Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:39 PM GMT

PDB ID	:	4CZY
Title	:	Complex of Neurospora crassa PAN2 (WD40-CS1) with PAN3 (pseudokinase and C-term)
Authors	:	Jonas, S.; Izaurralde, E.; Weichenrieder, O.
Deposited on	:	2014-04-22
Resolution	:	3.40 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 ⓘ symbol.

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

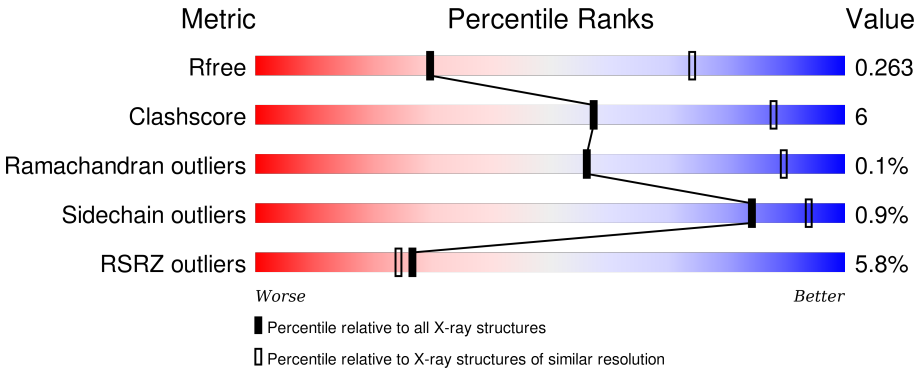
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	354	10% 82% 9% 9%
1	C	354	8% 80% 11% 9%
2	B	429	3% 74% 20% 6%
2	D	429	2% 76% 17% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11650 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 PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2516	1600	441	460	15			
1	C	323	Total	C	N	O	S	0	0	0
			2529	1609	444	461	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	EXPRESSION TAG	UNP P0C581
A	-1	HIS	-	EXPRESSION TAG	UNP P0C581
A	0	MET	-	EXPRESSION TAG	UNP P0C581
C	-2	PRO	-	EXPRESSION TAG	UNP P0C581
C	-1	HIS	-	EXPRESSION TAG	UNP P0C581
C	0	MET	-	EXPRESSION TAG	UNP P0C581

- Molecule 2 is a protein called PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3262	2073	580	598	11			
2	D	403	Total	C	N	O	S	0	0	0
			3255	2072	577	595	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	228	GLY	-	EXPRESSION TAG	UNP Q7SDP4
B	229	PRO	-	EXPRESSION TAG	UNP Q7SDP4
B	230	HIS	-	EXPRESSION TAG	UNP Q7SDP4
B	231	MET	-	EXPRESSION TAG	UNP Q7SDP4

