



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:35 am GMT

PDB ID : 2IEI  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

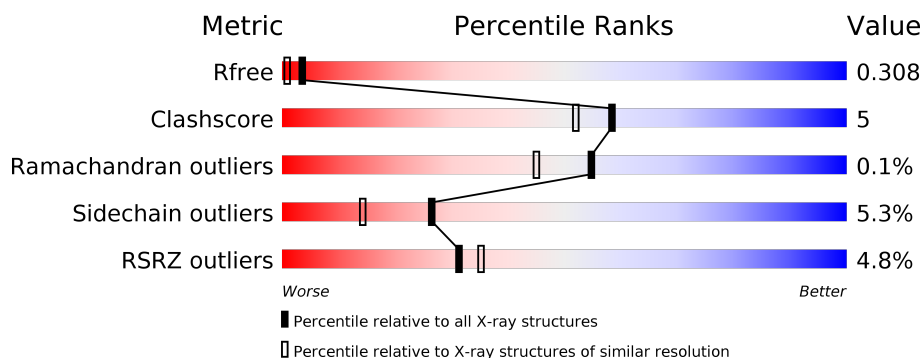
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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))
$R_{free}$	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	842	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	842	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLR	A	901	-	-	X	-
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.

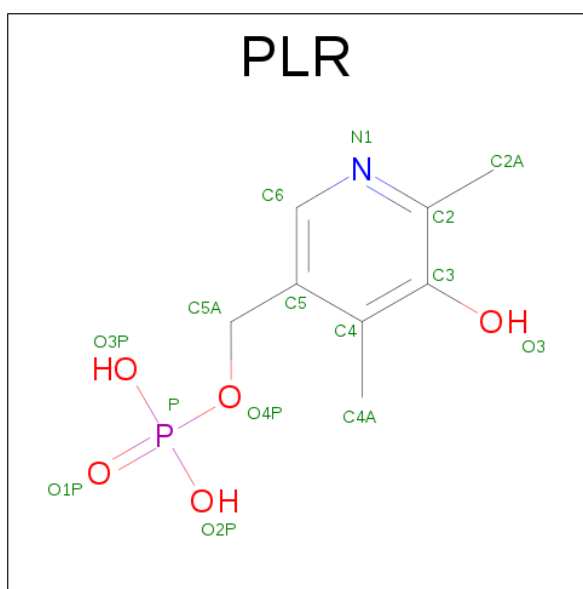
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

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 (three-letter code: PLR) (formula: C<sub>8</sub>H<sub>12</sub>NO<sub>5</sub>P).



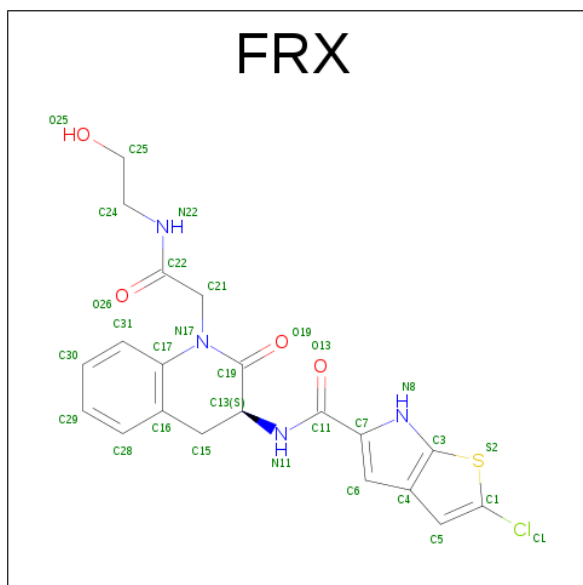
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

*Continued on next page...*

Continued from previous page...

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 (three-letter code: FRX) (formula: C<sub>20</sub>H<sub>19</sub>ClN<sub>4</sub>O<sub>4</sub>S).

