Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:55 am BST

PDB ID	:	4I6M
Title	:	Structure of Arp7-Arp9-Snf2(HSA)-RTT102 subcomplex of SWI/SNF chromatin remodeler.
Authors	:	Schubert, H.L.; Cairns, B.R.; Hill, C.P.
Deposited on	:	2012-11-29
Resolution	:	2.80 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 following versions of software and data (see references ①) were used in the production of this report:

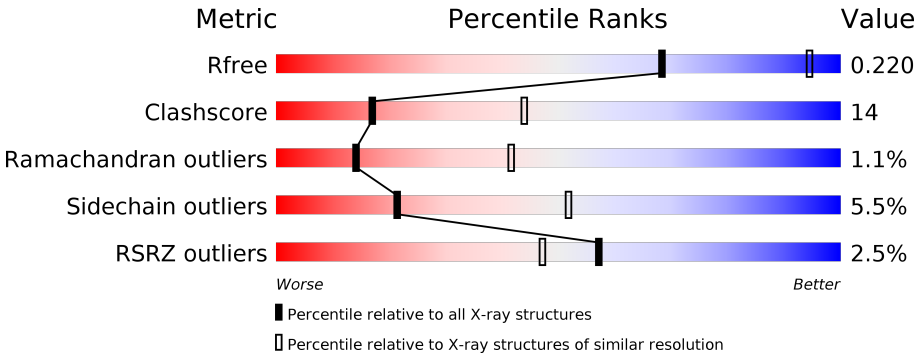
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 <=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	477	2% 55% 26% • 16%
2	B	439	2% 65% 24% • 10%
3	C	106	3% 46% 16% • 35%
4	D	157	% 20% 13% • 66%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7660 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 Actin-related protein 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	399	3227	2081	528	603	4	11	0	3	0

- Molecule 2 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	396	3198	2053	523	615	4	3	0	1	0

- Molecule 3 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
3	C	69	594	365	127	101	1	0	2	0

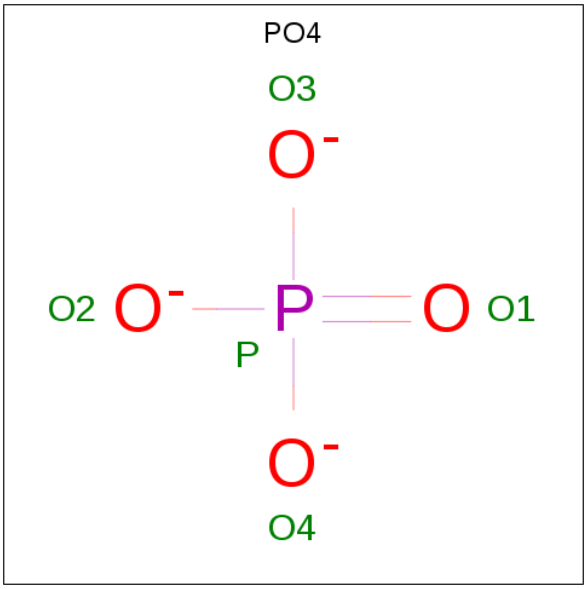
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	562	MSE	-	EXPRESSION TAG	UNP P22082
C	563	GLY	-	EXPRESSION TAG	UNP P22082
C	564	HIS	-	EXPRESSION TAG	UNP P22082
C	565	HIS	-	EXPRESSION TAG	UNP P22082
C	566	HIS	-	EXPRESSION TAG	UNP P22082
C	567	HIS	-	EXPRESSION TAG	UNP P22082
C	568	HIS	-	EXPRESSION TAG	UNP P22082
C	569	HIS	-	EXPRESSION TAG	UNP P22082
C	570	HIS	-	EXPRESSION TAG	UNP P22082
C	571	HIS	-	EXPRESSION TAG	UNP P22082
C	572	HIS	-	EXPRESSION TAG	UNP P22082
C	573	HIS	-	EXPRESSION TAG	UNP P22082
C	574	GLY	-	EXPRESSION TAG	UNP P22082

- Molecule 4 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	54	Total	C	N	O	Se	0	0	0
			490	313	84	92	1			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	O	P		0	0
			5	4	1			
5	A	1	Total	O	P		0	0
			5	4	1			
5	A	1	Total	O	P		0	0
			5	4	1			
5	A	1	Total	O	P		0	0
			5	4	1			
5	A	1	Total	O	P		0	0
			5	4	1			
5	A	1	Total	O	P		0	0
			5	4	1			
5	B	1	Total	O	P		0	0
			5	4	1			
5	B	1	Total	O	P		0	0
			5	4	1			
5	B	1	Total	O	P		0	0
			5	4	1			
5	B	1	Total	O	P		0	0
			5	4	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