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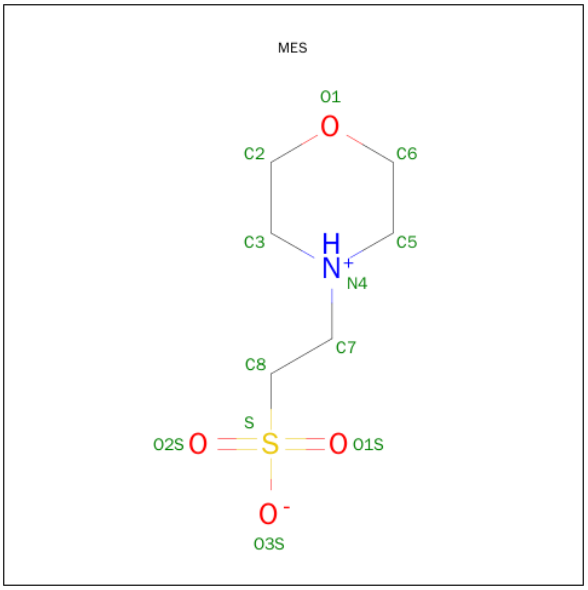
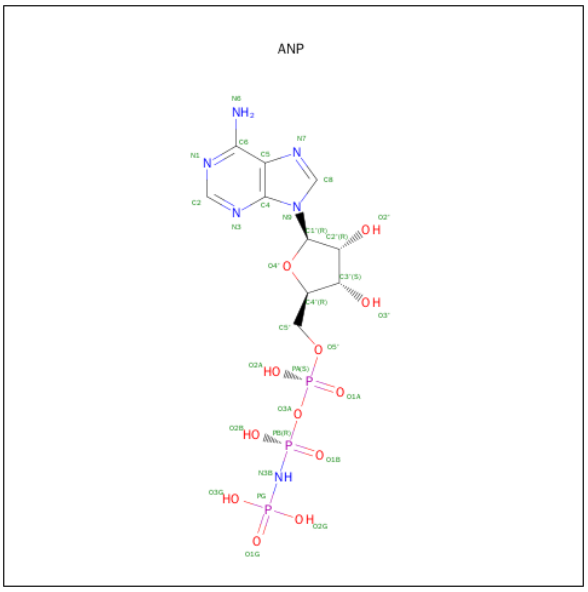
Chain	Residue	Modelled	Actual	Comment	Reference
B	232	LEU	-	EXPRESSION TAG	UNP Q7SDP4
B	233	GLU	-	EXPRESSION TAG	UNP Q7SDP4
D	228	GLY	-	EXPRESSION TAG	UNP Q7SDP4
D	229	PRO	-	EXPRESSION TAG	UNP Q7SDP4
D	230	HIS	-	EXPRESSION TAG	UNP Q7SDP4
D	231	MET	-	EXPRESSION TAG	UNP Q7SDP4
D	232	LEU	-	EXPRESSION TAG	UNP Q7SDP4
D	233	GLU	-	EXPRESSION TAG	UNP Q7SDP4

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

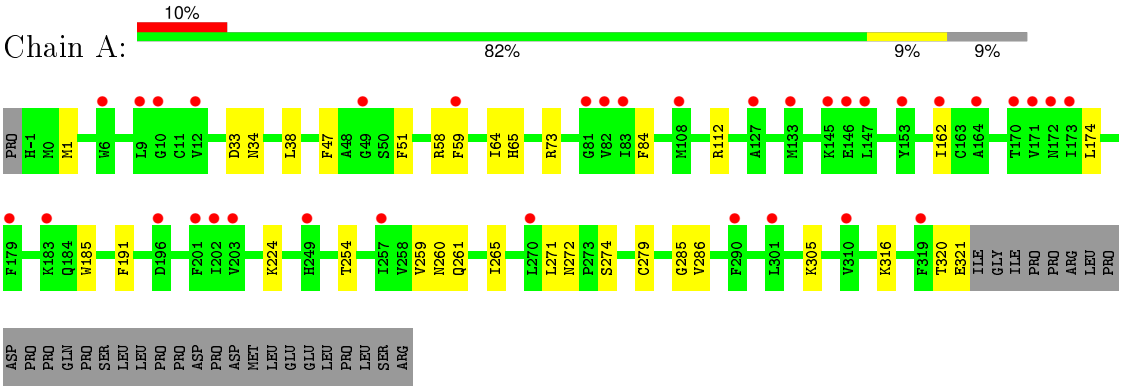
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

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.

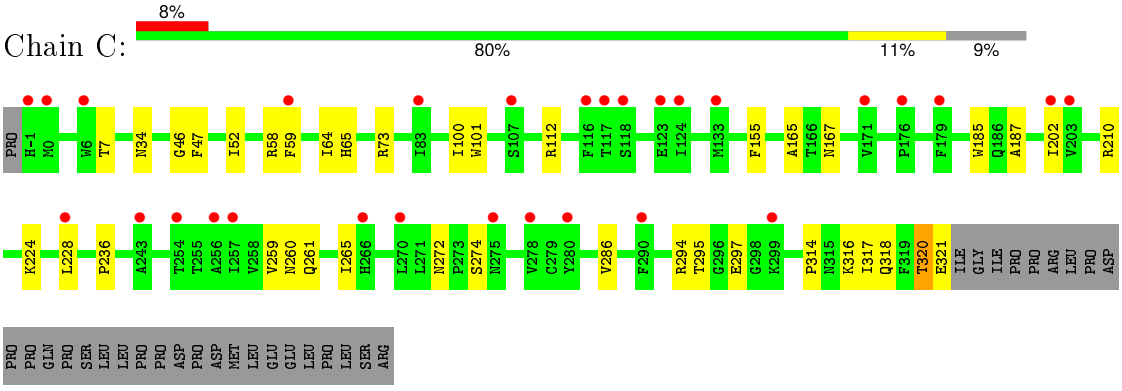
• Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN2

