Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:57 AM GMT

PDB ID	:	3NMN
Title	:	Crystal structure of pyrabactin-bound abscisic acid receptor PYL1 in complex with type 2C protein phosphatase ABI1
Authors	:	Zhou, X.E.; Melcher, K.; Ng, L.-M.; Soon, F.-F.; Xu, Y.; Suino-Powell, K.M.; Kovach, A.; Li, J.; Yong, E.-L.; Xu, H.E.
Deposited on	:	2010-06-22
Resolution	:	2.15 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

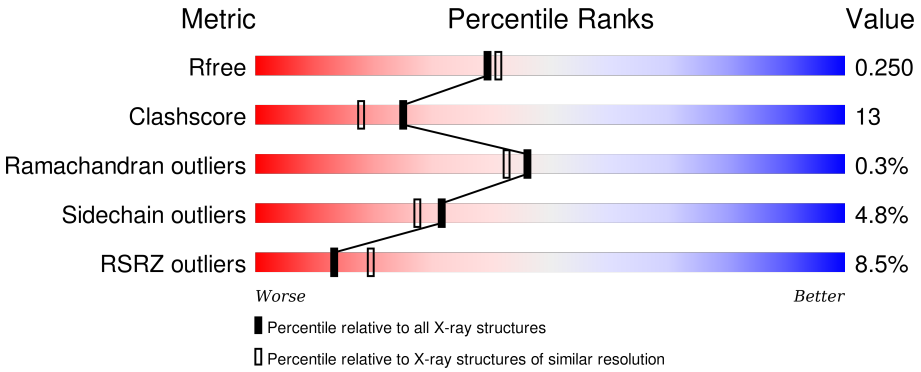
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 >=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 <=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	178	6%, 62%, 28%, 6%
1	C	178	6%, 71%, 23%
2	B	319	8%, 63%, 20%, 15%
2	D	319	9%, 68%, 18%, 13%

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
3	PYV	C	900	-	-	-	X
4	MG	D	999	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7184 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 Abscisic acid receptor PYL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1354	843	246	260	5			
1	C	171	Total	C	N	O	S	0	0	0
			1384	859	256	264	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	EXPRESSION TAG	UNP Q8VZS8
A	35	SER	-	EXPRESSION TAG	UNP Q8VZS8
C	34	GLY	-	EXPRESSION TAG	UNP Q8VZS8
C	35	SER	-	EXPRESSION TAG	UNP Q8VZS8

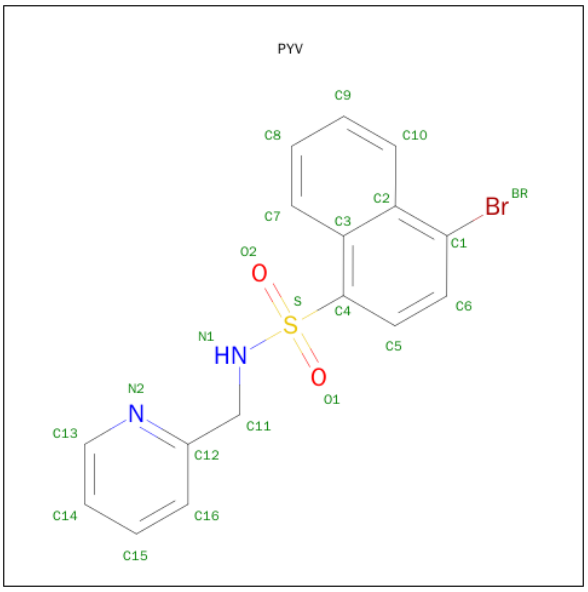
- Molecule 2 is a protein called Protein phosphatase 2C 56.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	271	Total	C	N	O	S	0	0	0
			2092	1318	366	395	13			
2	D	276	Total	C	N	O	S	0	0	0
			2126	1337	373	402	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	116	GLY	-	EXPRESSION TAG	UNP P49597
D	116	GLY	-	EXPRESSION TAG	UNP P49597

- Molecule 3 is 4-BROMO-N-(PYRIDIN-2-YLMETHYL)NAPHTHALENE-1-SULFONAMIDE (three-letter code: PYV) (formula: $C_{16}H_{13}BrN_2O_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Br C N O S 22 1 16 2 2 1	0	0
3	C	1	Total Br C N O S 22 1 16 2 2 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

