH:O	2.61	0.49
1:B:338:ASN:OD1	1:B:377:HIS:NE2	2.46	0.48
1:A:178:GLU:CD	1:B:250:ASN:O	2.56	0.48
1:A:260:GLY:HA2	1:A:264:GLN:HG3	1.93	0.48
1:A:184:ARG:HB2	1:A:184:ARG:HH21	1.77	0.48
1:B:574:LYS:NZ	2:B:904:PLR:O2P	2.46	0.48
1:B:575:ARG:HD2	1:B:666:ILE:O	2.14	0.48
1:A:205:ARG:NH2	1:A:217:ASP:OD2	2.45	0.48
1:B:759:LYS:HG3	1:B:760:ASP:N	2.28	0.48
1:A:235:ASN:HA	1:A:833:ARG:CG	2.38	0.48
1:A:328:ALA:O	1:A:331:ASP:HB2	2.14	0.48
1:A:138:ARG:HD3	1:A:138:ARG:C	2.38	0.48
1:A:430:LEU:HD22	1:A:444:LEU:N	2.29	0.48
1:B:97:ASN:ND2	4:B:1015:HOH:O	2.47	0.48
1:B:430:LEU:CD2	1:B:444:LEU:N	2.77	0.47
1:B:466:THR:HG22	1:B:467:ILE:HD13	1.96	0.47
1:A:363:LYS:CE	1:A:366:GLU:OE2	2.62	0.47
1:A:274:ASN:HA	1:A:277:ARG:HD2	1.97	0.47
1:A:52:TYR:OH	1:A:126:GLU:HG3	2.14	0.47
1:B:124:GLU:OE1	4:B:1059:HOH:O	2.20	0.47
1:B:431:VAL:CG1	1:B:437:LYS:HE2	2.45	0.47
1:B:678:ASN:HD22	1:B:678:ASN:N	2.12	0.47
1:B:155:TYR:N	1:B:155:TYR:CD1	2.83	0.47
1:B:350:MET:HE1	1:B:364:ALA:HB3	1.96	0.46
1:B:379:VAL:HG22	1:B:467:ILE:HG13	1.98	0.46
1:B:738:LEU:O	1:B:742:ILE:HG12	2.15	0.46
1:A:823:GLU:OE1	4:A:1160:HOH:O	2.21	0.46
1:A:13:ILE:HD12	1:A:501:GLU:HB2	1.98	0.45
1:B:363:LYS:HA	1:B:363:LYS:HE3	1.98	0.45
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.98	0.45
1:B:821:ALA:HB1	1:B:827:VAL:HG23	1.99	0.45
1:B:181:ASP:OD2	1:B:184:ARG:HG3	2.16	0.45
1:B:730:GLU:O	1:B:734:ARG:HD2	2.16	0.45
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.99	0.45
1:A:678:ASN:HD22	1:A:679:MET:H	1.65	0.45
1:A:29:LYS:HD2	4:A:1170:HOH:O	2.17	0.45
1:A:29:LYS:HD3	1:A:29:LYS:C	2.42	0.45
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.49	0.45
