



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:43 AM GMT

PDB ID : 2IEG  
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](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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

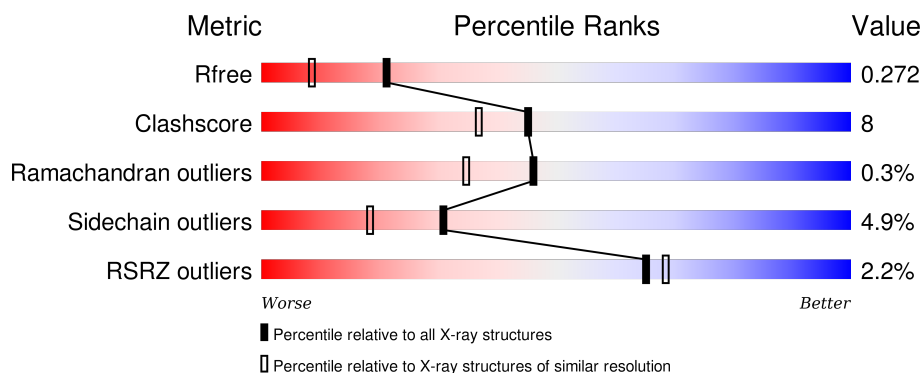
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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></div> <div>80% 12% 5%</div> </div>
1	B	842	<div> <div>3%</div> <div>78% 15%</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	903	-	-	X	-
2	PLR	B	904	-	-	X	-
3	FRY	B	902	-	-	-	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.

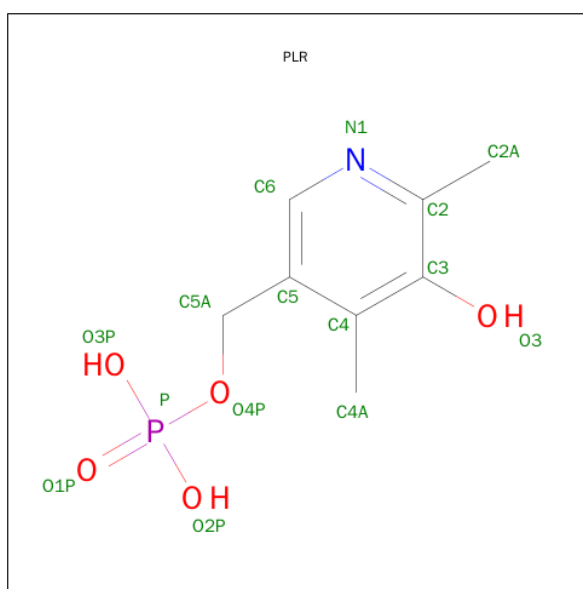
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

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



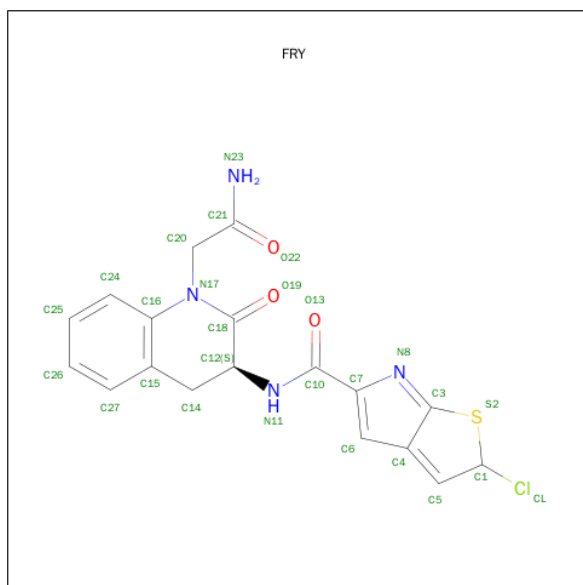
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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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 (2S)-N-[(3S)-1-(2-AMINO-2-OXOETHYL)-2-OXO-1,2,3,4-TETRAHYDROQUINOLIN-3-YL]-2-CHLORO-2H-THIENO[2,3-B]PYRROLE-5-CARBOXAMIDE (three-letter code: FRY) (formula: C<sub>18</sub>H<sub>15</sub>ClN<sub>4</sub>O<sub>3</sub>S).



