



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:31 PM UTC

PDB ID : 2IEI / pdb_00002iei
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 : 1.91 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)
Xtriage (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

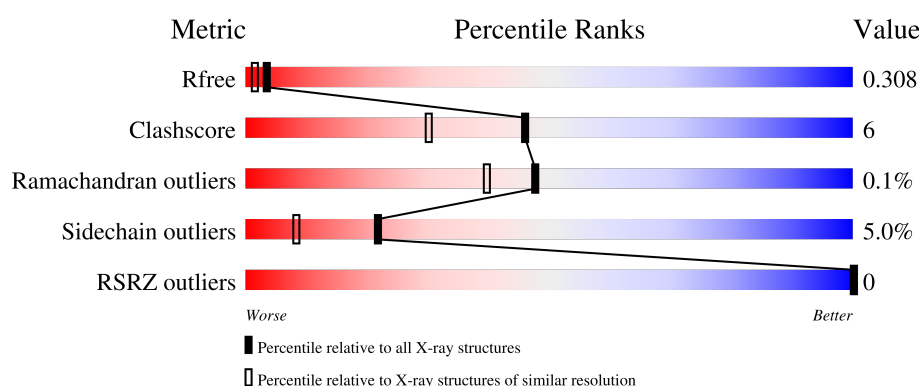
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. 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	
1	B	842	

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	B	902	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13536 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.

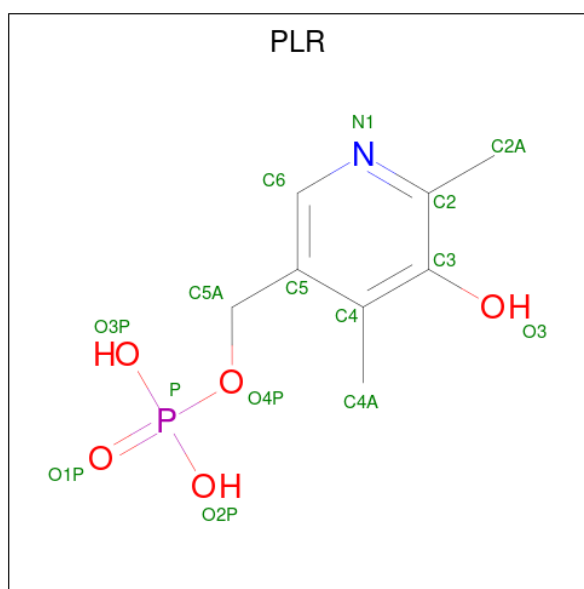
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	794	Total	C	N	O	S	0	0	0
			6416	4102	1124	1161	29			
1	B	796	Total	C	N	O	S	0	0	0
			6413	4094	1119	1171	29			

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).



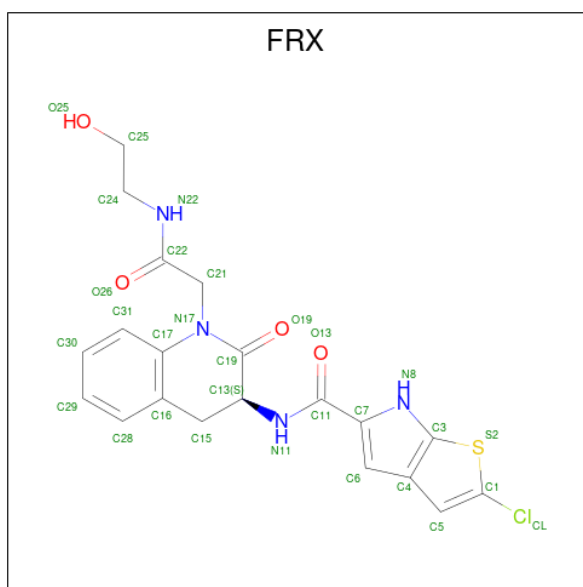
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- Molecule 3 is (S)-2-CHLORO-N-(1-(2-(2-HYDROXYETHYLAMINO)-2-OXOETHYL)-2-OXO-1,2,3,4-TETRAHYDROQUINOLIN-3-YL)-6H-THIENO[2,3-B]PYRROLE-5-CARBOXAMIDE (CCD ID: FRX) (formula: C₂₀H₁₉ClN₄O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			30	20	1	4	4	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			30	20	1	4	4	1		