1:B:641:ARG:HG3	4:B:1020:HOH:O	2.16	0.45
1:A:13:ILE:CG1	1:A:16:ARG:HG3	2.47	0.45
1:B:437:LYS:HB3	1:B:437:LYS:NZ	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:TYR:CZ	1:B:739:ARG:HG3	2.52	0.45
1:A:562:LEU:C	1:A:562:LEU:HD23	2.41	0.44
1:B:363:LYS:HE2	1:B:363:LYS:O	2.17	0.44
1:A:424:ARG:NH2	1:A:473:GLU:OE1	2.33	0.44
1:B:78:ASP:OD2	1:B:332[A]:LYS:HE2	2.16	0.44
1:B:677:GLY:HA2	1:B:680:LYS:HD2	1.98	0.44
1:A:282:ASN:HB2	4:A:1068:HOH:O	2.17	0.44
1:B:282:ASN:OD1	1:B:287:GLU:HB2	2.17	0.43
1:A:72:GLN:HG3	1:A:76:GLU:OE1	2.18	0.43
1:A:147:MET:HG2	1:A:152:LEU:HD12	2.00	0.43
1:A:513:SER:OG	1:A:831:ARG:NH1	2.51	0.43
1:B:247:LYS:NZ	4:B:1088:HOH:O	2.52	0.43
1:A:789:ALA:HA	1:A:792:LYS:HD3	2.00	0.43
1:B:363:LYS:NZ	1:B:366:GLU:CD	2.76	0.43
1:B:488:PRO:O	1:B:492:LEU:HB3	2.19	0.43
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.53	0.43
1:B:224:MET:CE	1:B:247:LYS:HG3	2.49	0.43
1:A:159:ILE:HG13	1:A:299:VAL:HG21	2.00	0.43
1:A:558:ASN:OD1	1:A:559:PRO:HD2	2.18	0.43
1:B:390:HIS:ND1	1:B:391:LEU:N	2.67	0.43
1:A:34:HIS:O	1:A:38:THR:HB	2.19	0.43
1:B:430:LEU:HD22	1:B:444:LEU:N	2.34	0.43
1:B:568:LYS:HE3	4:B:1081:HOH:O	2.19	0.43
1:A:233:TYR:CE1	1:A:234:ARG:HD3	2.54	0.42
1:B:235:ASN:HD22	1:B:235:ASN:N	2.09	0.42
1:A:575:ARG:HD3	1:A:666:ILE:O	2.19	0.42
1:A:760:ASP:HB2	4:A:1271:HOH:O	2.19	0.42
1:A:380[A]:ILE:HG23	1:A:382:GLU:CD	2.44	0.42
1:A:680:LYS:CE	2:A:903:PLR:H4A2	2.47	0.42
1:B:692:MET:HE1	1:B:710:ILE:HD13	2.01	0.42
1:A:329:PHE:HB3	1:A:330:PRO:HD3	2.00	0.42
1:A:764:MET:SD	1:A:764:MET:C	3.02	0.42
1:B:274:ASN:HA	1:B:277:ARG:HD2	2.00	0.42
1:B:34:HIS:HD2	1:B:38:THR:OG1	2.03	0.42
1:B:325:ASN:OD1	1:B:327:ASP:HB2	2.19	0.42