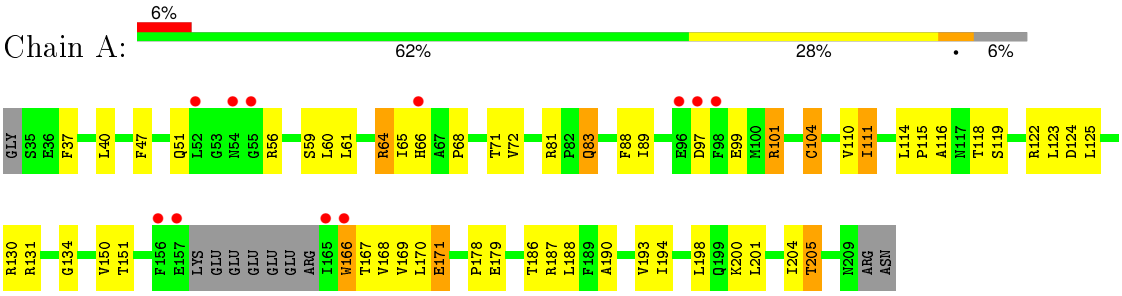
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	45	Total O 45 45	0	0
5	C	40	Total O 40 40	0	0
5	D	64	Total O 64 64	0	0

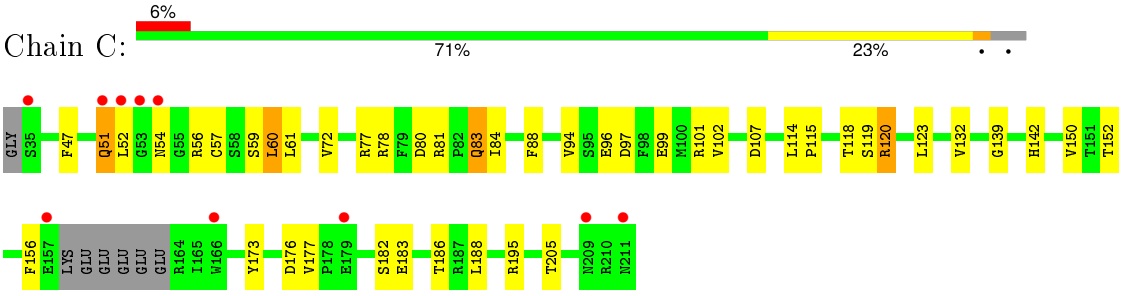
3 Residue-property plots (i)

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.

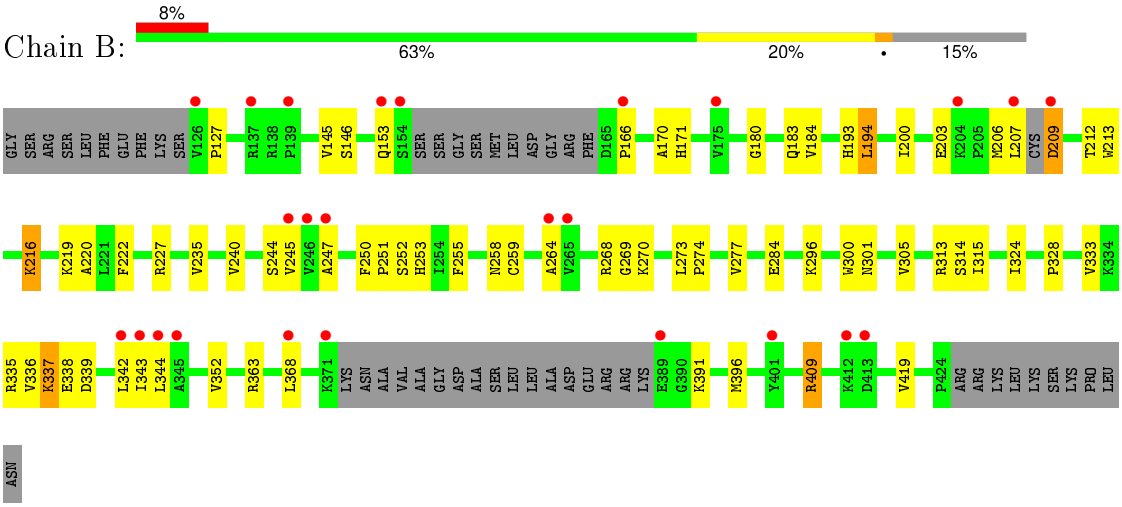
- Molecule 1: Abscisic acid receptor PYL1