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

- Molecule 4 is water.

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

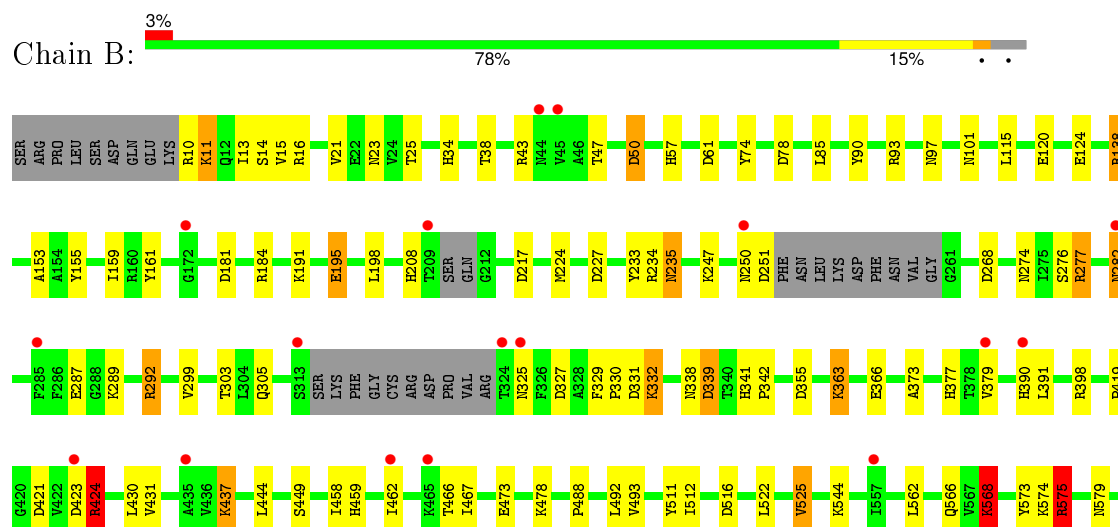
### 3 Residue-property plots

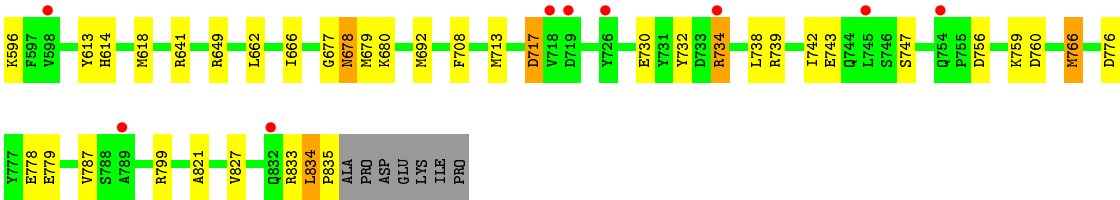
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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, $\alpha$ , $\beta$ , $\gamma$	114.12Å 125.16Å 128.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.97 – 1.90 33.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	81.3 (32.97-1.90) 77.2 (33.02-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 1.89Å)	Xtriage
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 (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.9	EDS
Estimated twinning fraction	0.085 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 117695 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage'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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.57	0/6719	0.88	25/9092 (0.3%)
1	B	0.54	0/6754	0.84	16/9139 (0.2%)
All	All	0.56	0/13473	0.86	41/18231 (0.2%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	277	ARG	NE-CZ-NH1	-8.33	116.13	120.30
1	A	601	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	283	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	292	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	138	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	277	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	B	423	ASP	CB-CG-OD2	7.14	124.72	118.30
1	A	833	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	423	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	138	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	601	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	526	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	533	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	339	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	633	ASP	CB-CG-OD2	6.32	123.98	118.30
1	B	331	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	638	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	739	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	575	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	421	ASP	CB-CG-OD2	5.98	123.69	118.30
1	A	128	ASP	CB-CG-OD2	5.86	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	776	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	292	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	424	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	739	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	227	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	717	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	50	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	470	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	292	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	693	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	234	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	717	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	795	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	268	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	649	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	575	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	516	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	424	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	6538	0	6493	98	0