1:B:329:PHE:N	1:B:330:PRO:CD	2.83	0.42
3:A:901:FRY:H231	3:A:901:FRY:C18	2.31	0.41
1:A:770[A]:ARG:HB3	1:A:771:PHE:CD2	2.55	0.41
1:B:380:ILE:HG22	1:B:382:GLU:CD	2.45	0.41
1:A:16:ARG:HB3	1:A:105:GLU:HB3	2.01	0.41
1:A:13:ILE:HG12	1:A:16:ARG:HG3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD12	1:A:82:ILE:N	2.34	0.41
1:A:380[B]:ILE:CG2	1:A:382:GLU:CD	2.93	0.41
1:A:553:TYR:O	1:A:554:LYS:HB2	2.20	0.41
1:B:74:TYR:CE2	1:B:153:ALA:HA	2.56	0.41
1:A:450:HIS:HE1	4:A:949:HOH:O	2.04	0.41
1:B:181:ASP:CG	1:B:184:ARG:HG3	2.46	0.41
1:A:234:ARG:NH2	4:A:1070:HOH:O	2.54	0.41
1:B:161:TYR:HA	1:B:276:SER:O	2.21	0.41
1:B:458:ILE:HG22	4:B:1030:HOH:O	2.19	0.41
1:A:90:TYR:CE1	1:A:650:VAL:HG23	2.56	0.41
1:A:380[A]:ILE:CG2	1:A:382:GLU:CD	2.93	0.41
1:B:699:MET:HE2	1:B:708:PHE:HZ	1.84	0.41
1:A:241:MET:HE3	1:A:243:LEU:CD1	2.51	0.41
1:A:743:GLU:O	1:A:747:SER:HB3	2.21	0.41
1:A:195:GLU:H	1:A:195:GLU:HG3	1.61	0.41
3:A:901:FRY:H24	3:A:901:FRY:H201	1.88	0.41
1:B:568:LYS:CE	4:B:1081:HOH:O	2.69	0.41
1:A:16:ARG:HA	4:A:1032:HOH:O	2.20	0.40
1:B:191:LYS:CE	3:B:902:FRY:O19	2.68	0.40
1:B:198:LEU:HD13	1:B:305:GLN:HB3	2.04	0.40
1:A:34:HIS:CE1	1:A:57:HIS:HB3	2.57	0.40
1:A:157:TYR:CD1	1:A:303:THR:HG23	2.56	0.40
1:A:732:TYR:CZ	1:A:739:ARG:HG3	2.56	0.40

All (1) 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)
4:A:1302:HOH:O	4:B:1135:HOH:O[1_455]	1.77	0.43

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	802/842 (95%)	773 (96%)	27 (3%)	2 (0%)	43	36
1	B	806/842 (96%)	777 (96%)	27 (3%)	2 (0%)	43	36
All	All	1608/1684 (96%)	1550 (96%)	54 (3%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	LYS
1	A	284	ASN
1	B	568	LYS