- Molecule 1: Abscisic acid receptor PYL1

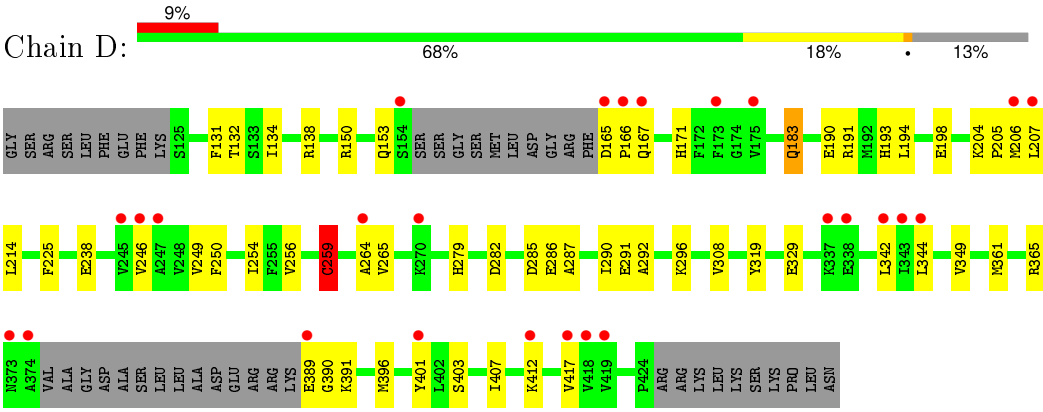


- Molecule 2: Protein phosphatase 2C 56



- Molecule 2: Protein phosphatase 2C 56

Chain D:


9%
68%
18%
13%
GLY SER ARG SER LEU PHE GLU PHE LYS S125 F131 T132 S133 I134 R138 R150 Q153 S154 SER SER GLY SER MET LEU ASP GLY ARG PHE D165 P166 Q167 H171 F172 F173 G174 V175 Q183 E190 R191 M192 H193 L194 E198 K204 P205 M206 L207 C208 D209 W213
L214 F225 E238 V245 V246 A247 V248 V249 F250 I254 F255 V256 C259 A264 V265 K270 H279 D282 D285 E286 A287 I290 E291 A292 K296 V308 Y319 E329 K337 E338 L342 I343 L344 V349 M361 R365 L368 K372
N373 A374 VAL ALA GLY ASP ALA SER LEU LEU ALA ASP GLU ARG ARG LYS E389 G390 K391 M396 Y401 L402 S403 I407 K412 V417 V418 V419 P424 ARG ARG LYS LEU LYS SER LYS PRO LEU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.98Å 66.71Å 72.60Å 115.78° 95.43° 105.60°	Depositor
Resolution (Å)	29.62 – 2.15 29.62 – 2.14	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.62-2.15) 79.9 (29.62-2.14)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.210 , 0.248 0.217 , 0.250	Depositor DCC
R_{free} test set	3617 reflections (7.81%)	DCC
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 50071 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7184	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: MG, PYV

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	0.95	2/1378 (0.1%)	0.83	2/1865 (0.1%)
1	C	1.04	0/1408	0.88	2/1904 (0.1%)
2	B	0.98	1/2132 (0.0%)	0.79	0/2881
2	D	0.96	1/2167 (0.0%)	0.81	1/2929 (0.0%)
All	All	0.98	4/7085 (0.1%)	0.82	5/9579 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	259	CYS	CB-SG	-9.61	1.66	1.82
1	A	104	CYS	CB-SG	-9.09	1.66	1.82
2	D	259	CYS	CB-SG	-8.34	1.68	1.82
1	A	171	GLU	CG-CD	5.04	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	130	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	176	ASP	CB-CG-OD1	5.18	122.96	118.30
2	D	390	GLY	N-CA-C	-5.09	100.36	113.10
1	A	56	ARG	NE-CZ-NH1	5.09	122.85	120.30

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	1354	0	1325	53	0
1	C	1384	0	1357	44	1
2	B	2092	0	2080	44	0
2	D	2126	0	2113	46	1
3	A	22	0	13	0	0
3	C	22	0	13	1	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	A	31	0	0	6	0
5	B	45	0	0	3	0
5	C	40	0	0	11	0
5	D	64	0	0	7	0
All	All	7184	0	6901	177	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 13.