Chain A:



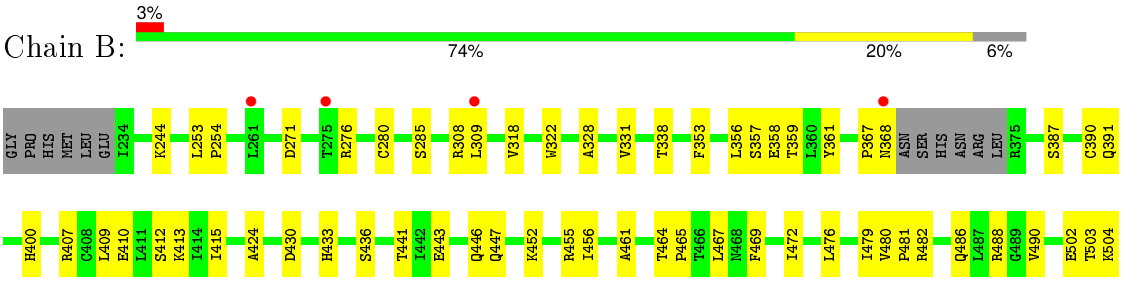
• Molecule 1: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN2

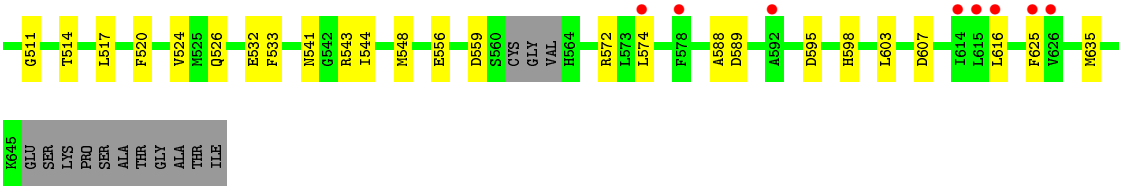
Chain C:



• Molecule 2: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3

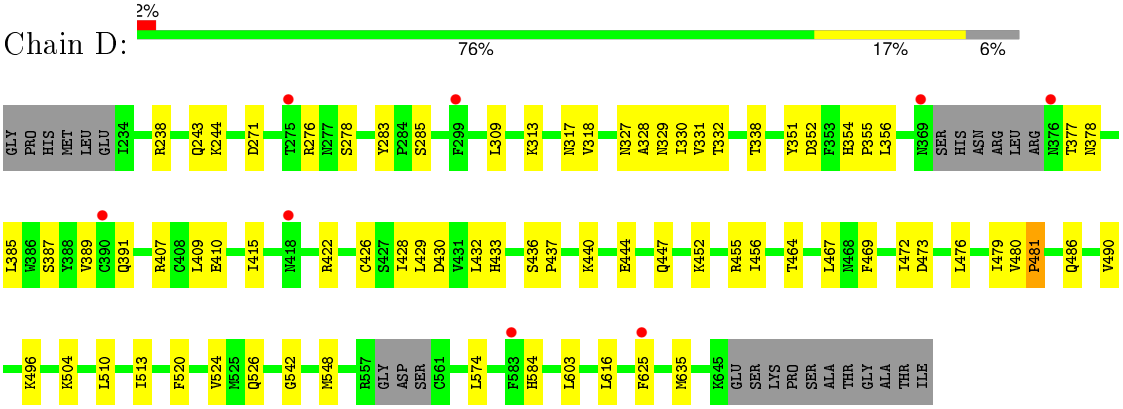
Chain B:





• Molecule 2: PAB-DEPENDENT POLY(A)-SPECIFIC RIBONUCLEASE SUBUNIT PAN3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.27Å 139.98Å 157.44Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	48.74 – 3.40 48.74 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.74-3.40) 99.0 (48.74-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE 1.8.4_1496)	Depositor
R, R_{free}	0.221 , 0.263 0.223 , 0.263	Depositor DCC
R_{free} test set	1669 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	106.6	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 77.9	EDS
Estimated twinning fraction	0.084 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 33303 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11650	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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, ANP, MES

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	0.24	0/2582	0.50	0/3512
1	C	0.25	0/2596	0.51	0/3530
2	B	0.26	0/3332	0.48	0/4512
2	D	0.26	0/3325	0.48	0/4504
All	All	0.25	0/11835	0.49	0/16058

There are no bond length outliers.