1	A	568	LYS

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	697/731 (95%)	663 (95%)	34 (5%)	22	14
1	B	699/731 (96%)	664 (95%)	35 (5%)	22	14
All	All	1396/1462 (96%)	1327 (95%)	69 (5%)	22	14

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	25	THR
1	A	128	ASP
1	A	138	ARG
1	A	184	ARG
1	A	195	GLU
1	A	209	THR
1	A	234	ARG
1	A	235	ASN
1	A	277	ARG
1	A	282	ASN
1	A	289	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	292	ARG
1	A	305	GLN
1	A	309	ARG
1	A	332	LYS
1	A	363	LYS
1	A	379	VAL
1	A	437	LYS
1	A	512	ILE
1	A	518	LEU
1	A	554	LYS
1	A	556	HIS
1	A	568	LYS
1	A	575	ARG
1	A	596	LYS
1	A	638	ASP
1	A	678	ASN
1	A	692	MET
1	A	708	PHE
1	A	716	GLU
1	A	746	SER
1	A	754	GLN
1	A	833	ARG
1	B	14	SER
1	B	15	VAL
1	B	23	ASN
1	B	93	ARG
1	B	138	ARG
1	B	195	GLU
1	B	217	ASP
1	B	234	ARG
1	B	235	ASN
1	B	247	LYS
1	B	264	GLN
1	B	277	ARG
1	B	282	ASN
1	B	292	ARG
1	B	332[A]	LYS
1	B	332[B]	LYS
1	B	363	LYS
1	B	379	VAL
1	B	384	LEU
1	B	398	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	437	LYS
1	B	525	VAL
1	B	544	LYS
1	B	568	LYS
1	B	575	ARG
1	B	596	LYS
1	B	678	ASN
1	B	692	MET
1	B	708	PHE
1	B	734	ARG
1	B	756	ASP
1	B	766	MET
1	B	778	GLU
1	B	833	ARG
1	B	834	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	101	ASN
1	A	211	GLN
1	A	219	GLN
1	A	235	ASN
1	A	282	ASN
1	A	376	ASN
1	A	412	ASN
1	A	477	HIS
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	614	HIS
1	A	678	ASN
1	A	767	HIS
1	B	34	HIS
1	B	72	GLN
1	B	101	ASN
1	B	219	GLN
1	B	235	ASN
1	B	282	ASN
1	B	412	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	481	ASN
1	B	484	ASN
1	B	566	GLN
1	B	579	ASN
1	B	614	HIS
1	B	678	ASN
1	B	740	GLN