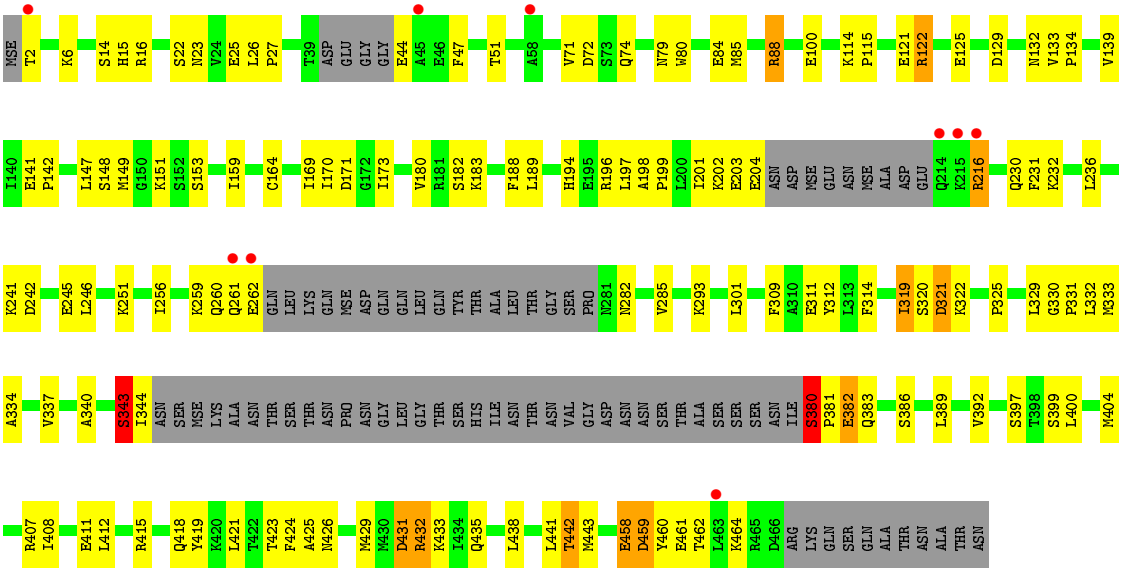
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	33	Total O 33 33	0	0
6	B	51	Total O 51 51	0	0
6	C	5	Total O 5 5	0	0
6	D	2	Total O 2 2	0	0

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 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.

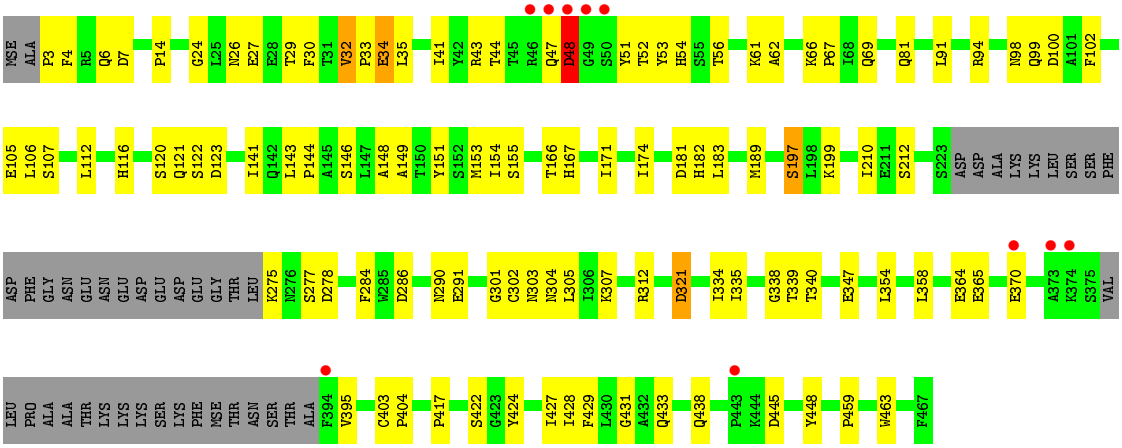
- Molecule 1: Actin-related protein 7

Chain A:



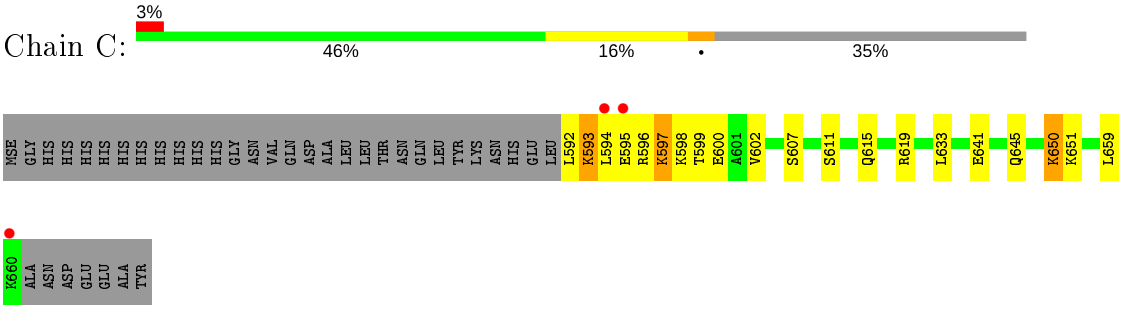
- Molecule 2: Actin-like protein ARP9

Chain B:



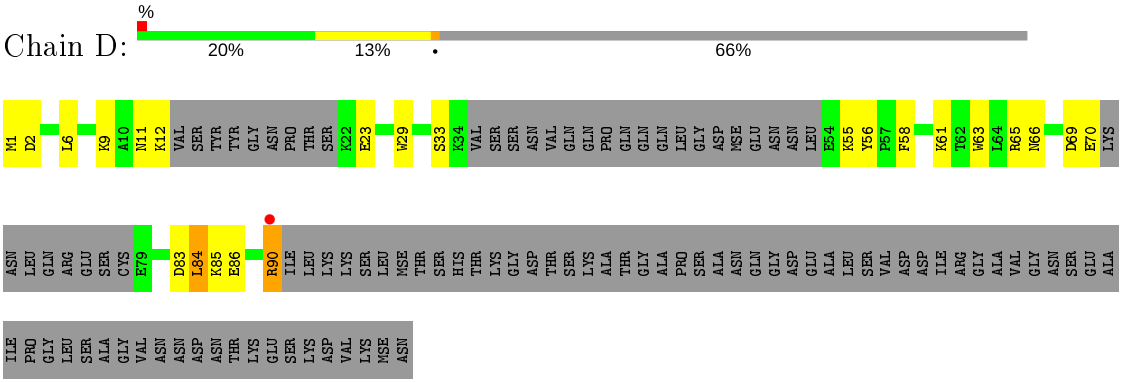
• Molecule 3: Actin-like protein ARP9

Chain C:



• Molecule 4: Regulator of Ty1 transposition protein 102

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.37Å 104.14Å 81.32Å 90.00° 93.78° 90.00°	Depositor
Resolution (Å)	29.90 – 2.80 29.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.90-2.80) 98.1 (29.96-2.80)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.184 , 0.223 0.180 , 0.220	Depositor DCC
R_{free} test set	2288 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7660	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.333 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: PO4

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	0.44	0/3292	0.61	1/4432 (0.0%)
2	B	0.45	0/3266	0.59	0/4423
3	C	0.44	0/602	0.58	0/790
4	D	0.41	0/501	0.57	0/669
All	All	0.44	0/7661	0.59	1/10314 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	380	SER	C-N-CD	5.94	140.88	128.40

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	3227	0	3251	114	1
2	B	3198	0	3187	72	1
3	C	594	0	652	13	0
4	D	490	0	467	22	0
5	A	30	0	0	0	0
5	B	30	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	33	0	0	3	0
6	B	51	0	0	4	0
6	C	5	0	0	0	0
6	D	2	0	0	0	0
All	All	7660	0	7557	212	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 14.