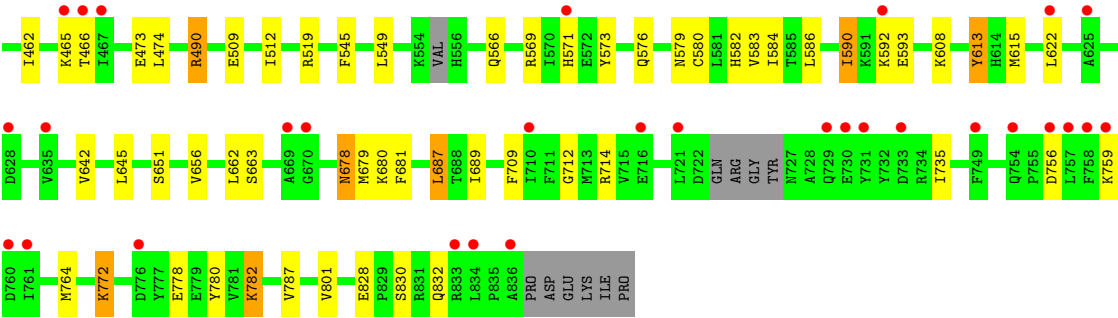


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	S	0	0
			30	20	1	4	4	1		
3	A	1	Total	C	Cl	N	O	S	0	0
			30	20	1	4	4	1		

- 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		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.40Å 125.34Å 129.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 1.91 32.65 – 1.91	Depositor EDS
% Data completeness (in resolution range)	80.5 (33.00-1.91) 75.0 (32.65-1.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FRX, 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	0.41	0/6559	0.57	1/8880 (0.0%)
1	B	0.39	0/6553	0.55	0/8873
All	All	0.40	0/13112	0.56	1/17753 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LEU	CA-CB-CG	5.99	129.08	115.30

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	68	0
1	B	6413	0	6319	70	0
2	A	15	0	10	8	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	7	0
4	B	260	0	0	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13536	0	12716	138	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 5.

All (138) 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:H4A2	1.28	1.42
1:B:680:LYS:HZ2	2:B:902:PLR:C4A	1.58	1.11
1:A:680:LYS:HZ1	2:A:901:PLR:H4A3	1.27	0.99
1:B:680:LYS:HZ1	2:B:902:PLR:H4A3	1.29	0.96
1:B:680:LYS:HZ1	2:B:902:PLR:C4A	1.69	0.95
1:A:138:ARG:HD3	1:A:138:ARG:O	1.71	0.91
1:A:680:LYS:NZ	2:A:901:PLR:H4A3	1.88	0.86
1:A:571:HIS:HB2	1:A:574:LYS:HG2	1.60	0.84
1:A:680:LYS:HZ2	2:A:901:PLR:H4A2	1.45	0.82
1:A:680:LYS:NZ	2:A:901:PLR:H4A2	1.99	0.77
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:A:680:LYS:HZ2	2:A:901:PLR:C4A	2.00	0.71
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: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:509:GLU:O	1:B:512:ILE:HG12	1.97	0.65
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
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:HD3	1:B:138:ARG:O	2.03	0.58
1:A:610:ALA:HB3	1:A:613:TYR:HB2	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:680:LYS:HZ2	2:B:902:PLR:H4A2	0.63	0.57
1:B:85:LEU:HD13	1:B:335:ILE:HG23	1.86	0.57
1:A:226:TYR:HE1	1:A:245:SER:HG	1.53	0.56
1:A:568:LYS:CE	4:A:993:HOH:O	2.52	0.56
1:A:13:ILE:HG22	1:A:15:VAL:HG12	1.87	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: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:B:83:TYR:HE1	1:B:310:ARG:HH21	1.57	0.53
1:A:93:ARG:NH2	1:A:124:GLU:HA	2.20	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
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:793:ASN:C	1:A:793:ASN:HD22	2.16	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:138:ARG:HG3	2:B:902:PLR:H4A3	1.96	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:B:778:GLU:CD	1:B:778:GLU:H	2.17	0.47
1:A:680:LYS:CE	2:A:901:PLR:C4A	2.93	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:A:680:LYS:CE	2:A:901:PLR:H4A2	2.45	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:B:455:VAL:H	1:B:459:HIS:HD2	1.64	0.44
1:A:380:ILE:HG23	1:A:382:GLU:CD	2.38	0.43
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:N	1:B:82:ILE:HD12	2.34	0.43
1:A:283:ASP:O	1:A:571:HIS:HE1	2.02	0.42
1:B:379:VAL:HG21	1:B:462:ILE:HD11	2.01	0.42
1:B:93:ARG:NH1	4:B:967:HOH:O	2.52	0.42
1:B:292:ARG:O	1:B:292:ARG:HD3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:29:LYS:HG2	1:A:30:ASN:N	2.35	0.41
1:B:712:GLY:O	1:B:714:ARG:NH1	2.54	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:689:ILE:HA	1:B:709:PHE:HB2	2.02	0.40
2:A:901:PLR:H5A1	2:A:901:PLR:H4A1	1.82	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