All (177) 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:A:151:THR:HG23	5:A:215:HOH:O	1.52	1.10
1:C:118:THR:HB	5:C:20:HOH:O	1.54	1.05
2:D:249:VAL:HG22	5:D:51:HOH:O	1.59	0.99
1:C:83:GLN:H	1:C:83:GLN:HE21	1.12	0.98
2:B:333:VAL:HG12	2:D:292:ALA:HB1	1.51	0.91
2:B:209:ASP:HB2	2:B:213:TRP:HB2	1.52	0.90
2:D:361:MET:CE	2:D:401:TYR:HB3	2.05	0.87
1:C:77:ARG:HG2	5:C:215:HOH:O	1.74	0.87
2:D:132:THR:HB	5:D:59:HOH:O	1.76	0.85
1:C:81:ARG:HA	1:C:83:GLN:HE22	1.42	0.83
2:D:254:ILE:HG23	5:D:51:HOH:O	1.77	0.83
1:C:182:SER:O	1:C:186:THR:HG23	1.80	0.82
2:B:391:LYS:HD3	2:B:396:MET:HE2	1.62	0.81
2:D:361:MET:HE2	2:D:401:TYR:HB3	1.62	0.80
1:C:72:VAL:HG22	1:C:205:THR:HG21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LEU:HD13	2:B:296:LYS:HD2	1.66	0.77
1:C:132:VAL:HG22	1:C:152:THR:HG22	1.67	0.76
1:A:111:ILE:HG23	2:B:180:GLY:HA2	1.68	0.75
1:C:83:GLN:H	1:C:83:GLN:NE2	1.85	0.74
1:A:72:VAL:HG22	1:A:205:THR:HG21	1.70	0.73
2:D:134:ILE:CD1	2:D:407:ILE:HD11	2.19	0.73
1:A:99:GLU:HB3	5:A:232:HOH:O	1.91	0.71
2:D:391:LYS:HD3	2:D:396:MET:HE3	1.74	0.69
1:A:60:LEU:C	1:A:60:LEU:HD23	2.12	0.69
1:A:201:LEU:O	1:A:205:THR:HB	1.93	0.68
1:A:60:LEU:HD23	1:A:61:LEU:N	2.09	0.68
2:D:183:GLN:H	2:D:183:GLN:HE21	1.42	0.67
1:C:78:ARG:N	5:C:215:HOH:O	2.26	0.67
2:B:209:ASP:HB3	2:B:212:THR:HB	1.76	0.67
1:A:125:LEU:N	1:A:125:LEU:HD23	2.10	0.67
1:A:110:VAL:HG21	1:A:116:ALA:O	1.96	0.66
2:D:403:SER:HB3	5:D:59:HOH:O	1.95	0.66
1:A:72:VAL:HG21	1:A:167:THR:HG21	1.79	0.65
1:C:78:ARG:HG2	5:C:215:HOH:O	1.96	0.64
1:C:81:ARG:CZ	1:C:84:ILE:HD11	2.28	0.64
1:C:114:LEU:HB3	1:C:115:PRO:HD2	1.80	0.64
2:B:203:GLU:HB3	2:B:216:LYS:HG3	1.79	0.63
1:C:52:LEU:HB2	5:C:235:HOH:O	1.98	0.63
2:D:206:MET:HB2	2:D:209:ASP:OD1	2.00	0.62
2:B:391:LYS:CD	2:B:396:MET:HE2	2.28	0.62
2:B:343:ILE:HD12	2:B:419:VAL:HG22	1.82	0.62
1:A:81:ARG:HA	1:A:83:GLN:HE22	1.63	0.61
1:C:78:ARG:NH1	1:C:81:ARG:HD3	2.15	0.61
1:A:47:PHE:HB3	1:A:150:VAL:HG11	1.83	0.61
2:B:258:ASN:ND2	5:B:438:HOH:O	2.33	0.60
2:B:193:HIS:CE1	2:B:194:LEU:HD13	2.37	0.60
1:A:60:LEU:HD21	1:A:170:LEU:HD22	1.83	0.60
1:A:188:LEU:CD1	2:B:296:LYS:HD2	2.32	0.60
2:B:277:VAL:HG21	2:D:285:ASP:HA	1.82	0.59
2:B:315:ILE:N	2:B:315:ILE:HD12	2.18	0.59
1:C:88:PHE:CD2	1:C:114:LEU:HD11	2.37	0.58
2:B:207:LEU:HD13	2:B:207:LEU:C	2.23	0.58
2:D:134:ILE:HD11	2:D:407:ILE:HD11	1.85	0.58
2:D:193:HIS:CE1	2:D:194:LEU:HD13	2.39	0.58
2:B:352:VAL:HB	2:B:409:ARG:HB3	1.85	0.58
1:C:47:PHE:HB3	1:C:150:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:ASP:HB2	2:D:213:TRP:HB2	1.86	0.57
2:D:249:VAL:HA	5:D:51:HOH:O	2.05	0.57