1	B	6562	0	6508	104	0
2	A	15	0	10	9	0
2	B	15	0	10	11	0
3	A	27	0	14	6	0
3	B	27	0	14	1	0
4	A	403	0	0	11	1
4	B	340	0	0	11	1
All	All	13927	0	13049	202	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 (202) 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	1.41	1.31
1:A:680:LYS:NZ	2:A:903:PLR:H4A3	1.45	1.30
1:A:680:LYS:HZ1	2:A:903:PLR:C4A	1.50	1.19
1:B:680:LYS:HZ1	2:B:904:PLR:C4A	1.62	1.05
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:680:LYS:NZ	2:A:903:PLR:H4A2	1.76	0.99
1:B:680:LYS:HZ1	2:B:904:PLR:H4A3	0.82	0.97
1:A:680:LYS:HZ1	2:A:903:PLR:H4A3	0.82	0.97
1:B:680:LYS:HZ2	2:B:904:PLR:C4A	1.70	0.95
1:A:379:VAL:HG22	1:A:467:ILE:HG13	1.48	0.94
1:B:680:LYS:HZ2	2:B:904:PLR:H4A2	1.31	0.92
1:A:680:LYS:HZ2	2:A:903:PLR:H4A2	1.30	0.90
1:A:90:TYR:HE1	4:A:1146:HOH:O	1.55	0.89
1:A:680:LYS:HZ2	2:A:903:PLR:C4A	1.75	0.88
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: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:B:680:LYS:NZ	2:B:904:PLR:H4A2	1.87	0.79
1:A:101:ASN:HD22	1:A:233:TYR:HA	1.48	0.79
1:B:138:ARG:HD3	1:B:138:ARG:O	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: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
1:B:766:MET:HA	1:B:766:MET:HE3	1.71	0.73
1:A:379:VAL:CG2	1:A:467:ILE:HG13	2.18	0.71
1:A:138:ARG:O	1:A:138:ARG:HD3	1.91	0.70
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:209:THR:OG1	1:A:211:GLN:N	2.27	0.67
1:A:184:ARG:HB2	1:A:184:ARG:NH2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	1:A:282:ASN:HD22	1.98	0.62
1:B:437:LYS:HZ3	1:B:437:LYS:HB3	1.63	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: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:536[B]:LYS:NZ	1:A:536[B]:LYS:HB2	2.18	0.59
1:A:196:PHE:HD2	1:A:242:ARG:HH12	1.49	0.59
1:B:47:THR:HG23	1:B:50:ASP:OD2	2.02	0.58
1:A:680:LYS:CE	2:A:903:PLR:H4A2	2.34	0.58
1:B:678:ASN:HD22	1:B:679:MET:H	1.50	0.58
1:B:159:ILE:HG13	1:B:299:VAL:CG2	2.33	0.58
1:A:568:LYS:NZ	2:A:903:PLR:O1P	2.33	0.57
1:A:159:ILE:HG13	1:A:299:VAL:CG2	2.34	0.57
1:B:282:ASN:N	1:B:282:ASN:HD22	2.02	0.57
1:B:511:TYR:CE1	1:B:512:ILE:HD13	2.39	0.57
1:B:159:ILE:CG1	1:B:299:VAL:CG2	2.82	0.57
1:B:363:LYS:HA	1:B:363:LYS:CE	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:B:662:LEU:HD22	1:B:787:VAL:HG11	1.89	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:A:536[B]:LYS:HB2	1:A:536[B]:LYS:HZ2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:743:GLU:O	1:B:747:SER:OG	2.05	0.53
4:A:1262:HOH:O	1:B:195:GLU:HG3	2.08	0.53
1:A:455:VAL:H	1:A:459:HIS:HD2	1.57	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: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: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:A:96:GLN:CD	1:A:494:LEU:HG	2.32	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: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:B:459:HIS:O	1:B:462:ILE:HG22	2.12	0.49