All (212) 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:216:ARG:HG2	1:A:216:ARG:HH11	1.17	1.08
1:A:343:SER:CB	1:A:344:ILE:HA	1.81	1.07
1:A:343:SER:HB3	1:A:344:ILE:HA	1.09	1.06
3:C:592:LEU:HD11	3:C:594:LEU:HD12	1.37	1.06
1:A:114:LYS:HG3	1:A:115:PRO:HD3	1.37	1.05
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.25	1.00
1:A:25:GLU:O	3:C:619:ARG:NH2	1.96	0.98
1:A:343:SER:HB3	1:A:344:ILE:CA	1.95	0.96
3:C:592:LEU:HD12	3:C:594:LEU:H	1.32	0.92
1:A:84:GLU:OE2	1:A:88:ARG:NH1	2.05	0.89
2:B:303:ASN:HD21	2:B:307:LYS:HZ1	1.24	0.82
2:B:459:PRO:HG2	4:D:63:TRP:CD2	2.18	0.79
1:A:159:ILE:HD11	1:A:408:ILE:HD11	1.65	0.78
1:A:216:ARG:NH1	1:A:216:ARG:HG2	1.94	0.77
1:A:114:LYS:HG3	1:A:115:PRO:CD	2.14	0.76
2:B:303:ASN:HD21	2:B:307:LYS:NZ	1.85	0.74
1:A:100:GLU:HG2	1:A:132:ASN:HB3	1.68	0.74
1:A:122:ARG:HH11	1:A:122:ARG:CG	1.99	0.73
5:B:504:PO4:O2	6:B:627:HOH:O	2.06	0.73
2:B:14:PRO:O	2:B:116[B]:HIS:HE1	1.72	0.72
4:D:84:LEU:O	4:D:85:LYS:HB2	1.89	0.72
4:D:1:MSE:HG2	4:D:2:ASP:N	2.06	0.71
1:A:51:THR:HB	6:A:633:HOH:O	1.91	0.70
1:A:14:SER:HA	1:A:71:VAL:HB	1.74	0.69
2:B:98:ASN:O	2:B:99:GLN:HG2	1.93	0.69
1:A:183:LYS:HG2	1:A:183:LYS:O	1.91	0.68
1:A:344:ILE:O	1:A:344:ILE:HG23	1.92	0.68
1:A:392:VAL:HB	1:A:423:THR:HG22	1.75	0.68
1:A:139:VAL:HG11	1:A:443:MSE:HG3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:LYS:HB3	2:B:278:ASP:OD2	1.94	0.67
2:B:107:SER:O	4:D:11:ASN:HA	1.95	0.67
1:A:311:GLU:OE2	1:A:407:ARG:NH2	2.28	0.67
1:A:458:GLU:HG2	1:A:459:ASP:N	2.10	0.66
2:B:303:ASN:ND2	2:B:307:LYS:NZ	2.43	0.66
1:A:180:VAL:HG11	1:A:332:LEU:HG	1.78	0.66
1:A:148:SER:HB2	1:A:442:THR:HG21	1.79	0.64
1:A:153:SER:HA	1:A:169:ILE:O	1.99	0.62
1:A:121:GLU:O	1:A:125:GLU:HG3	1.98	0.62
1:A:382:GLU:H	1:A:382:GLU:CD	2.03	0.62
1:A:216:ARG:CG	1:A:216:ARG:HH11	2.04	0.62
1:A:343:SER:CB	1:A:344:ILE:CA	2.66	0.62
2:B:47:GLN:O	2:B:48:ASP:HB3	1.99	0.62
2:B:14:PRO:O	2:B:116[B]:HIS:CE1	2.53	0.61
1:A:429:MSE:HE3	2:B:321:ASP:O	2.01	0.61
1:A:203:GLU:O	1:A:204:GLU:HB2	2.00	0.60
2:B:189:MSE:HE2	2:B:305:LEU:HA	1.82	0.60
1:A:389:LEU:HB3	1:A:421:LEU:HD23	1.84	0.60
1:A:256:ILE:O	1:A:260:GLN:HB2	2.01	0.60
1:A:330:GLY:HA2	1:A:333:MSE:HE2	1.83	0.60
2:B:53:TYR:CD1	2:B:81:GLN:HG3	2.37	0.60
2:B:44:THR:OG1	2:B:62:ALA:HB2	2.02	0.60
1:A:400:LEU:HD12	1:A:433:LYS:HE2	1.84	0.59
2:B:35:LEU:HD11	4:D:84:LEU:HD13	1.84	0.59
2:B:141:ILE:HG12	2:B:448:TYR:HB3	1.85	0.59
2:B:199:LYS:HD2	2:B:210:ILE:HD13	1.85	0.58
4:D:29:TRP:CD2	4:D:61:LYS:HD3	2.38	0.58
1:A:380:SER:O	1:A:383:GLN:HB2	2.03	0.58
1:A:159:ILE:HG23	1:A:164:CYS:SG	2.44	0.58
1:A:418:GLN:HG3	1:A:418:GLN:O	2.03	0.58
1:A:334:ALA:HB2	1:A:415:ARG:HD3	1.86	0.57
1:A:44:GLU:HG2	1:A:44:GLU:O	2.04	0.57
2:B:182:HIS:HE1	6:B:628:HOH:O	1.85	0.57
1:A:381:PRO:HG2	1:A:382:GLU:OE2	2.04	0.57
1:A:72:ASP:OD1	1:A:74:GLN:HB2	2.05	0.57
1:A:122:ARG:NH1	1:A:122:ARG:HG2	2.06	0.57
1:A:216:ARG:HA	1:A:216:ARG:NE	2.20	0.56
1:A:194:HIS:NE2	1:A:203:GLU:OE1	2.39	0.56
1:A:241:LYS:NZ	1:A:245:GLU:HB3	2.19	0.56
3:C:593:LYS:O	3:C:597:LYS:HG2	2.05	0.56