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	784/842 (93%)	758 (97%)	26 (3%)	0	100	100
1	B	784/842 (93%)	750 (96%)	33 (4%)	1 (0%)	55	45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1568/1684 (93%)	1508 (96%)	59 (4%)	1 (0%)	55 45

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%)	633 (94%)	42 (6%)	21 10
1	B	676/731 (92%)	646 (96%)	30 (4%)	33 20
All	All	1351/1462 (92%)	1279 (95%)	72 (5%)	26 14

All (72) 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
1	A	90	TYR
1	A	115	LEU
1	A	121	GLU
1	A	127	GLU
1	A	128	ASP
1	A	198	LEU
1	A	234	ARG
1	A	277	ARG
1	A	292	ARG
1	A	344	LEU
1	A	358	ARG
1	A	359	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	380	ILE
1	A	384	LEU
1	A	386	ARG
1	A	390	HIS
1	A	400	LEU
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	573	TYR
1	A	579	ASN
1	A	586	LEU
1	A	596	LYS
1	A	613	TYR
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	A	793	ASN
1	B	42	ASP
1	B	60	ARG
1	B	90	TYR
1	B	119	MET
1	B	127	GLU
1	B	138	ARG
1	B	176	MET
1	B	198	LEU
1	B	234	ARG
1	B	289	LYS
1	B	292	ARG
1	B	344	LEU
1	B	363	LYS
1	B	400	LEU
1	B	444	LEU
1	B	474	LEU
1	B	490	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	549	LEU
1	B	573	TYR
1	B	579	ASN
1	B	590	ILE
1	B	613	TYR
1	B	622	LEU
1	B	645	LEU
1	B	678	ASN
1	B	687	LEU
1	B	764	MET
1	B	772	LYS
1	B	782	LYS
1	B	828	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	101	ASN
1	A	239	ASN
1	A	453	ASN
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	566	GLN
1	A	579	ASN
1	A	723	GLN
1	A	754	GLN
1	A	793	ASN
1	B	12	GLN
1	B	34	HIS
1	B	97	ASN
1	B	211	GLN
1	B	219	GLN
1	B	408	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	595	ASN
1	B	678	ASN
1	B	696	ASN
1	B	754	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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$
2	PLR	A	901	1	15,15,15	1.10	2 (13%)	20,22,22	1.39	2 (10%)
3	FRX	A	904	-	29,33,33	2.29	4 (13%)	33,47,47	3.59	10 (30%)
2	PLR	B	902	1	15,15,15	1.06	2 (13%)	20,22,22	1.51	3 (15%)
3	FRX	B	903	-	29,33,33	2.36	4 (13%)	33,47,47	3.63	9 (27%)