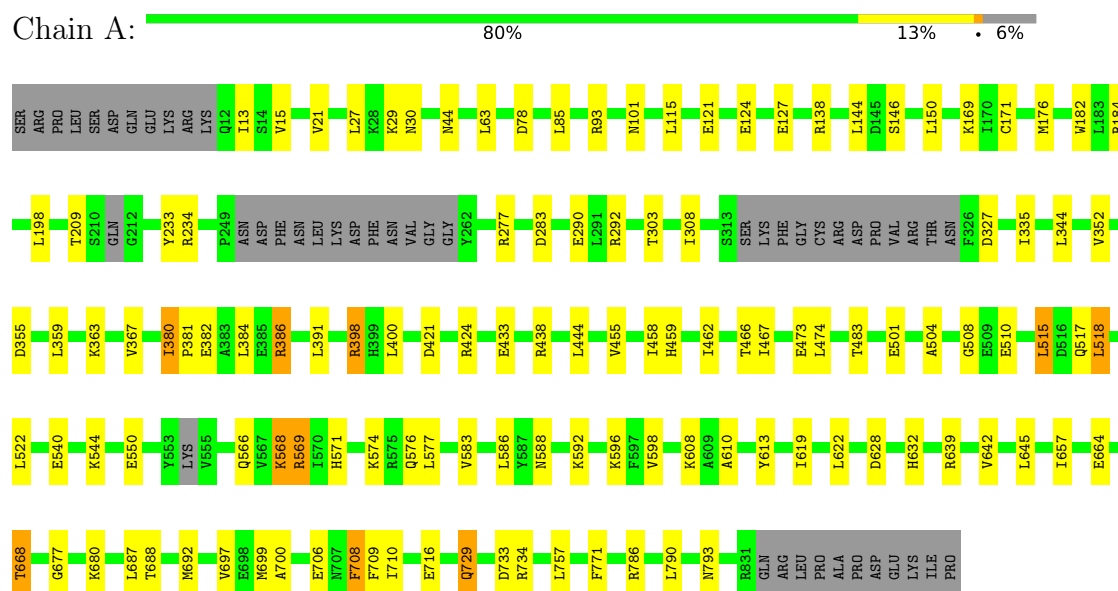
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	357	Total	O	0	0
			357	357		
4	B	260	Total	O	0	0
			260	260		

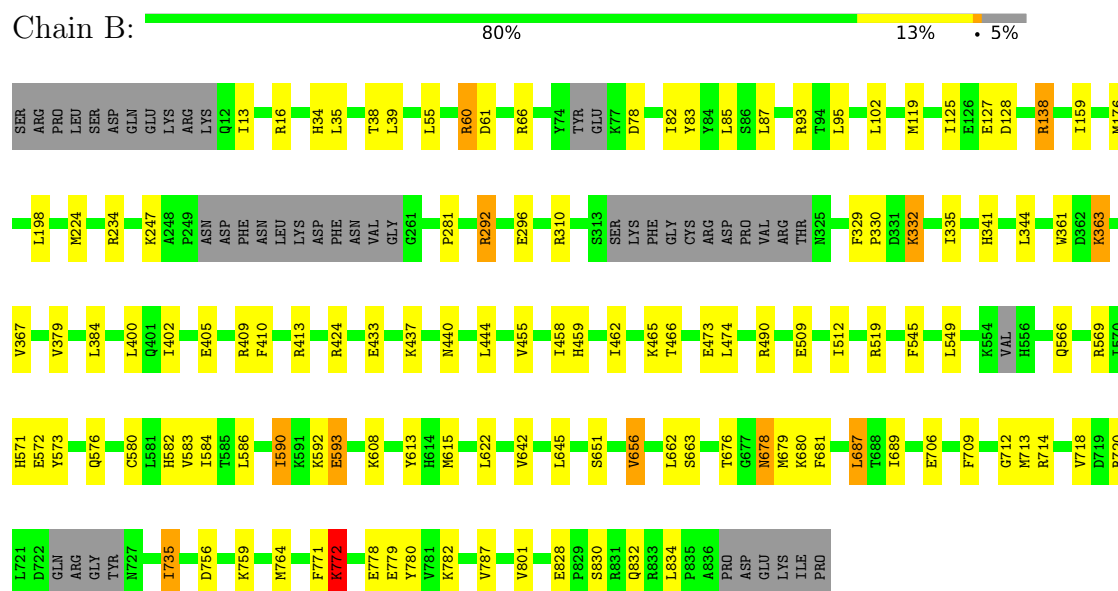
3 Residue-property plots

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



- Molecule 1: Glycogen phosphorylase, muscle form



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.40Å 125.34Å 129.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 1.91 33.00 – 1.91	Depositor EDS
% Data completeness (in resolution range)	80.5 (33.00-1.91) 75.0 (33.00-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.255 , 0.297 0.268 , 0.308	Depositor DCC
R_{free} test set	5805 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.197 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13536	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLR, FRX

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	0.53	1/6559 (0.0%)	0.85	1/8880 (0.0%)
1	B	0.51	0/6553	0.84	2/8873 (0.0%)
All	All	0.52	1/13112 (0.0%)	0.85	3/17753 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	657	ILE	CA-CB	5.25	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	ILE	CA-C-N	6.02	125.90	119.28
1	B	735	ILE	C-N-CA	6.02	125.90	119.28
1	A	757	LEU	N-CA-C	5.30	117.47	111.11

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	6416	0	6339	71	0
1	B	6413	0	6319	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	10	5	0
2	B	15	0	10	6	0
3	A	30	0	19	1	0
3	B	30	0	19	1	0
4	A	357	0	0	8	0
4	B	260	0	0	4	0
All	All	13536	0	12716	146	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 6.