1:B:159:ILE:HG13	1:B:299:VAL:HG21	1.94	0.49
1:B:85[B]:LEU:HD11	1:B:303:THR:HG21	1.93	0.49
1:B:522:LEU:O	1:B:525:VAL:HG22	2.13	0.49
1:B:799:ARG:CZ	4:B:1171:HOH:O	2.61	0.49
1:A:362:ASP:OD1	1:A:409:ARG:NH1	2.46	0.49
1:B:338:ASN:OD1	1:B:377:HIS:NE2	2.46	0.48
1:A:260:GLY:HA2	1:A:264:GLN:HG3	1.93	0.48
1:A:184:ARG:HH21	1:A:184:ARG:HB2	1.77	0.48
1:B:575:ARG:HD2	1:B:666:ILE:O	2.14	0.48
1:B:759:LYS:HG3	1:B:760:ASP:N	2.28	0.48
1:A:205:ARG:NH2	1:A:217:ASP:OD2	2.45	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:B:97:ASN:ND2	4:B:1015:HOH:O	2.47	0.48
1:A:430:LEU:HD22	1:A:444:LEU:N	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:HA	1:A:277:ARG:HD2	1.97	0.47
1:B:431:VAL:CG1	1:B:437:LYS:HE2	2.45	0.47
1:B:124:GLU:OE1	4:B:1059:HOH:O	2.20	0.47
1:A:52:TYR:OH	1:A:126:GLU:HG3	2.14	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: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:B:363:LYS:HE3	1:B:363:LYS:HA	1.98	0.45
1:A:13:ILE:HD12	1:A:501:GLU:HB2	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:B:562:LEU:C	1:B:562:LEU:HD23	2.37	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:B:437:LYS:HB3	1:B:437:LYS:NZ	2.31	0.45
1:A:13:ILE:CG1	1:A:16:ARG:HG3	2.47	0.45
1:B:732:TYR:CZ	1:B:739:ARG:HG3	2.52	0.45
1:B:363:LYS:O	1:B:363:LYS:HE2	2.17	0.44
1:A:424:ARG:NH2	1:A:473:GLU:OE1	2.33	0.44
1:A:282:ASN:N	1:A:282:ASN:ND2	2.65	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:178:GLU:CD	1:B:250:ASN:O	2.56	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:A:789:ALA:HA	1:A:792:LYS:HD3	2.00	0.43
1:B:488:PRO:O	1:B:492:LEU:HB3	2.19	0.43
1:A:138:ARG:C	1:A:138:ARG:HD3	2.38	0.43
1:B:224:MET:CE	1:B:247:LYS:HG3	2.49	0.43
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.53	0.43
1:A:159:ILE:HG13	1:A:299:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:568:LYS:HE3	4:B:1081:HOH:O	2.19	0.43
1:B:430:LEU:HD22	1:B:444:LEU:N	2.34	0.43
1:A:34:HIS:O	1:A:38:THR:HB	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
2:B:904:PLR:H4A1	2:B:904:PLR:H5A1	1.91	0.42
1:A:760:ASP:HB2	4:A:1271:HOH:O	2.19	0.42
1:A:575:ARG:HD3	1:A:666:ILE:O	2.19	0.42
1:A:329:PHE:HB3	1:A:330:PRO:HD3	2.00	0.42
1:B:680:LYS:CE	2:B:904:PLR:H4A2	2.48	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: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
1:B:74:TYR:CE2	1:B:153:ALA:HA	2.56	0.41
1:A:82:ILE:HD12	1:A:82:ILE:N	2.34	0.41
1:A:553:TYR:O	1:A:554:LYS:HB2	2.20	0.41
1:A:450:HIS:HE1	4:A:949:HOH:O	2.04	0.41
1:B:574:LYS:NZ	2:B:904:PLR:O2P	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:743:GLU:O	1:A:747:SER:HB3	2.21	0.41
1:B:568:LYS:CE	4:B:1081:HOH:O	2.69	0.41
3:A:901:FRY:H201	3:A:901:FRY:H24	1.88	0.41
1:A:195:GLU:H	1:A:195:GLU:HG3	1.61	0.41
1:A:16:ARG:HA	4:A:1032:HOH:O	2.20	0.40
1:A:29:LYS:C	1:A:29:LYS:HD3	2.42	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:157:TYR:CD1	1:A:303:THR:HG23	2.56	0.40
1:A:34:HIS:CE1	1:A:57:HIS:HB3	2.57	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 sym-