1:A:65:ILE:HB	1:A:167:THR:HG23	1.85	0.57
1:A:111:ILE:CG2	2:B:180:GLY:HA2	2.36	0.56
2:B:264:ALA:HB2	2:B:344:LEU:HD22	1.87	0.55
1:C:72:VAL:CG2	1:C:205:THR:HG21	2.35	0.55
1:A:122:ARG:NH1	1:A:124:ASP:OD1	2.39	0.55
2:B:270:LYS:HA	2:B:363:ARG:NH2	2.22	0.55
1:A:83:GLN:HE21	1:A:83:GLN:H	1.54	0.54
1:A:171:GLU:HB2	5:A:215:HOH:O	2.07	0.54
2:D:287:ALA:O	2:D:291:GLU:HG2	2.07	0.54
1:A:125:LEU:HD21	1:A:134:GLY:HA3	1.91	0.53
2:D:150:ARG:H	2:D:171:HIS:HD2	1.56	0.53
1:A:59:SER:HB2	1:A:187:ARG:HD3	1.91	0.53
2:D:167:GLN:HA	2:D:250:PHE:HE1	1.72	0.53
2:B:337:LYS:HG3	2:B:338:GLU:OE2	2.08	0.53
1:A:122:ARG:NH1	5:A:216:HOH:O	2.31	0.53
2:D:132:THR:HG22	2:D:134:ILE:HG23	1.90	0.52
1:C:188:LEU:HD13	2:D:296:LYS:HD2	1.90	0.52
1:C:114:LEU:HB3	1:C:115:PRO:CD	2.38	0.52
1:A:200:LYS:HG2	1:A:204:ILE:HD13	1.91	0.52
2:B:333:VAL:CG1	2:D:292:ALA:HB1	2.33	0.52
1:C:59:SER:HB3	1:C:173:TYR:CE2	2.45	0.52
2:D:365:ARG:HA	2:D:368:LEU:HD22	1.91	0.51
2:D:391:LYS:CD	2:D:396:MET:HE3	2.40	0.51
1:A:99:GLU:HB2	1:A:101:ARG:HD2	1.92	0.51
1:A:178:PRO:HG2	2:B:300:TRP:CH2	2.46	0.51
1:C:96:GLU:H	1:C:96:GLU:CD	2.13	0.51
1:C:78:ARG:HH12	1:C:81:ARG:HD3	1.76	0.51
2:D:365:ARG:HD3	5:D:437:HOH:O	2.11	0.51
1:C:61:LEU:HD12	1:C:61:LEU:N	2.26	0.51
1:A:110:VAL:CG2	1:A:116:ALA:O	2.59	0.50
2:D:138:ARG:HG2	2:D:412:LYS:O	2.11	0.50
2:B:222:PHE:CD1	2:B:328:PRO:HD2	2.46	0.50
2:D:225:PHE:HE2	2:D:259:CYS:HB3	1.77	0.50
1:A:83:GLN:HG3	1:A:89:ILE:HG21	1.94	0.49
1:C:81:ARG:CA	1:C:83:GLN:HE22	2.20	0.49
2:D:254:ILE:HG12	5:D:51:HOH:O	2.12	0.49
2:D:361:MET:HE3	2:D:401:TYR:HB3	1.88	0.49
2:B:274:PRO:HD2	5:B:17:HOH:O	2.12	0.49
1:C:77:ARG:CG	5:C:215:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:NE2	1:A:83:GLN:H	2.10	0.48
1:A:114:LEU:HB3	1:A:115:PRO:HD2	1.95	0.48
2:B:305:VAL:HG21	2:B:324:ILE:HD11	1.96	0.48
1:C:80:ASP:OD2	1:C:94:VAL:HG11	2.14	0.47
1:C:114:LEU:HD22	2:D:308:VAL:HG13	1.96	0.47
1:C:52:LEU:HD13	1:C:54:ASN:O	2.14	0.47
1:C:51:GLN:HB3	5:C:233:HOH:O	2.14	0.47
2:B:368:LEU:HD12	2:B:368:LEU:C	2.35	0.47
2:B:127:PRO:HB3	2:B:171:HIS:CD2	2.49	0.47
1:A:64:ARG:HG3	1:A:168:VAL:HG22	1.95	0.47
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.80	0.47
2:B:203:GLU:OE2	2:B:219:LYS:HD3	2.14	0.47
1:A:97:ASP:O	5:A:224:HOH:O	2.20	0.47
2:D:131:PHE:H	2:D:396:MET:HE1	1.80	0.47
1:A:114:LEU:HB3	1:A:115:PRO:CD	2.45	0.47
1:A:101:ARG:O	1:A:101:ARG:HD3	2.15	0.46
2:B:313:ARG:O	2:B:314:SER:HB3	2.15	0.46
2:D:403:SER:O	2:D:407:ILE:HG13	2.16	0.46
2:B:273:LEU:HD23	5:B:17:HOH:O	2.16	0.46
1:C:56:ARG:NE	5:C:227:HOH:O	2.49	0.46
2:D:265:VAL:O	2:D:342:LEU:HD12	2.16	0.46
2:B:251:PRO:O	2:B:335:ARG:HD3	2.15	0.46