All (146) 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:902:PLR:H4A1	1.03	1.35
1:A:680:LYS:NZ	2:A:901:PLR:H4A3	1.50	1.26
1:B:680:LYS:HZ1	2:B:902:PLR:C4A	1.55	1.16
1:A:680:LYS:HZ1	2:A:901:PLR:C4A	1.73	1.02
1:A:680:LYS:HZ1	2:A:901:PLR:H4A3	0.78	0.91
1:A:138:ARG:O	1:A:138:ARG:HD3	1.71	0.91
1:B:680:LYS:HZ2	2:B:902:PLR:C4A	1.72	0.84
1:A:571:HIS:HB2	1:A:574:LYS:HG2	1.60	0.84
1:B:680:LYS:HZ1	2:B:902:PLR:H4A1	0.94	0.75
1:A:93:ARG:HH21	1:A:124:GLU:HA	1.51	0.75
1:B:87:LEU:HD11	1:B:296:GLU:HG2	1.69	0.74
4:A:1193:HOH:O	1:B:60:ARG:HD3	1.88	0.73
1:B:55:LEU:HD23	1:B:95:LEU:HD21	1.71	0.72
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.71	0.71
1:B:680:LYS:HZ2	2:B:902:PLR:H4A1	0.88	0.70
1:A:569:ARG:NH1	1:A:608:LYS:O	2.25	0.69
1:B:778:GLU:O	1:B:782:LYS:HE2	1.93	0.68
1:B:13:ILE:HG13	1:B:16:ARG:HG3	1.74	0.67
1:B:224:MET:HE2	1:B:247:LYS:HD2	1.75	0.67
1:A:515:LEU:HD22	1:A:518:LEU:HD22	1.77	0.67
3:A:904:FRX:H151	3:B:903:FRX:O26	1.95	0.67
1:A:455:VAL:H	1:A:459:HIS:HD2	1.43	0.66
1:B:680:LYS:HZ1	2:B:902:PLR:H4A2	1.59	0.66
1:B:509:GLU:O	1:B:512:ILE:HG12	1.97	0.65
1:B:713:MET:HE1	1:B:772:LYS:HG3	1.80	0.64
1:A:184:ARG:HD3	1:B:247:LYS:HZ1	1.63	0.63
1:B:281:PRO:O	1:B:569:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.02	0.60
1:A:540:GLU:O	1:A:544:LYS:HG2	2.00	0.60
1:B:592:LYS:HG3	1:B:593:GLU:HG2	1.84	0.60
1:A:588:ASN:O	1:A:592:LYS:HG2	2.02	0.59
1:A:709:PHE:HE1	1:A:786:ARG:HG3	1.67	0.59
1:B:545:PHE:CE1	1:B:656:VAL:HG22	2.38	0.58
1:B:138:ARG:O	1:B:138:ARG:HD3	2.03	0.58
1:A:610:ALA:HB3	1:A:613:TYR:HB2	1.85	0.58
1:B:361:TRP:CH2	1:B:402:ILE:HG23	2.40	0.57
1:B:586:LEU:O	1:B:590:ILE:HG23	2.03	0.57
1:B:85:LEU:HD13	1:B:335:ILE:HG23	1.86	0.57
1:A:13:ILE:HG22	1:A:15:VAL:HG12	1.87	0.56
1:A:568:LYS:CE	4:A:993:HOH:O	2.52	0.56
1:A:184:ARG:HD3	1:B:247:LYS:NZ	2.20	0.55
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.88	0.55
1:A:568:LYS:HE2	4:A:993:HOH:O	2.07	0.55
1:B:361:TRP:HH2	1:B:402:ILE:HG23	1.70	0.55
1:B:410:PHE:O	1:B:413:ARG:HB3	2.07	0.55
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.90	0.54
1:A:734:ARG:HG2	4:A:1175:HOH:O	2.07	0.54
1:B:582:HIS:HB2	1:B:780:TYR:CE2	2.43	0.54
1:A:793:ASN:HD22	1:A:793:ASN:C	2.16	0.54
1:B:87:LEU:HD12	1:B:341:HIS:HB3	1.90	0.53
1:B:138:ARG:HB3	4:B:971:HOH:O	2.08	0.53
1:A:699:MET:HE2	1:A:708:PHE:HZ	1.74	0.53
1:B:83:TYR:HE1	1:B:310:ARG:HH21	1.57	0.53
1:B:572:GLU:OE2	1:B:764:MET:HE3	2.09	0.53
1:A:93:ARG:NH2	1:A:124:GLU:HA	2.20	0.52
1:B:778:GLU:H	1:B:778:GLU:CD	2.17	0.52
1:A:598:VAL:HG22	1:A:639:ARG:HD2	1.92	0.51
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.92	0.51
1:A:93:ARG:NH2	1:A:124:GLU:OE2	2.42	0.51
1:A:571:HIS:HB2	1:A:574:LYS:CG	2.38	0.51
1:B:678:ASN:HD22	1:B:678:ASN:N	2.07	0.51
1:A:455:VAL:O	1:A:483:THR:HA	2.10	0.51
1:A:569:ARG:NH1	4:A:1070:HOH:O	2.44	0.50
1:B:55:LEU:CD2	1:B:95:LEU:HD21	2.41	0.50
1:B:424:ARG:NH2	1:B:473:GLU:OE1	2.45	0.50
1:A:458:ILE:O	1:A:462:ILE:HG13	2.12	0.49
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.93	0.49
1:A:424:ARG:NH2	1:A:473:GLU:OE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HD13	1:A:352:VAL:HG11	1.93	0.49
1:A:327:ASP:OD1	1:A:363:LYS:HE2	2.12	0.49
1:B:519:ARG:NH1	4:B:1010:HOH:O	2.44	0.49
1:A:127:GLU:HG2	1:A:182:TRP:HA	1.94	0.49
1:B:462:ILE:HA	1:B:465:LYS:HG2	1.95	0.49
1:A:680:LYS:CE	2:A:901:PLR:H4A3	2.38	0.49