metry 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%)	52	42
1	B	806/842 (96%)	777 (96%)	27 (3%)	2 (0%)	52	42
All	All	1608/1684 (96%)	1550 (96%)	54 (3%)	4 (0%)	46	42

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%)	665 (95%)	32 (5%)	33	21
1	B	699/731 (96%)	662 (95%)	37 (5%)	28	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1396/1462 (96%)	1327 (95%)	69 (5%)	31	18

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	ASN
1	A	90	TYR
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	292	ARG
1	A	309	ARG
1	A	313	SER
1	A	363	LYS
1	A	379	VAL
1	A	518	LEU
1	A	554	LYS
1	A	556	HIS
1	A	568	LYS
1	A	579	ASN
1	A	596	LYS
1	A	613	TYR
1	A	638	ASP
1	A	678	ASN
1	A	692	MET
1	A	708	PHE
1	A	746	SER
1	A	770[A]	ARG
1	A	770[B]	ARG
1	A	833	ARG
1	B	14	SER
1	B	15	VAL
1	B	23	ASN
1	B	90	TYR
1	B	138	ARG

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Mol	Chain	Res	Type
1	B	195	GLU
1	B	217	ASP
1	B	235	ASN
1	B	277	ARG
1	B	282	ASN
1	B	289	LYS
1	B	292	ARG
1	B	332[A]	LYS
1	B	332[B]	LYS
1	B	339	ASP
1	B	363	LYS
1	B	419	PRO
1	B	424	ARG
1	B	437	LYS
1	B	478	LYS
1	B	525	VAL
1	B	544	LYS
1	B	568	LYS
1	B	573	TYR
1	B	575	ARG
1	B	579	ASN
1	B	596	LYS
1	B	613	TYR
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	459	HIS
1	A	477	HIS
1	A	481	ASN
1	A	484	ASN
1	A	560	ASN
1	A	566	GLN
1	A	579	ASN
1	A	678	ASN
1	B	34	HIS
1	B	62	HIS
1	B	101	ASN
1	B	219	GLN
1	B	235	ASN
1	B	282	ASN
1	B	412	ASN
1	B	481	ASN
1	B	484	ASN
1	B	566	GLN
1	B	579	ASN
1	B	614	HIS
1	B	678	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	A	901	1	24,30,30	2.51	2 (8%)	26,44,44	2.18	7 (26%)
2	PLR	A	903	1	15,15,15	1.15	2 (13%)	21,22,22	1.31	3 (14%)
3	FRY	B	902	-	24,30,30	2.68	1 (4%)	26,44,44	1.77	4 (15%)
2	PLR	B	904	1	15,15,15	1.38	2 (13%)	21,22,22	1.28	2 (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
3	FRY	A	901	1	-	3/12/48/48	0/4/4/4
2	PLR	A	903	1	-	0/6/6/6	0/1/1/1
3	FRY	B	902	-	-	3/12/48/48	0/4/4/4
2	PLR	B	904	1	-	0/6/6/6	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	PLR	C3-C2	-3.64	1.38	1.40
2	A	903	PLR	C3-C2	-2.23	1.39	1.40
3	A	901	FRY	C14-C12	-2.20	1.49	1.53
2	B	904	PLR	C2-N1	2.09	1.38	1.34
2	A	903	PLR	C2-N1	2.22	1.38	1.34
3	A	901	FRY	O19-C18	11.55	1.43	1.22
3	B	902	FRY	O19-C18	12.67	1.45	1.22