1:A:426:ASN:HB3	1:A:432:ARG:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:CD2	1:A:443:MSE:SE	3.04	0.55
1:A:16[A]:ARG:NH2	6:A:627:HOH:O	2.40	0.55
1:A:333:MSE:HE3	1:A:412:LEU:HD13	1.87	0.55
1:A:26:LEU:HB3	1:A:27:PRO:HD2	1.88	0.55
4:D:69:ASP:O	4:D:70:GLU:HG3	2.07	0.54
1:A:196:ARG:NH2	1:A:312:TYR:OH	2.39	0.54
1:A:438:LEU:O	1:A:442:THR:HG23	2.08	0.54
2:B:275:LYS:HE3	2:B:277:SER:H	1.73	0.54
2:B:43:ARG:HG3	2:B:53:TYR:CE2	2.42	0.54
1:A:381:PRO:C	1:A:383:GLN:H	2.11	0.53
2:B:43:ARG:HD3	2:B:51:TYR:CD1	2.43	0.53
4:D:1:MSE:HG2	4:D:2:ASP:H	1.72	0.53
1:A:261:GLN:HB2	1:A:262:GLU:OE1	2.09	0.52
1:A:147:LEU:HD22	1:A:443:MSE:SE	2.59	0.52
1:A:80:TRP:NE1	1:A:122:ARG:HD3	2.25	0.52
2:B:34:GLU:H	2:B:34:GLU:CD	2.13	0.52
1:A:197:LEU:HD11	1:A:231:PHE:CZ	2.45	0.52
1:A:399:SER:OG	1:A:432:ARG:NH1	2.42	0.52
2:B:32:VAL:HG23	2:B:33:PRO:HD2	1.92	0.52
3:C:595:GLU:O	3:C:599:THR:HG23	2.11	0.52
1:A:399:SER:HA	1:A:404:MSE:HG2	1.92	0.51
3:C:641:GLU:O	3:C:645:GLN:HG3	2.10	0.51
2:B:189:MSE:HE2	2:B:305:LEU:CA	2.41	0.51
1:A:201:ILE:O	1:A:202:LYS:HB2	2.11	0.51
1:A:133:VAL:HG13	1:A:134:PRO:HD2	1.91	0.51
4:D:85:LYS:O	4:D:90:ARG:NH1	2.44	0.51
1:A:418:GLN:HG2	1:A:419:TYR:CE1	2.46	0.51
1:A:6:LYS:HE3	2:B:121:GLN:OE1	2.09	0.51
1:A:426:ASN:O	1:A:432:ARG:NE	2.35	0.51
1:A:418:GLN:HB3	6:A:605:HOH:O	2.10	0.50
1:A:320:SER:OG	1:A:322:LYS:N	2.38	0.50
1:A:407:ARG:O	1:A:411:GLU:HB2	2.12	0.50
2:B:47:GLN:O	2:B:48:ASP:CB	2.59	0.50
1:A:22:SER:HA	1:A:441:LEU:CD1	2.42	0.50
2:B:335:ILE:HG22	2:B:340:THR:HG21	1.93	0.49
2:B:102:PHE:HZ	4:D:6:LEU:CD2	2.25	0.49
1:A:141:GLU:HB3	1:A:142:PRO:HD3	1.94	0.49
3:C:650:LYS:HE2	3:C:650:LYS:HA	1.94	0.49
1:A:122:ARG:NH1	1:A:122:ARG:CG	2.66	0.49
1:A:460:TYR:CZ	1:A:464:LYS:HE3	2.47	0.49
1:A:389:LEU:O	1:A:421:LEU:HA	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ILE:HD13	2:B:312:ARG:CG	2.42	0.49
3:C:592:LEU:CD1	3:C:594:LEU:HD12	2.26	0.48
1:A:458:GLU:O	1:A:461:GLU:N	2.47	0.48
2:B:286:ASP:HB3	2:B:290:ASN:H	1.79	0.48
1:A:241:LYS:O	1:A:242:ASP:C	2.52	0.48
1:A:15:HIS:ND1	1:A:16[B]:ARG:HG2	2.29	0.47
1:A:170:ILE:O	1:A:173:ILE:HG22	2.13	0.47
2:B:120:SER:HB2	2:B:123:ASP:H	1.78	0.47
2:B:370:GLU:HG3	2:B:395:VAL:HG21	1.97	0.47
2:B:151:TYR:CD1	3:C:633:LEU:HD12	2.50	0.47
2:B:364:GLU:HG2	2:B:365:GLU:N	2.29	0.47
2:B:417:PRO:HD2	6:B:633:HOH:O	2.15	0.47
2:B:148:ALA:O	2:B:431:GLY:HA3	2.14	0.47
1:A:259:LYS:O	1:A:259:LYS:HD2	2.14	0.47
2:B:26:ASN:O	2:B:27:GLU:HB2	2.15	0.47
2:B:286:ASP:HB2	2:B:290:ASN:HB2	1.95	0.47
1:A:216:ARG:CG	1:A:216:ARG:NH1	2.69	0.47
1:A:337:VAL:O	1:A:340:ALA:HB3	2.15	0.47
1:A:188:PHE:HZ	1:A:319:ILE:HD13	1.80	0.47
1:A:325:PRO:O	1:A:331:PRO:HG2	2.15	0.47
1:A:6:LYS:HD2	1:A:23:ASN:ND2	2.30	0.46
2:B:153:MSE:HG3	2:B:334:ILE:HD13	1.97	0.46
2:B:30:PHE:HB3	2:B:433:GLN:OE1	2.14	0.46
1:A:241:LYS:HZ2	1:A:245:GLU:HB3	1.80	0.46
2:B:3:PRO:HA	2:B:4:PHE:HA	1.67	0.46
1:A:183:LYS:O	1:A:183:LYS:CG	2.61	0.46
4:D:83:ASP:C	4:D:84:LEU:O	2.52	0.46
2:B:403:CYS:HB2	2:B:404:PRO:HA	1.97	0.46
2:B:66:LYS:HA	2:B:67:PRO:HD3	1.78	0.46
1:A:419:TYR:CD1	1:A:419:TYR:N	2.84	0.46
2:B:212:SER:HB3	2:B:284:PHE:HE2	1.81	0.45
4:D:9:LYS:HD2	4:D:12:LYS:HE2	1.97	0.45