1:B:756:ASP:HB3	1:B:759:LYS:HD2	1.94	0.49
1:B:363:LYS:O	1:B:367:VAL:HG23	2.12	0.49
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.78	0.49
1:B:678:ASN:HD22	1:B:679:MET:H	1.61	0.49
1:A:568:LYS:HE2	4:A:915:HOH:O	2.13	0.48
1:B:458:ILE:O	1:B:462:ILE:HG23	2.14	0.48
1:A:380:ILE:HG23	1:A:382:GLU:CD	2.38	0.48
1:B:569:ARG:HD2	1:B:608:LYS:O	2.12	0.48
1:B:128:ASP:OD1	1:B:651:SER:HB3	2.13	0.48
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.96	0.47
1:A:577:LEU:HD13	1:A:619:ILE:HG12	1.95	0.47
1:B:830:SER:HB3	1:B:832:GLN:HG3	1.97	0.47
1:A:668:THR:HG21	1:A:771:PHE:HB3	1.96	0.47
1:A:680:LYS:CE	2:A:901:PLR:C4A	2.93	0.47
1:A:138:ARG:HD3	1:A:138:ARG:C	2.40	0.47
1:B:363:LYS:O	1:B:363:LYS:HE2	2.15	0.47
1:A:677:GLY:HA2	1:A:680:LYS:HD2	1.96	0.47
1:A:729:GLN:NE2	1:A:733:ASP:OD2	2.48	0.46
1:B:405:GLU:OE2	1:B:409:ARG:NH2	2.47	0.46
1:B:433:GLU:OE1	1:B:437:LYS:NZ	2.48	0.46
1:B:571:HIS:CD2	1:B:613:TYR:HE2	2.33	0.46
1:A:13:ILE:HG23	1:A:501:GLU:OE2	2.15	0.46
1:B:687:LEU:HD13	1:B:801:VAL:HG22	1.97	0.46
1:A:363:LYS:O	1:A:367:VAL:HG23	2.15	0.46
1:B:465:LYS:HG3	1:B:466:THR:HG23	1.98	0.46
1:B:663:SER:HB2	1:B:681:PHE:HB3	1.97	0.45
1:A:13:ILE:CG2	1:A:15:VAL:HG12	2.45	0.45
1:A:504:ALA:HA	1:A:508:GLY:O	2.16	0.45
1:A:628:ASP:O	1:A:632:HIS:ND1	2.47	0.45
1:B:490:ARG:HD2	4:B:1123:HOH:O	2.15	0.45
1:A:786:ARG:HH12	1:A:790:LEU:HD13	1.82	0.45
1:B:66:ARG:NH1	1:B:102:LEU:HD22	2.32	0.44
1:A:169:LYS:NZ	4:A:1029:HOH:O	2.50	0.44
1:B:455:VAL:H	1:B:459:HIS:HD2	1.64	0.44
1:A:510:GLU:CD	1:A:517:GLN:HE22	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:TYR:HE1	1:B:615:MET:HB3	1.82	0.43
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.83	0.43
1:A:146:SER:O	1:A:150:LEU:HG	2.18	0.43
1:A:700:ALA:HB1	1:A:710:ILE:HD11	1.99	0.43
1:A:85:LEU:HD11	1:A:303:THR:HG21	2.00	0.43
1:B:82:ILE:HD12	1:B:82:ILE:N	2.34	0.43
1:A:283:ASP:O	1:A:571:HIS:HE1	2.02	0.42
1:B:93:ARG:NH1	4:B:967:HOH:O	2.52	0.42
1:B:379:VAL:HG21	1:B:462:ILE:HD11	2.01	0.42
1:B:292:ARG:O	1:B:292:ARG:HD3	2.19	0.42
1:A:380:ILE:HA	1:A:381:PRO:HD3	1.81	0.42
1:A:386:ARG:HB2	1:A:438:ARG:HD3	2.01	0.42
1:B:35:LEU:HA	1:B:39:LEU:HD12	2.01	0.42
1:A:688:THR:HB	1:A:708:PHE:CE2	2.55	0.42
1:B:384:LEU:HD21	1:B:440:ASN:HD21	1.85	0.42
1:A:583:VAL:HG11	1:A:642:VAL:HG21	2.01	0.42
1:A:700:ALA:CB	1:A:710:ILE:HD11	2.50	0.42
1:A:716:GLU:H	1:A:716:GLU:CD	2.28	0.42
1:B:138:ARG:HD3	1:B:138:ARG:C	2.44	0.42
1:A:171:CYS:HB3	1:A:176:MET:CG	2.50	0.41
1:B:78:ASP:OD2	1:B:332:LYS:HE2	2.21	0.41
1:B:580:CYS:O	1:B:584:ILE:HG13	2.20	0.41
1:B:583:VAL:HG11	1:B:642:VAL:HG21	2.03	0.41
1:A:101:ASN:HD22	1:A:233:TYR:HA	1.85	0.41
1:A:566:GLN:HA	4:A:975:HOH:O	2.20	0.41
1:B:735:ILE:HD13	1:B:778:GLU:OE2	2.20	0.41
1:A:566:GLN:HB2	1:A:664:GLU:HB2	2.03	0.41
1:B:718:VAL:C	1:B:720:ARG:H	2.28	0.41
1:A:29:LYS:HG2	1:A:30:ASN:N	2.35	0.41
1:B:771:PHE:O	1:B:772:LYS:C	2.63	0.41
1:A:466:THR:OG1	1:A:467:ILE:N	2.53	0.41
1:B:87:LEU:CD2	1:B:159:ILE:HD12	2.51	0.41
1:B:712:GLY:O	1:B:714:ARG:NH1	2.54	0.41
1:B:689:ILE:HA	1:B:709:PHE:HB2	2.02	0.40
1:B:384:LEU:HD21	1:B:440:ASN:ND2	2.37	0.40
1:B:662:LEU:HD22	1:B:787:VAL:HG11	2.03	0.40
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	784/842 (93%)	758 (97%)	26 (3%)	0	100	100
1	B	784/842 (93%)	750 (96%)	33 (4%)	1 (0%)	48	40
All	All	1568/1684 (93%)	1508 (96%)	59 (4%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	772	LYS