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
2	PLR	A	901	1	-	0/6/6/6	0/1/1/1
3	FRX	A	904	-	-	0/13/32/32	0/4/4/4
2	PLR	B	902	1	-	0/6/6/6	0/1/1/1
3	FRX	B	903	-	-	0/13/32/32	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	FRX	C6-C7	-9.02	1.23	1.39
3	A	904	FRX	C6-C7	-8.89	1.24	1.39
3	B	903	FRX	C4-C3	-6.42	1.31	1.42
3	A	904	FRX	C4-C3	-6.15	1.31	1.42
3	B	903	FRX	C6-C4	-4.97	1.22	1.41
3	A	904	FRX	C6-C4	-4.74	1.23	1.41
2	A	901	PLR	C3-C2	-2.35	1.39	1.40
2	B	902	PLR	C3-C2	-2.27	1.39	1.40
3	A	904	FRX	C5-C4	-2.06	1.33	1.41
3	B	903	FRX	C5-C4	-2.06	1.33	1.41
2	B	902	PLR	C2-N1	2.25	1.38	1.33
2	A	901	PLR	C2-N1	2.44	1.39	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	PLR	C4A-C4-C5	-4.16	116.65	120.86
3	A	904	FRX	C25-C24-N22	-3.83	103.74	111.79
3	A	904	FRX	C21-N17-C17	-3.81	115.98	120.03
2	A	901	PLR	C4A-C4-C5	-3.23	117.59	120.86
2	B	902	PLR	C5-C6-N1	-3.01	118.77	123.87
3	B	903	FRX	C21-N17-C17	-2.93	116.92	120.03
3	B	903	FRX	C6-C4-C3	-2.80	97.48	105.38
2	A	901	PLR	C5-C6-N1	-2.72	119.27	123.87
3	A	904	FRX	O13-C11-C7	-2.65	115.46	121.13
3	A	904	FRX	C6-C4-C3	-2.48	98.39	105.38
3	B	903	FRX	C25-C24-N22	-2.41	106.72	111.79
3	A	904	FRX	C16-C17-N17	2.50	119.64	117.35
2	B	902	PLR	C6-C5-C4	2.64	120.38	118.18
3	B	903	FRX	C13-N11-C11	3.31	130.13	121.56
3	B	903	FRX	C16-C17-N17	3.59	120.65	117.35
3	A	904	FRX	C5-C4-C3	3.76	115.96	105.38
3	A	904	FRX	C24-N22-C22	3.89	130.31	122.84
3	B	903	FRX	C5-C4-C3	3.95	116.51	105.38
3	B	903	FRX	C21-N17-C19	4.21	123.16	118.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904	FRX	C7-C11-N11	4.21	123.79	115.20
3	B	903	FRX	C19-C13-N11	4.82	118.67	109.95
3	A	904	FRX	C21-N17-C19	5.14	124.22	118.38
3	A	904	FRX	C7-C6-C4	16.86	127.58	106.55
3	B	903	FRX	C7-C6-C4	17.37	128.22	106.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	PLR	8	0
3	A	904	FRX	1	0
2	B	902	PLR	6	0
3	B	903	FRX	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	794/842 (94%)	0.45	25 (3%)	49 54	20, 29, 39, 49	10 (1%)
1	B	796/842 (94%)	0.63	51 (6%)	20 23	23, 33, 47, 53	8 (1%)
All	All	1590/1684 (94%)	0.54	76 (4%)	31 35	20, 31, 44, 53	18 (1%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	ASN	5.3
1	B	284	ASN	5.0
1	B	836	ALA	4.4
1	A	285	PHE	4.4
1	B	285	PHE	4.3
1	A	435	ALA	4.3
1	A	20	GLY	4.0
1	B	435	ALA	3.8
1	B	466	THR	3.8
1	B	749	PHE	3.6
1	B	19	ALA	3.6
1	A	75	TYR	3.5
1	B	18	LEU	3.4
1	B	756	ASP	3.4
1	B	716	GLU	3.4
1	B	833	ARG	3.3
1	A	13	ILE	3.2
1	A	45	VAL	3.2
1	B	380	ILE	3.2
1	B	758	PHE	3.1
1	B	721	LEU	3.1
1	B	733	ASP	3.0
1	B	625	ALA	3.0
1	A	44	ASN	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	414	VAL	3.0
1	A	21	VAL	2.9
1	B	729	GLN	2.9
1	A	710	ILE	2.9
1	B	23	ASN	2.9
1	B	408	GLN	2.7
1	B	211	GLN	2.7
1	A	287	GLU	2.6
1	A	76	GLU	2.6
1	B	834	LEU	2.6
1	B	465	LYS	2.5
1	B	185	TYR	2.5
1	B	571	HIS	2.5
1	A	537	VAL	2.5
1	B	731	TYR	2.5
1	B	628	ASP	2.5
1	B	761	ILE	2.4
1	B	760	ASP	2.4
1	B	21	VAL	2.4
1	A	25	THR	2.4
1	A	209	THR	2.4
1	A	18	LEU	2.4
1	A	613	TYR	2.4
1	B	425	LEU	2.4
1	A	718	VAL	2.4
1	B	360	ASP	2.3
1	B	730	GLU	2.3
1	A	638	ASP	2.3
1	B	42	ASP	2.3
1	A	115	LEU	2.3
1	B	622	LEU	2.3
1	B	467	ILE	2.2
1	B	669	ALA	2.2
1	B	592	LYS	2.2
1	B	171	CYS	2.2
1	A	361	TRP	2.2
1	A	723	GLN	2.2
1	B	754	GLN	2.2
1	B	757	LEU	2.2
1	A	465	LYS	2.2
1	B	759	LYS	2.1
1	A	284	ASN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	434	GLY	2.1
1	B	418	PHE	2.1
1	B	710	ILE	2.1
1	A	283	ASP	2.1
1	A	103	ALA	2.1
1	B	13	ILE	2.1
1	B	776	ASP	2.0
1	B	116	GLY	2.0
1	B	670	GLY	2.0
1	B	635	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FRX	B	903	30/30	0.93	0.14	0.78	25,34,39,39	0
3	FRX	A	904	30/30	0.90	0.14	0.54	28,33,41,43	0
2	PLR	B	902	15/15	0.95	0.10	-0.83	20,23,26,26	0
2	PLR	A	901	15/15	0.96	0.10	-1.31	20,21,23,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.