1:A:169:VAL:HG12	5:A:215:HOH:O	2.16	0.45
1:C:107:ASP:OD1	1:C:120:ARG:HG3	2.16	0.45
1:A:40:LEU:O	1:A:40:LEU:HD23	2.16	0.45
1:C:118:THR:HG22	1:C:119:SER:N	2.31	0.45
2:B:268:ARG:HH11	2:B:336:VAL:HG22	1.81	0.45
1:A:190:ALA:O	1:A:193:VAL:HG22	2.16	0.45
2:B:245:VAL:O	2:B:245:VAL:HG13	2.16	0.45
2:B:244:SER:HB3	2:B:315:ILE:HD11	1.99	0.44
2:B:252:SER:OG	2:B:253:HIS:HD2	2.00	0.44
2:B:184:VAL:HG23	2:B:240:VAL:HG12	1.99	0.44
1:A:81:ARG:HA	1:A:83:GLN:NE2	2.30	0.44
2:B:268:ARG:HD3	2:B:339:ASP:OD1	2.17	0.44
2:D:286:GLU:O	2:D:290:ILE:HG12	2.16	0.44
1:C:56:ARG:CZ	5:C:227:HOH:O	2.65	0.44
1:C:139:GLY:O	1:C:142:HIS:HE1	2.00	0.44
1:C:81:ARG:NH2	1:C:84:ILE:HD11	2.33	0.44
2:D:191:ARG:HH22	2:D:198:GLU:CD	2.21	0.44
1:A:88:PHE:C	1:A:111:ILE:HD12	2.39	0.43
2:D:207:LEU:HD13	2:D:213:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD23	5:C:235:HOH:O	2.18	0.43
2:D:264:ALA:HB2	2:D:344:LEU:CD2	2.47	0.43
1:A:99:GLU:O	1:A:104:CYS:SG	2.73	0.43
2:D:238:GLU:O	2:D:319:TYR:HD2	2.01	0.43
2:D:166:PRO:O	2:D:207:LEU:HD22	2.18	0.43
1:A:40:LEU:HD23	1:A:40:LEU:C	2.38	0.43
1:A:166:TRP:CE3	1:A:166:TRP:HA	2.54	0.43
2:B:207:LEU:HD22	2:B:207:LEU:O	2.18	0.43
2:D:349:VAL:HG21	2:D:417:VAL:HG22	2.00	0.43
2:D:204:LYS:N	2:D:205:PRO:HD3	2.35	0.42
1:C:57:CYS:HB3	1:C:183:GLU:HG2	2.01	0.42
1:C:177:VAL:HG13	1:C:186:THR:HG21	2.00	0.42
1:A:68:PRO:HG2	1:A:71:THR:OG1	2.19	0.42
2:B:170:ALA:HB2	2:B:250:PHE:CZ	2.55	0.42
1:A:65:ILE:HG21	1:A:205:THR:CG2	2.49	0.42
1:C:114:LEU:HD13	3:C:900:PYV:BR	2.75	0.42
1:C:120:ARG:HD3	1:C:120:ARG:N	2.34	0.42
1:A:193:VAL:HG23	1:A:194:ILE:N	2.33	0.42
1:A:99:GLU:HB2	1:A:101:ARG:CD	2.49	0.42
2:B:200:ILE:HD12	2:B:220:ALA:HB1	2.02	0.42
1:A:118:THR:HG22	1:A:119:SER:N	2.35	0.42
1:C:101:ARG:O	1:C:102:VAL:C	2.57	0.41
1:A:65:ILE:HG21	1:A:205:THR:HG21	2.03	0.41
2:B:264:ALA:CB	2:B:344:LEU:HD22	2.50	0.41
1:A:66:HIS:HB3	1:A:166:TRP:CH2	2.56	0.41
1:A:99:GLU:HG3	1:A:104:CYS:SG	2.61	0.41
2:D:368:LEU:C	2:D:368:LEU:HD23	2.40	0.41
1:C:60:LEU:C	1:C:61:LEU:HD12	2.40	0.41
1:C:118:THR:CB	5:C:20:HOH:O	2.35	0.41
2:D:165:ASP:HB3	2:D:166:PRO:HD3	2.02	0.41
2:B:247:ALA:HA	2:B:255:PHE:O	2.21	0.41
2:D:214:LEU:O	2:D:214:LEU:HD23	2.21	0.41
1:A:198:LEU:HA	1:A:198:LEU:HD23	1.90	0.41
1:C:81:ARG:HA	1:C:83:GLN:NE2	2.23	0.41
2:B:342:LEU:O	2:B:343:ILE:HD13	2.21	0.41
2:B:145:VAL:HG12	2:B:146:SER:N	2.36	0.40
2:D:246:VAL:O	2:D:256:VAL:HA	2.20	0.40
1:A:166:TRP:HE3	1:A:166:TRP:HA	1.86	0.40
2:D:279:HIS:HE2	2:D:329:GLU:CG	2.35	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)
1:C:54:ASN:ND2	2:D:389:GLU:O[1_455]	2.16	0.04