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	675/731 (92%)	637 (94%)	38 (6%)	19	6
1	B	676/731 (92%)	646 (96%)	30 (4%)	25	10
All	All	1351/1462 (92%)	1283 (95%)	68 (5%)	22	8

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	27	LEU
1	A	44	ASN
1	A	63	LEU
1	A	78	ASP

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	121	GLU
1	A	144	LEU
1	A	198	LEU
1	A	209	THR
1	A	234	ARG
1	A	277	ARG
1	A	292	ARG
1	A	344	LEU
1	A	359	LEU
1	A	380	ILE
1	A	384	LEU
1	A	386	ARG
1	A	398	ARG
1	A	400	LEU
1	A	433	GLU
1	A	444	LEU
1	A	474	LEU
1	A	515	LEU
1	A	518	LEU
1	A	522	LEU
1	A	550	GLU
1	A	568	LYS
1	A	569	ARG
1	A	586	LEU
1	A	596	LYS
1	A	622	LEU
1	A	645	LEU
1	A	668	THR
1	A	687	LEU
1	A	706	GLU
1	A	708	PHE
1	A	729	GLN
1	B	60	ARG
1	B	119	MET
1	B	125	ILE
1	B	127	GLU
1	B	138	ARG
1	B	176	MET
1	B	198	LEU
1	B	234	ARG
1	B	292	ARG

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Mol	Chain	Res	Type
1	B	332	LYS
1	B	344	LEU
1	B	363	LYS
1	B	400	LEU
1	B	444	LEU
1	B	474	LEU
1	B	549	LEU
1	B	573	TYR
1	B	590	ILE
1	B	593	GLU
1	B	622	LEU
1	B	645	LEU
1	B	656	VAL
1	B	676	THR
1	B	678	ASN
1	B	687	LEU
1	B	706	GLU
1	B	772	LYS
1	B	779	GLU
1	B	828	GLU
1	B	834	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	282	ASN
1	A	453	ASN
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	496	ASN
1	A	541	ASN
1	A	566	GLN
1	A	579	ASN
1	A	684	ASN
1	A	723	GLN
1	A	729	GLN
1	A	754	GLN
1	A	763	ASN
1	A	767	HIS