2:B:424:TYR:CD1	2:B:427:ILE:HD12	2.51	0.45
4:D:33:SER:HB3	4:D:55:LYS:HD3	1.98	0.45
4:D:56:TYR:HB3	4:D:58:PHE:CE2	2.51	0.45
2:B:102:PHE:HZ	4:D:6:LEU:HD23	1.82	0.45
4:D:33:SER:HB3	4:D:55:LYS:CD	2.46	0.45
1:A:164:CYS:HB2	1:A:182:SER:HB3	1.98	0.45
1:A:236:LEU:HD22	1:A:309:PHE:CD2	2.51	0.45
2:B:121:GLN:HG2	2:B:463:TRP:CH2	2.52	0.45
2:B:146:SER:HB2	2:B:174:ILE:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:O	1:A:285:VAL:HG22	2.16	0.45
2:B:302:CYS:HB2	6:B:604:HOH:O	2.16	0.45
4:D:23:GLU:OE2	4:D:65:ARG:HD3	2.16	0.45
1:A:334:ALA:CB	1:A:415:ARG:HD3	2.46	0.44
4:D:66:ASN:HB3	4:D:70:GLU:HB2	1.98	0.44
1:A:320:SER:OG	1:A:321:ASP:N	2.49	0.44
2:B:30:PHE:N	2:B:30:PHE:CD1	2.84	0.44
2:B:143:LEU:HD12	2:B:144:PRO:HD2	1.98	0.44
2:B:354:LEU:HD22	2:B:358:LEU:HD22	1.99	0.44
2:B:197:SER:HB3	2:B:301:GLY:HA2	1.99	0.44
2:B:286:ASP:CB	2:B:290:ASN:H	2.29	0.44
1:A:232:LYS:HA	1:A:236:LEU:HG	1.99	0.44
1:A:151:LYS:HE3	1:A:424:PHE:CE1	2.53	0.43
1:A:203:GLU:O	1:A:204:GLU:CB	2.66	0.43
1:A:381:PRO:HG2	1:A:382:GLU:CD	2.39	0.43
1:A:80:TRP:CE2	1:A:122:ARG:HD3	2.53	0.43
2:B:189:MSE:HG2	2:B:305:LEU:CD1	2.49	0.43
1:A:381:PRO:C	1:A:383:GLN:N	2.72	0.43
4:D:84:LEU:O	4:D:85:LYS:CB	2.61	0.43
4:D:83:ASP:O	4:D:86:GLU:HG3	2.18	0.43
1:A:47:PHE:CD2	1:A:85:MSE:HE1	2.54	0.43
1:A:314:PHE:CZ	1:A:407:ARG:HG3	2.54	0.43
1:A:129:ASP:OD2	1:A:460:TYR:HE2	2.01	0.43
1:A:180:VAL:CG1	1:A:332:LEU:HG	2.48	0.43
1:A:458:GLU:O	1:A:459:ASP:C	2.57	0.43
4:D:9:LYS:HD2	4:D:12:LYS:NZ	2.34	0.43
1:A:153:SER:HG	1:A:171:ASP:H	1.66	0.42
2:B:189:MSE:HE1	2:B:304:ASN:OD1	2.18	0.42
2:B:6:GLN:O	2:B:24:GLY:HA2	2.19	0.42
3:C:598:LYS:O	3:C:602:VAL:HG23	2.18	0.42
3:C:594:LEU:O	3:C:595:GLU:C	2.55	0.42
1:A:381:PRO:O	1:A:383:GLN:N	2.53	0.42
2:B:286:ASP:HB2	2:B:290:ASN:O	2.18	0.42
2:B:112:LEU:HD12	2:B:141:ILE:HD12	2.02	0.42
1:A:198:ALA:N	1:A:199:PRO:HD2	2.34	0.42
1:A:431:ASP:O	1:A:435:GLN:HB2	2.19	0.42
2:B:91:LEU:CD2	2:B:106:LEU:HD22	2.50	0.42
2:B:312:ARG:HD3	2:B:312:ARG:HA	1.79	0.42
2:B:445:ASP:HA	2:B:448:TYR:CE1	2.55	0.42
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.84	0.41
2:B:183:LEU:HD23	2:B:183:LEU:HA	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:ASN:ND2	2:B:307:LYS:HZ2	2.18	0.41
2:B:26:ASN:HB3	2:B:29:THR:O	2.21	0.41
1:A:197:LEU:HD11	1:A:231:PHE:CE1	2.55	0.41
2:B:429:PHE:HE1	2:B:433:GLN:HE21	1.68	0.41
1:A:458:GLU:O	1:A:460:TYR:N	2.53	0.41
2:B:154:ILE:O	2:B:154:ILE:HG22	2.21	0.41
2:B:338:GLY:O	2:B:339:THR:C	2.59	0.41
2:B:166:THR:HG22	2:B:167:HIS:CE1	2.56	0.41
3:C:633:LEU:HA	3:C:633:LEU:HD23	1.82	0.41
1:A:149:MSE:HE1	1:A:425:ALA:CA	2.51	0.41
1:A:381:PRO:HG2	1:A:382:GLU:H	1.86	0.41
1:A:314:PHE:CE1	1:A:329:LEU:HD23	2.57	0.40
1:A:418:GLN:HG2	1:A:419:TYR:CD1	2.56	0.40
2:B:148:ALA:HB1	2:B:428:ILE:O	2.21	0.40
3:C:611:SER:O	3:C:615:GLN:HG3	2.21	0.40
1:A:389:LEU:HD22	1:A:421:LEU:CD2	2.52	0.40
2:B:146:SER:O	2:B:149:ALA:HB3	2.21	0.40
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.97	0.40
2:B:459:PRO:HG2	4:D:63:TRP:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLN:NE2	2:B:61:LYS:O[1_554]	2.03	0.17