1	B	767	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FRY	B	902	-	28,30,30	2.64	2 (7%)	30,44,44	2.04	8 (26%)
3	FRY	A	901	-	28,30,30	2.50	3 (10%)	30,44,44	2.32	10 (33%)
2	PLR	A	903	1	15,15,15	1.18	1 (6%)	21,22,22	1.38	3 (14%)
2	PLR	B	904	1	15,15,15	1.30	2 (13%)	21,22,22	1.34	3 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRY	B	902	-	-	5/12/48/48	0/4/4/4
3	FRY	A	901	-	-	6/12/48/48	0/4/4/4
2	PLR	A	903	1	-	0/6/6/6	0/1/1/1
2	PLR	B	904	1	-	2/6/6/6	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	FRY	O19-C18	13.01	1.45	1.22
3	A	901	FRY	O19-C18	11.87	1.43	1.22
3	B	902	FRY	C5-C4	3.30	1.47	1.34
3	A	901	FRY	C5-C4	3.10	1.46	1.34
2	A	903	PLR	C2-N1	2.76	1.38	1.33
2	B	904	PLR	C3-C2	-2.62	1.38	1.41
2	B	904	PLR	C2-N1	2.60	1.38	1.33
3	A	901	FRY	C14-C12	-2.43	1.49	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	FRY	C7-C10-N11	5.90	123.60	115.22
3	B	902	FRY	O19-C18-N17	-5.40	117.14	122.66
3	A	901	FRY	C20-N17-C18	5.37	124.23	118.31
3	A	901	FRY	C15-C14-C12	-4.70	105.26	111.17
3	A	901	FRY	C7-C10-N11	4.53	121.66	115.22
3	A	901	FRY	C7-N8-C3	-4.15	102.96	110.10
3	B	902	FRY	C20-N17-C18	3.89	122.59	118.31
3	A	901	FRY	O19-C18-N17	-3.75	118.83	122.66
3	B	902	FRY	C15-C14-C12	-3.34	106.97	111.17
3	A	901	FRY	C18-C12-N11	-3.31	104.09	110.15
3	A	901	FRY	C6-C7-C10	3.20	129.24	123.92
2	B	904	PLR	C5-C6-N1	-2.92	119.08	123.83
3	A	901	FRY	C5-C4-C3	2.76	113.27	107.66
2	A	903	PLR	C5-C6-N1	-2.76	119.34	123.83
2	A	903	PLR	C4A-C4-C3	-2.71	116.01	120.52
3	B	902	FRY	C7-N8-C3	-2.68	105.49	110.10
2	A	903	PLR	C3-C4-C5	2.44	121.51	118.59
3	B	902	FRY	C5-C4-C3	2.43	112.60	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	904	PLR	C3-C4-C5	2.41	121.48	118.59