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Mol	Chain	Res	Type
1	A	793	ASN
1	B	12	GLN
1	B	34	HIS
1	B	73	HIS
1	B	97	ASN
1	B	219	GLN
1	B	412	ASN
1	B	450	HIS
1	B	459	HIS
1	B	481	ASN
1	B	484	ASN
1	B	566	GLN
1	B	579	ASN
1	B	595	ASN
1	B	678	ASN
1	B	696	ASN
1	B	754	GLN
1	B	763	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 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	FRX	A	904	-	33,33,33	2.17	6 (18%)	40,47,47	3.88	13 (32%)
2	PLR	A	901	1	15,15,15	1.13	1 (6%)	21,22,22	1.44	3 (14%)
3	FRX	B	903	-	33,33,33	2.29	6 (18%)	40,47,47	3.90	13 (32%)
2	PLR	B	902	1	15,15,15	1.08	1 (6%)	21,22,22	1.56	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	FRX	A	904	-	-	1/16/32/32	0/4/4/4
2	PLR	A	901	1	-	0/6/6/6	0/1/1/1
3	FRX	B	903	-	-	4/16/32/32	0/4/4/4
2	PLR	B	902	1	-	0/6/6/6	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	FRX	C6-C4	-7.60	1.22	1.42
3	A	904	FRX	C6-C4	-7.26	1.23	1.42
3	B	903	FRX	C6-C7	-6.60	1.23	1.38
3	A	904	FRX	C6-C7	-6.50	1.24	1.38
3	B	903	FRX	C3-S2	-5.78	1.66	1.73
3	A	904	FRX	C3-S2	-5.08	1.67	1.73
3	A	904	FRX	C5-C4	-3.41	1.33	1.42
3	B	903	FRX	C5-C4	-3.41	1.33	1.42
3	B	903	FRX	C4-C3	-3.20	1.31	1.38
3	A	904	FRX	C4-C3	-2.99	1.31	1.38
2	A	901	PLR	C2-N1	2.87	1.39	1.33
3	B	903	FRX	C1-CL	2.83	1.77	1.71
3	A	904	FRX	C1-CL	2.68	1.77	1.71
2	B	902	PLR	C2-N1	2.64	1.38	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	FRX	C4-C6-C7	14.66	128.22	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	FRX	C4-C6-C7	14.19	127.58	108.22
3	B	903	FRX	C6-C4-C3	-12.21	97.48	111.57
3	A	904	FRX	C6-C4-C3	-11.42	98.39	111.57
3	A	904	FRX	C4-C3-S2	7.71	115.59	111.69
3	B	903	FRX	C4-C3-S2	7.21	115.34	111.69
3	A	904	FRX	C6-C7-N8	-6.41	97.05	107.74
3	B	903	FRX	C6-C7-N8	-6.32	97.21	107.74
3	A	904	FRX	C21-N17-C19	5.37	124.22	118.31
3	A	904	FRX	C7-C11-N11	5.19	123.79	116.86
3	B	903	FRX	C13-N11-C11	4.83	130.13	122.00
3	B	903	FRX	C19-C13-N11	4.64	118.67	110.15
3	B	903	FRX	C21-N17-C19	4.41	123.16	118.31
3	A	904	FRX	O13-C11-C7	-4.37	115.46	121.09
3	B	903	FRX	C5-C4-C3	4.28	116.51	111.57
2	B	902	PLR	C4A-C4-C5	-4.16	116.65	120.94
3	A	904	FRX	C24-N22-C22	4.02	130.31	122.82
3	A	904	FRX	C5-C4-C3	3.80	115.96	111.57
3	A	904	FRX	C21-N17-C17	-3.78	115.98	120.20
3	A	904	FRX	C25-C24-N22	-3.33	103.74	111.60
2	A	901	PLR	C4A-C4-C5	-3.25	117.59	120.94
2	B	902	PLR	C5-C6-N1	-3.11	118.77	123.83
3	B	903	FRX	C21-N17-C17	-2.94	116.92	120.20
2	A	901	PLR	C5-C6-N1	-2.80	119.27	123.83
2	B	902	PLR	C6-C5-C4	2.79	120.38	118.10
3	B	903	FRX	C5-C1-S2	2.65	118.50	113.16
3	A	904	FRX	C5-C1-S2	2.65	118.50	113.16
3	B	903	FRX	O13-C11-C7	-2.42	117.97	121.09
3	B	903	FRX	C5-C1-CL	-2.21	123.02	127.00
3	A	904	FRX	C5-C1-CL	-2.13	123.16	127.00
2	A	901	PLR	C6-C5-C4	2.13	119.84	118.10
3	B	903	FRX	C25-C24-N22	-2.07	106.72	111.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