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	392/477 (82%)	369 (94%)	18 (5%)	5 (1%)	12 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	391/439 (89%)	368 (94%)	21 (5%)	2 (0%)	29 61
3	C	69/106 (65%)	64 (93%)	3 (4%)	2 (3%)	4 15
4	D	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	6 22
All	All	898/1179 (76%)	844 (94%)	44 (5%)	10 (1%)	14 41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	48	ASP
3	C	596	ARG
1	A	343	SER
1	A	382	GLU
1	A	459	ASP
3	C	597	LYS
4	D	84	LEU
1	A	431	ASP
1	A	458	GLU
2	B	155	SER

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	357/404 (88%)	338 (95%)	19 (5%)	22 54
2	B	363/393 (92%)	343 (94%)	20 (6%)	21 52
3	C	63/91 (69%)	57 (90%)	6 (10%)	8 25
4	D	53/136 (39%)	52 (98%)	1 (2%)	57 85
All	All	836/1024 (82%)	790 (94%)	46 (6%)	21 52

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	79	ASN
1	A	88	ARG
1	A	122	ARG
1	A	216	ARG
1	A	230	GLN
1	A	246	LEU
1	A	251	LYS
1	A	293	LYS
1	A	301	LEU
1	A	319	ILE
1	A	321	ASP
1	A	343	SER
1	A	380	SER
1	A	386	SER
1	A	397	SER
1	A	432	ARG
1	A	442	THR
1	A	462	THR
2	B	7	ASP
2	B	32	VAL
2	B	34	GLU
2	B	41	ILE
2	B	48	ASP
2	B	52	THR
2	B	54	HIS
2	B	56	THR
2	B	69	GLN
2	B	94	ARG
2	B	100	ASP
2	B	105	GLU
2	B	122	SER
2	B	181	ASP
2	B	197	SER
2	B	291	GLU
2	B	321	ASP
2	B	347	GLU
2	B	422	SER
2	B	438	GLN
3	C	593	LYS
3	C	600	GLU
3	C	607	SER
3	C	650	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	651	LYS
3	C	659	LEU
4	D	90	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	303	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	$\#\|Z\| > 2$
5	PO4	B	501	-	4,4,4	1.00	0	6,6,6	0.61	0
5	PO4	B	506	-	4,4,4	0.87	0	6,6,6	0.52	0
5	PO4	B	502	-	4,4,4	0.88	0	6,6,6	0.40	0
5	PO4	A	502	-	4,4,4	0.81	0	6,6,6	0.44	0
5	PO4	A	505	-	4,4,4	0.84	0	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PO4	B	505	-	4,4,4	0.88	0	6,6,6	0.42	0
5	PO4	A	501	-	4,4,4	0.89	0	6,6,6	0.64	0
5	PO4	B	504	-	4,4,4	0.85	0	6,6,6	0.50	0
5	PO4	A	506	-	4,4,4	0.88	0	6,6,6	0.44	0
5	PO4	B	503	-	4,4,4	0.84	0	6,6,6	0.56	0
5	PO4	A	503	-	4,4,4	0.89	0	6,6,6	0.51	0
5	PO4	A	504	-	4,4,4	0.79	0	6,6,6	0.80	0