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	164/178 (92%)	156 (95%)	8 (5%)	0	100 100
1	C	167/178 (94%)	159 (95%)	8 (5%)	0	100 100
2	B	263/319 (82%)	245 (93%)	15 (6%)	3 (1%)	17 10
2	D	270/319 (85%)	257 (95%)	13 (5%)	0	100 100
All	All	864/994 (87%)	817 (95%)	44 (5%)	3 (0%)	46 42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	153	GLN
2	B	269	GLY
2	B	166	PRO

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	153/162 (94%)	142 (93%)	11 (7%)	18 12
1	C	156/162 (96%)	148 (95%)	8 (5%)	29 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	225/265 (85%)	214 (95%)	11 (5%)	31 26
2	D	229/265 (86%)	222 (97%)	7 (3%)	47 47
All	All	763/854 (89%)	726 (95%)	37 (5%)	31 27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	51	GLN
1	A	64	ARG
1	A	83	GLN
1	A	101	ARG
1	A	111	ILE
1	A	123	LEU
1	A	166	TRP
1	A	179	GLU
1	A	186	THR
1	A	205	THR
2	B	183	GLN
2	B	194	LEU
2	B	206	MET
2	B	209	ASP
2	B	216	LYS
2	B	227	ARG
2	B	235	VAL
2	B	284	GLU
2	B	301	ASN
2	B	337	LYS
2	B	409	ARG
1	C	51	GLN
1	C	60	LEU
1	C	83	GLN
1	C	97	ASP
1	C	99	GLU
1	C	120	ARG
1	C	123	LEU
1	C	156	PHE
2	D	153	GLN
2	D	183	GLN
2	D	190	GLU
2	D	209	ASP