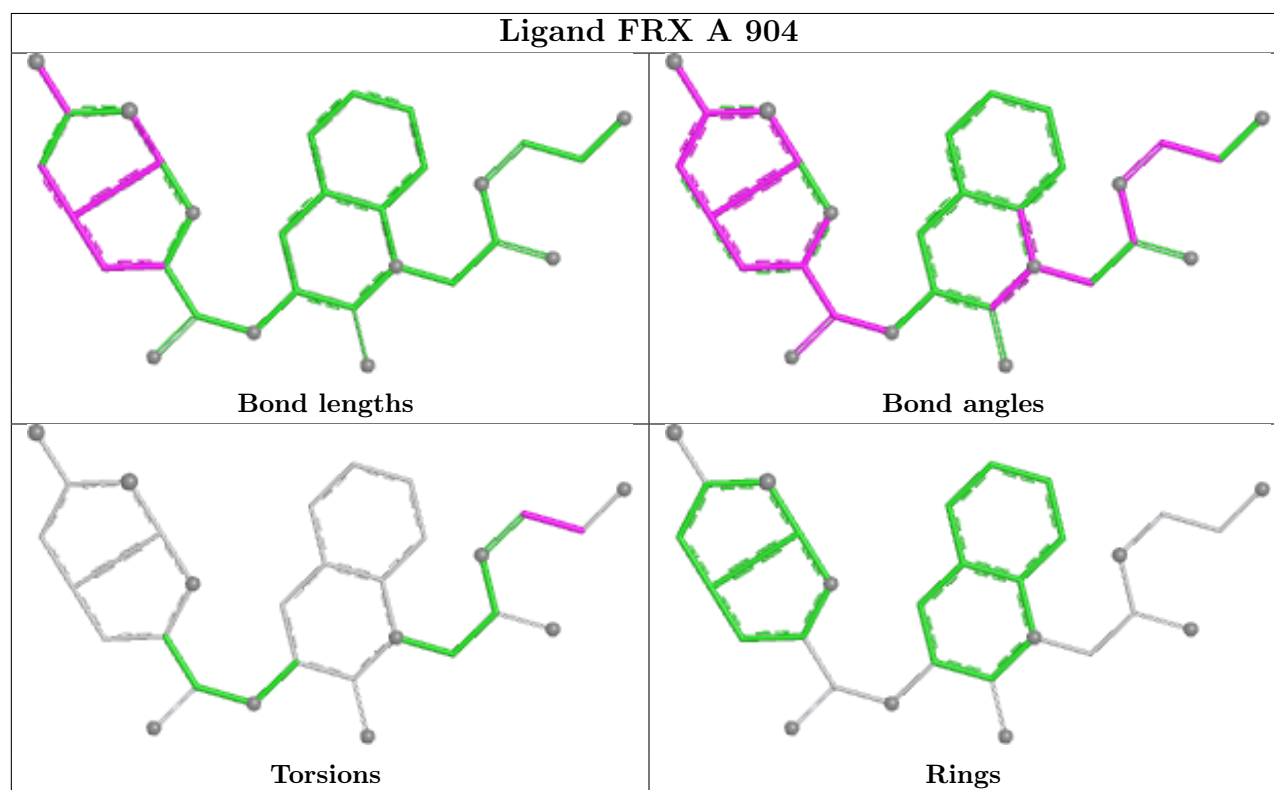
Mol	Chain	Res	Type	Atoms
3	B	903	FRX	C19-C13-N11-C11
3	B	903	FRX	O13-C11-N11-C13
3	B	903	FRX	N22-C24-C25-O25
3	B	903	FRX	C7-C11-N11-C13
3	A	904	FRX	N22-C24-C25-O25

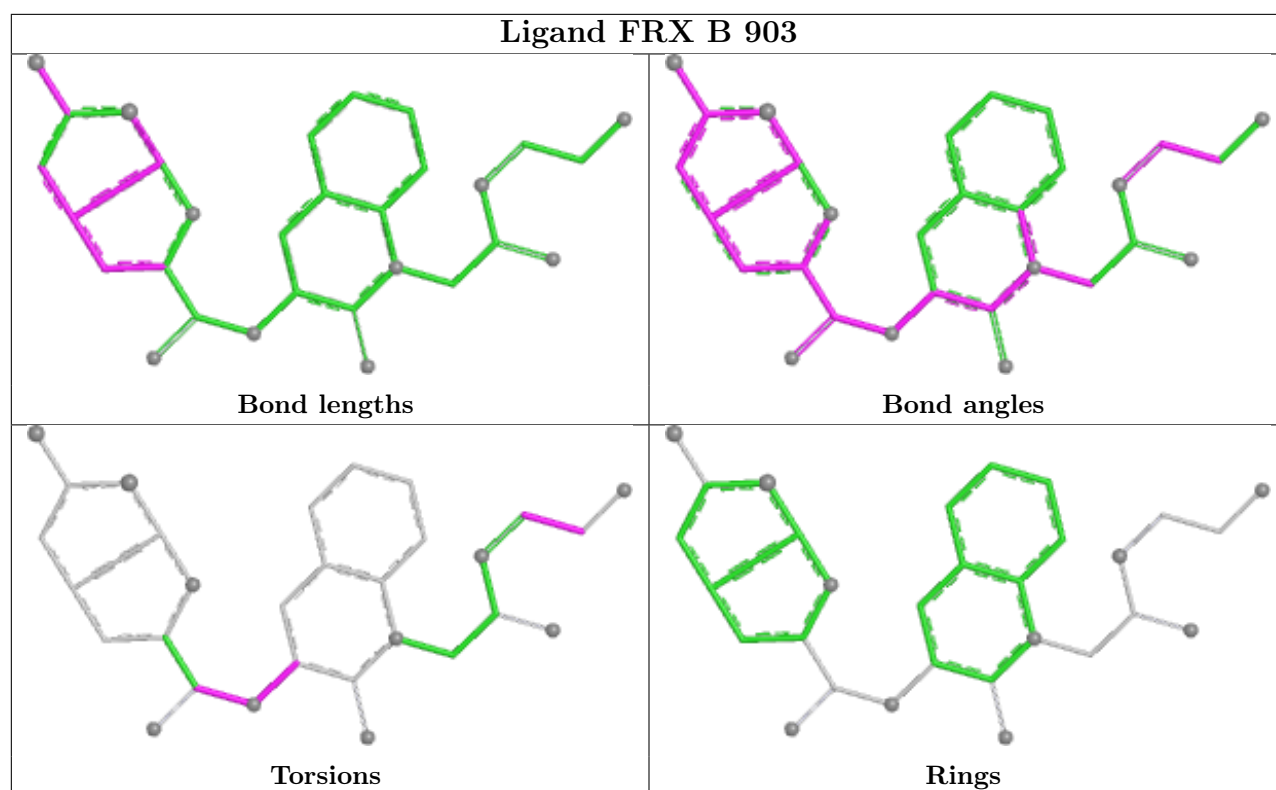
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	FRX	1	0
2	A	901	PLR	5	0
3	B	903	FRX	1	0
2	B	902	PLR	6	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	794/842 (94%)	-0.78	0 100 100	20, 29, 39, 49	10 (1%)
1	B	796/842 (94%)	-0.70	0 100 100	22, 33, 47, 53	8 (1%)
All	All	1590/1684 (94%)	-0.74	0 100 100	20, 31, 44, 53	18 (1%)