There are no bond length outliers.

There are no bond angle outliers.

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
5	B	504	PO4	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^{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	388/477 (81%)	-0.19	9 (2%) 60 51	36, 65, 110, 152	0
2	B	393/439 (89%)	-0.25	10 (2%) 57 47	31, 56, 115, 171	0
3	C	68/106 (64%)	0.03	3 (4%) 34 24	42, 66, 112, 127	0
4	D	53/157 (33%)	-0.09	1 (1%) 66 59	49, 82, 119, 164	0
All	All	902/1179 (76%)	-0.19	23 (2%) 57 47	31, 62, 114, 171	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	ASP	3.5
3	C	594	LEU	3.4
2	B	394	PHE	3.3
2	B	47	GLN	3.2
2	B	50	SER	3.2
2	B	49	GLY	3.1
1	A	214	GLN	3.1
2	B	374	LYS	3.0
3	C	660	LYS	3.0
1	A	58	ALA	2.8
2	B	373	ALA	2.8
4	D	90	ARG	2.5
1	A	215	LYS	2.5
1	A	262	GLU	2.3
1	A	261	GLN	2.3
1	A	45	ALA	2.3
1	A	463	LEU	2.2
1	A	216	ARG	2.2
1	A	2	THR	2.2
2	B	370	GLU	2.2
2	B	46	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	595	GLU	2.1
2	B	443	PRO	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. 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	B-factors(Å^2)	Q<0.9
5	PO4	B	503	5/5	0.81	0.14	145,147,148,149	0
5	PO4	B	505	5/5	0.82	0.18	153,154,156,160	0
5	PO4	B	504	5/5	0.84	0.29	153,154,155,156	0
5	PO4	B	502	5/5	0.88	0.20	125,126,127,127	0
5	PO4	A	504	5/5	0.88	0.18	121,121,123,123	0
5	PO4	A	506	5/5	0.92	0.44	148,148,151,151	0
5	PO4	B	506	5/5	0.92	0.24	152,152,153,154	0
5	PO4	A	505	5/5	0.92	0.34	135,136,138,139	0
5	PO4	A	502	5/5	0.95	0.15	91,95,97,98	0
5	PO4	A	503	5/5	0.98	0.17	86,89,92,94	0
5	PO4	A	501	5/5	0.98	0.17	63,69,72,72	0
5	PO4	B	501	5/5	0.99	0.12	64,68,73,78	0

6.5 Other polymers (i)

There are no such residues in this entry.