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FRY	C7-N8-C3	-4.30	102.96	110.40
3	A	901	FRY	C18-C12-N11	-3.32	104.09	110.23
3	A	901	FRY	C16-N17-C18	-2.86	115.45	121.46
3	B	902	FRY	C7-N8-C3	-2.84	105.49	110.40
2	B	904	PLR	C5-C6-N1	-2.75	119.08	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	903	PLR	C5-C6-N1	-2.60	119.34	123.86
2	A	903	PLR	C4A-C4-C3	-2.40	116.01	120.36
3	B	902	FRY	C16-N17-C18	-2.14	116.96	121.46
3	A	901	FRY	C14-C12-N11	2.31	115.68	112.02
2	B	904	PLR	C3-C4-C5	2.47	121.48	118.78
2	A	903	PLR	C3-C4-C5	2.50	121.51	118.78
3	A	901	FRY	C6-C7-C10	2.87	129.24	124.15
3	B	902	FRY	C20-N17-C18	3.67	122.59	118.15
3	A	901	FRY	C7-C10-N11	4.73	121.66	114.97
3	A	901	FRY	C20-N17-C18	5.01	124.23	118.15
3	B	902	FRY	C7-C10-N11	6.10	123.60	114.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	902	FRY	O13-C10-C7-C6
3	A	901	FRY	O13-C10-C7-C6
3	A	901	FRY	C6-C7-C10-N11
3	A	901	FRY	N8-C7-C10-N11
3	B	902	FRY	C6-C7-C10-N11
3	B	902	FRY	N8-C7-C10-N11

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FRY	6	0
2	A	903	PLR	9	0
3	B	902	FRY	1	0
2	B	904	PLR	11	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	803/842 (95%)	0.10	10 (1%) 81 83	27, 36, 47, 55	0
1	B	805/842 (95%)	0.25	26 (3%) 51 54	28, 39, 51, 58	0
All	All	1608/1684 (95%)	0.18	36 (2%) 65 68	27, 37, 49, 58	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	TYR	4.3
1	A	44	ASN	4.1
1	B	45	VAL	4.0
1	B	324	THR	3.9
1	B	734	ARG	3.4
1	B	557	ILE	3.2
1	A	21	VAL	3.1
1	A	724	ARG	3.0
1	A	835	PRO	3.0
1	B	745	LEU	2.9
1	B	250	ASN	2.8
1	A	638	ASP	2.8
1	B	379	VAL	2.7
1	B	598	VAL	2.7
1	B	285	PHE	2.6
1	B	726	TYR	2.6
1	A	211	GLN	2.5
1	A	113	TYR	2.5
1	B	832	GLN	2.4
1	B	282	ASN	2.4
1	B	313	SER	2.3
1	B	325	ASN	2.3
1	B	423	ASP	2.3
1	B	718	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	209	THR	2.3
1	B	390	HIS	2.3
1	A	18	LEU	2.2
1	B	44	ASN	2.2
1	B	465	LYS	2.2
1	A	832	GLN	2.2
1	B	754	GLN	2.1
1	B	719	ASP	2.1
1	B	435	ALA	2.1
1	B	789	ALA	2.0
1	B	172	GLY	2.0
1	B	462	ILE	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	FRY	B	902	27/27	0.91	0.15	2.34	33,42,50,52	0
3	FRY	A	901	27/27	0.93	0.13	0.94	28,34,45,47	0
2	PLR	B	904	15/15	0.96	0.09	-0.80	26,28,31,34	0
2	PLR	A	903	15/15	0.97	0.09	-0.97	26,30,31,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.