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Mol	Chain	Res	Type
2	D	259	CYS
2	D	282	ASP
2	D	368	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	83	GLN
1	A	146	ASN
1	A	199	GLN
2	B	167	GLN
2	B	183	GLN
2	B	193	HIS
2	B	253	HIS
2	B	258	ASN
2	B	299	GLN
2	B	408	GLN
1	C	42	GLN
1	C	51	GLN
1	C	83	GLN
1	C	87	HIS
1	C	142	HIS
1	C	146	ASN
1	C	154	HIS
1	C	199	GLN
2	D	171	HIS
2	D	183	GLN
2	D	193	HIS
2	D	223	ASN
2	D	253	HIS
2	D	299	GLN
2	D	408	GLN

5.3.3 RNA

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)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	PYV	A	900	-	24,24,24	4.31	8 (33%)	34,34,34	2.93	14 (41%)
3	PYV	C	900	-	24,24,24	4.24	7 (29%)	34,34,34	3.08	12 (35%)

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	PYV	A	900	-	-	0/12/12/12	0/3/3/3
3	PYV	C	900	-	-	0/12/12/12	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	PYV	BR-C1	-14.08	1.52	1.90
3	C	900	PYV	BR-C1	-13.35	1.54	1.90
3	C	900	PYV	C4-S	-13.18	1.63	1.77
3	A	900	PYV	C4-S	-12.43	1.64	1.77
3	C	900	PYV	C11-N1	-4.19	1.42	1.47
3	A	900	PYV	C11-N1	-3.91	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	900	PYV	C6-C5	2.18	1.42	1.38
3	C	900	PYV	O2-S	2.19	1.45	1.43
3	A	900	PYV	C9-C10	2.21	1.41	1.36
3	A	900	PYV	C6-C1	2.41	1.41	1.36
3	A	900	PYV	O2-S	2.73	1.46	1.43
3	C	900	PYV	C5-C4	3.23	1.41	1.37
3	A	900	PYV	C5-C4	3.46	1.41	1.37
3	C	900	PYV	C3-C2	5.17	1.53	1.43
3	A	900	PYV	C3-C2	5.72	1.54	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	900	PYV	O2-S-O1	-9.74	106.62	119.54
3	A	900	PYV	O2-S-O1	-7.59	109.47	119.54
3	C	900	PYV	C5-C4-C3	-6.51	115.25	121.04
3	C	900	PYV	C6-C1-C2	-6.42	112.31	121.91
3	A	900	PYV	C5-C4-C3	-6.21	115.50	121.04
3	A	900	PYV	C6-C1-C2	-6.10	112.79	121.91
3	C	900	PYV	O1-S-N1	-3.18	101.91	107.03
3	A	900	PYV	C16-C12-N2	-2.89	117.80	122.18
3	A	900	PYV	O2-S-N1	-2.88	102.39	107.03
3	A	900	PYV	C14-C13-N2	-2.19	119.78	123.44
3	C	900	PYV	C10-C2-C1	-2.12	119.15	124.84
3	C	900	PYV	O2-S-C4	2.11	111.59	108.01
3	A	900	PYV	C11-N1-S	2.36	123.97	119.75
3	C	900	PYV	C5-C6-C1	2.48	125.50	120.77
3	A	900	PYV	C3-C4-S	2.94	125.38	121.54
3	C	900	PYV	BR-C1-C2	3.06	127.42	119.71
3	A	900	PYV	BR-C1-C2	3.09	127.49	119.71
3	A	900	PYV	C6-C5-C4	3.12	125.43	121.77
3	A	900	PYV	C4-S-N1	3.14	112.94	106.55
3	A	900	PYV	O1-S-C4	3.15	113.37	108.01
3	C	900	PYV	C4-S-N1	3.37	113.42	106.55
3	C	900	PYV	C3-C4-S	4.09	126.89	121.54
3	C	900	PYV	O2-S-N1	4.37	114.06	107.03
3	A	900	PYV	C13-N2-C12	5.09	124.36	117.36
3	A	900	PYV	C1-C2-C3	5.99	123.42	117.60
3	C	900	PYV	C1-C2-C3	6.58	123.99	117.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	900	PYV	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	168/178 (94%)	0.59	11 (6%)	22	31	28, 47, 90, 107	0
1	C	171/178 (96%)	0.22	10 (5%)	26	36	21, 38, 74, 105	0
2	B	271/319 (84%)	0.33	25 (9%)	11	17	17, 42, 86, 123	0
2	D	276/319 (86%)	0.52	29 (10%)	8	13	24, 43, 92, 111	0
All	All	886/994 (89%)	0.42	75 (8%)	13	19	17, 43, 87, 123	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	374	ALA	9.1
1	C	211	ASN	7.7
2	D	208	CYS	7.4
1	A	52	LEU	7.1
1	A	165	ILE	7.1
1	A	97	ASP	5.7
2	D	167	GLN	5.5
2	D	165	ASP	5.3
2	D	209	ASP	5.2
2	B	209	ASP	5.1
2	D	401	TYR	4.9
2	D	270	LYS	4.6
1	A	166	TRP	4.6
1	A	54	ASN	4.4
2	B	368	LEU	4.3
1	A	98	PHE	4.2
2	B	344	LEU	4.2
2	D	344	LEU	4.0
2	B	389	GLU	4.0
1	C	52	LEU	4.0
2	D	206	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	53	GLY	4.0
2	D	207	LEU	3.9
1	A	156	PHE	3.8
2	B	154	SER	3.8
2	D	245	VAL	3.7
1	A	96	GLU	3.5
2	D	166	PRO	3.4
1	C	35	SER	3.2
2	B	401	TYR	3.2
2	B	166	PRO	3.1
2	D	246	VAL	3.1
2	B	371	LYS	3.1
2	B	412	LYS	3.0
2	B	247	ALA	3.0
1	C	179	GLU	3.0
2	D	154	SER	3.0
1	C	166	TRP	2.9
1	C	157	GLU	2.9
2	B	137	ARG	2.8
1	A	55	GLY	2.8
2	B	245	VAL	2.8
2	B	126	VAL	2.7
2	D	373	ASN	2.7
2	B	265	VAL	2.6
2	D	247	ALA	2.5
2	D	343	ILE	2.5
2	D	412	LYS	2.5
1	A	157	GLU	2.5
2	D	175	VAL	2.5
2	D	389	GLU	2.4
1	A	66	HIS	2.4
2	B	342	LEU	2.4
1	C	54	ASN	2.4
2	B	139	PRO	2.3
2	B	264	ALA	2.3
1	C	209	ASN	2.3
2	D	372	LYS	2.3
2	B	246	VAL	2.3
2	D	338	GLU	2.3
2	D	337	LYS	2.2
1	C	51	GLN	2.2
2	D	417	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	204	LYS	2.2
2	B	175	VAL	2.1
2	D	342	LEU	2.1
2	D	173	PHE	2.1
2	D	264	ALA	2.1
2	D	419	VAL	2.1
2	B	207	LEU	2.1
2	B	345	ALA	2.1
2	B	413	ASP	2.1
2	D	418	VAL	2.1
2	B	153	GLN	2.0
2	B	343	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	PYV	C	900	22/22	0.87	0.18	2.46	31,43,44,44	0
4	MG	D	999	1/1	0.55	0.26	2.44	64,64,64,64	0
3	PYV	A	900	22/22	0.89	0.19	1.52	25,43,46,49	0
4	MG	B	998	1/1	0.94	0.21	1.32	52,52,52,52	0
4	MG	D	998	1/1	0.99	0.08	-2.09	34,34,34,34	0
4	MG	B	999	1/1	0.98	0.07	-2.11	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.