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.

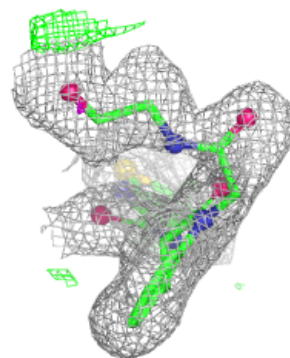
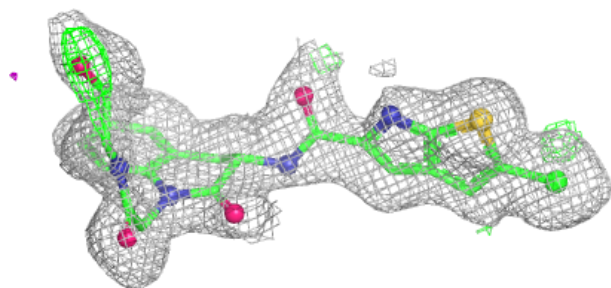
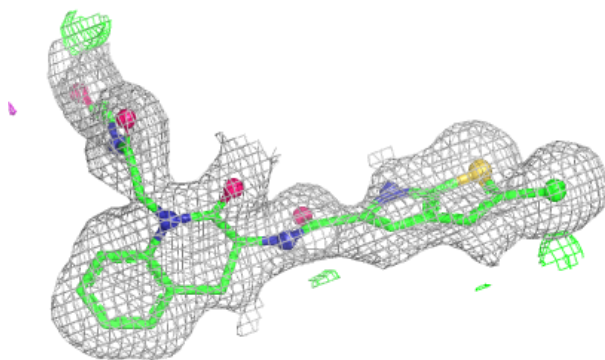
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLR	A	901	15/15	0.99	0.04	20,21,23,24	0
2	PLR	B	902	15/15	0.99	0.03	20,23,26,26	0
3	FRX	A	904	30/30	0.99	0.05	28,33,41,43	0
3	FRX	B	903	30/30	0.99	0.05	25,34,39,39	0

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.

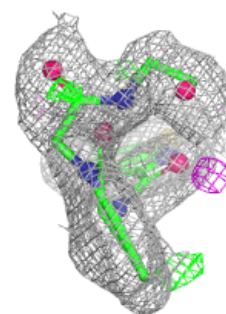
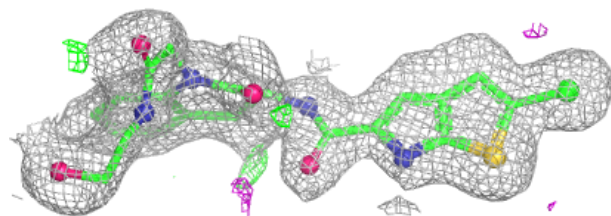
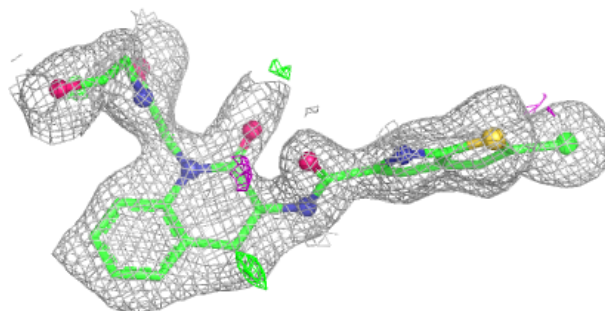
Electron density around FRX A 904:

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



Electron density around FRX B 903:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.