3	B	902	FRY	C6-C7-C10	2.24	127.65	123.92
3	A	901	FRY	O13-C10-C7	-2.21	115.61	121.15
3	A	901	FRY	O22-C21-C20	-2.05	117.16	120.77
2	B	904	PLR	C4A-C4-C3	-2.03	117.14	120.52
3	B	902	FRY	O13-C10-N11	-2.00	119.56	123.09

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	FRY	N11-C10-C7-C6
3	A	901	FRY	C21-C20-N17-C16
3	B	902	FRY	N11-C10-C7-C6
3	B	902	FRY	C21-C20-N17-C16
3	A	901	FRY	N11-C10-C7-N8
3	B	902	FRY	N11-C10-C7-N8
3	A	901	FRY	O13-C10-C7-C6
3	B	902	FRY	O13-C10-C7-C6
3	A	901	FRY	N17-C20-C21-N23
3	A	901	FRY	O13-C10-C7-N8
3	B	902	FRY	O13-C10-C7-N8
2	B	904	PLR	C4-C5-C5A-O4P
2	B	904	PLR	C6-C5-C5A-O4P

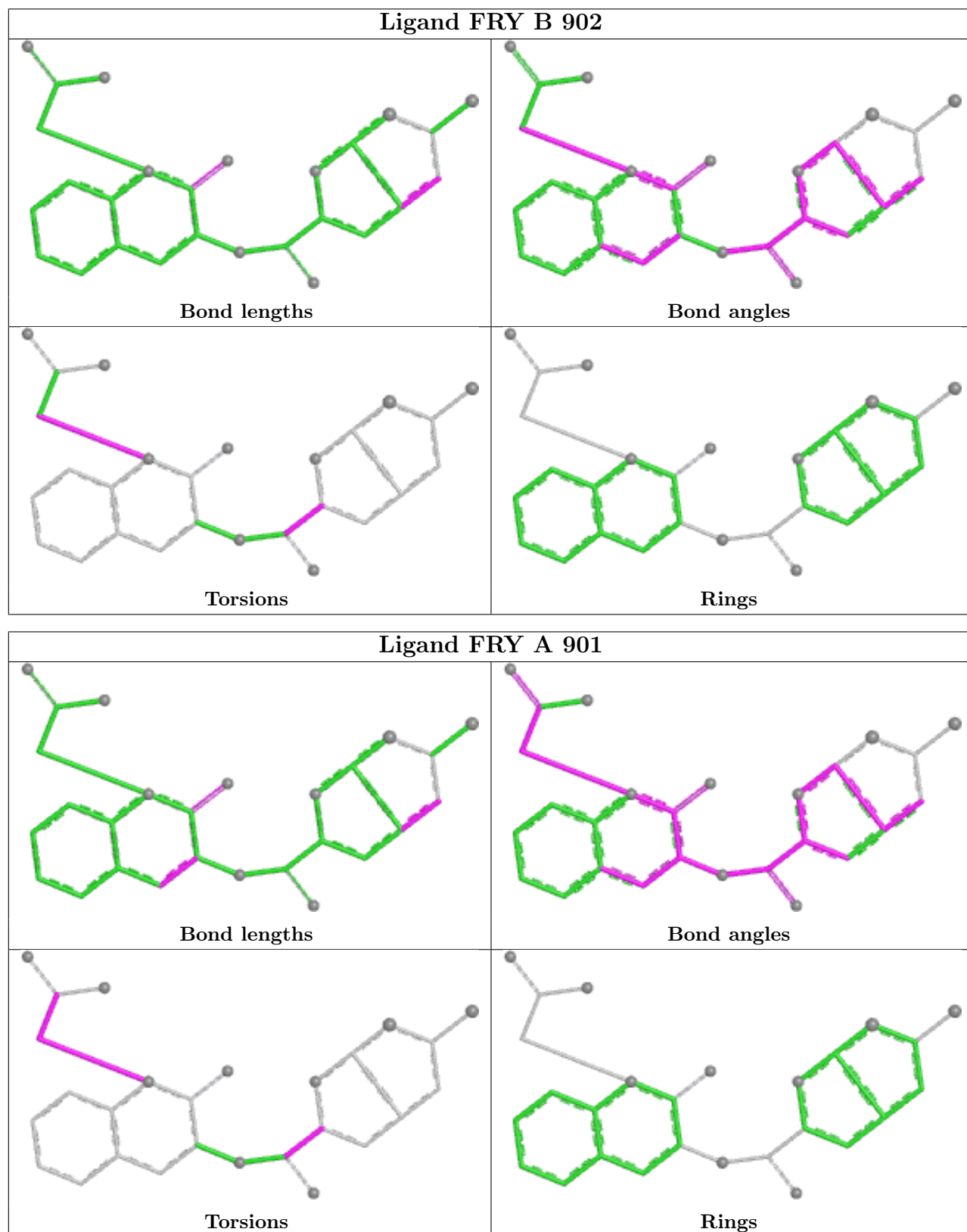
There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	FRY	1	0
3	A	901	FRY	7	0
2	A	903	PLR	10	0
2	B	904	PLR	8	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 than 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.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	803/842 (95%)	-1.03	0 100 100	21, 35, 47, 55	7 (0%)
1	B	805/842 (95%)	-0.96	0 100 100	24, 39, 51, 58	9 (1%)
All	All	1608/1684 (95%)	-1.00	0 100 100	21, 37, 49, 58	16 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

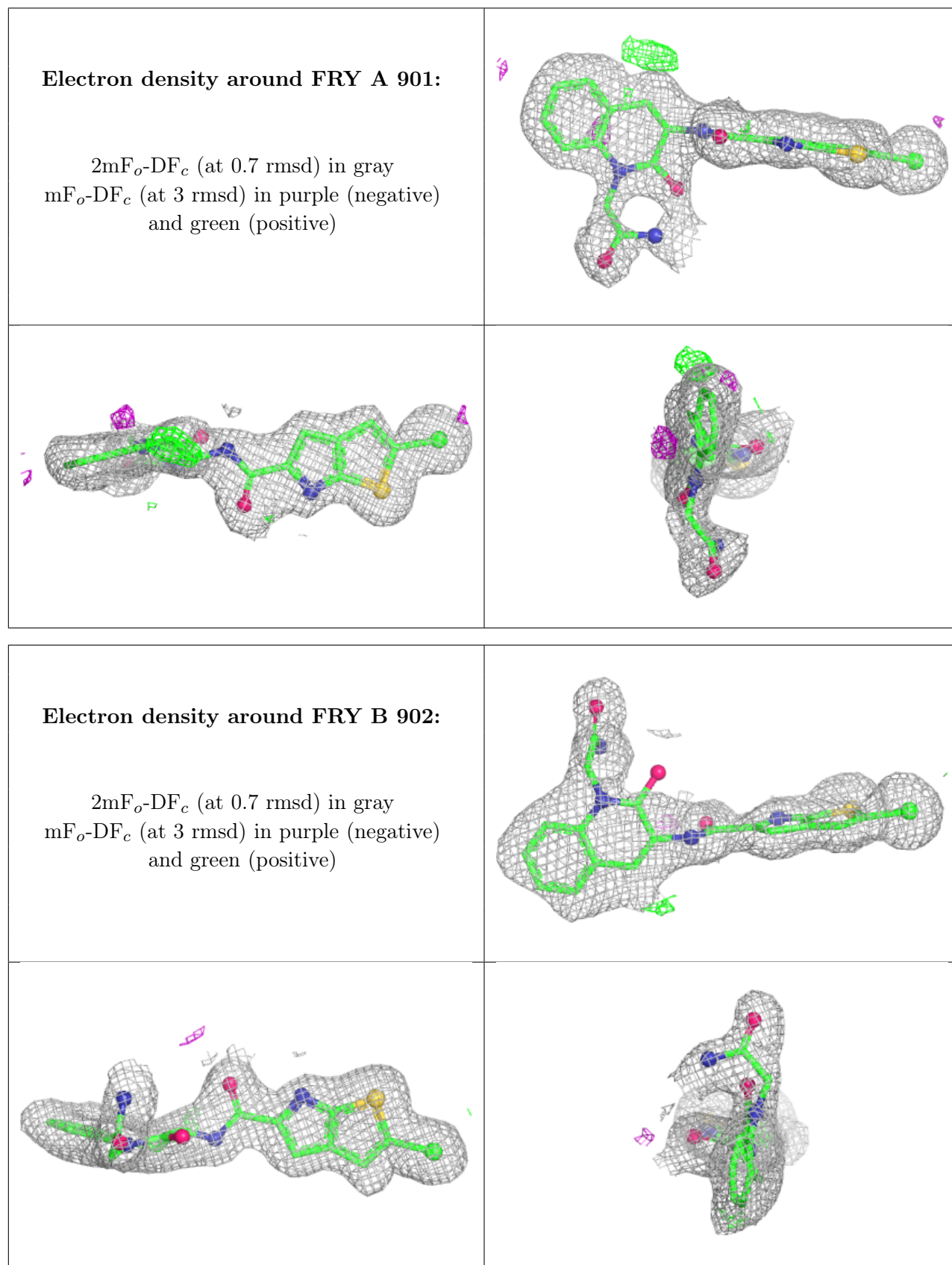
6.4 Ligands [i](#)

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, 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	B-factors(Å ²)	Q<0.9
2	PLR	A	903	15/15	0.99	0.03	26,30,31,32	0
2	PLR	B	904	15/15	0.99	0.03	26,28,31,34	0
3	FRY	A	901	27/27	0.99	0.04	28,34,45,47	0
3	FRY	B	902	27/27	0.99	0.04	33,42,50,52	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.