There are no bond angle outliers.

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	2516	0	2461	16	0
1	C	2529	0	2479	23	0
2	B	3262	0	3233	58	0
2	D	3255	0	3226	48	0
3	A	12	0	12	1	0
3	C	12	0	12	1	0
4	B	31	0	13	7	0
4	D	31	0	13	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
All	All	11650	0	11449	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (139) 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)
4:B:1650:ANP:H5'2	4:B:1650:ANP:H8	1.51	0.90
2:B:359:THR:HG23	4:B:1650:ANP:H3'	1.56	0.87
4:B:1650:ANP:C8	4:B:1650:ANP:H5'2	2.08	0.83
2:B:559:ASP:H	2:B:572:ARG:HH12	1.27	0.81
2:B:532:GLU:OE1	2:D:238:ARG:NH2	2.18	0.76
2:B:357:SER:O	4:B:1650:ANP:O2'	2.05	0.75
4:B:1650:ANP:C5'	4:B:1650:ANP:H8	2.23	0.68
2:D:377:THR:HG22	2:D:378:ASN:H	1.58	0.68
2:D:469:PHE:HA	2:D:472:ILE:HG23	1.78	0.65
2:B:556:GLU:HB2	2:D:584:HIS:NE2	2.13	0.63
2:B:574:LEU:HB3	2:B:635:MET:HE1	1.81	0.63
2:B:544:ILE:HD12	2:B:603:LEU:HB3	1.80	0.62
1:C:259:VAL:HG22	1:C:265:ILE:HG12	1.84	0.60
1:A:185:TRP:CZ2	1:A:224:LYS:HB3	2.37	0.59
2:D:473:ASP:OD1	2:D:496:LYS:NZ	2.32	0.59
2:B:461:ALA:O	2:B:482:ARG:NH2	2.29	0.57
2:B:452:LYS:O	2:B:456:ILE:HG13	2.06	0.56
2:B:328:ALA:HB2	2:D:526:GLN:HG3	1.88	0.55
2:B:253:LEU:HD12	2:B:254:PRO:HD2	1.87	0.55
2:B:447:GLN:HE22	2:B:504:LYS:H	1.56	0.54
2:B:556:GLU:HB2	2:D:584:HIS:CE1	2.43	0.54
2:B:520:PHE:O	2:B:524:VAL:HG23	2.07	0.54
2:D:574:LEU:HB3	2:D:635:MET:HE1	1.89	0.53
2:B:308:ARG:HD2	2:B:308:ARG:O	2.08	0.53
1:C:202:ILE:HG13	1:C:228:LEU:HG	1.90	0.53
2:D:616:LEU:HB2	2:D:625:PHE:HB2	1.90	0.53
2:B:400:HIS:CD2	2:B:446:GLN:HG2	2.44	0.52
2:B:616:LEU:HB2	2:B:625:PHE:HB2	1.90	0.52
2:B:353:PHE:CD1	4:B:1650:ANP:H2	2.44	0.52
1:A:1:MET:HG3	1:A:279:CYS:HB3	1.91	0.52
2:D:276:ARG:NH1	2:D:285:SER:O	2.42	0.52
2:B:548:MET:HB3	2:D:548:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:SER:O	2:D:391:GLN:HG3	2.11	0.51
2:D:407:ARG:NH1	2:D:430:ASP:OD2	2.43	0.51
2:B:543:ARG:CZ	2:D:243:GLN:HE22	2.25	0.50
1:C:297:GLU:HB3	1:C:317:ILE:HB	1.93	0.50
1:A:162:ILE:HB	1:A:174:LEU:HB2	1.92	0.49
2:D:447:GLN:HE22	2:D:504:LYS:H	1.59	0.49
2:B:441:THR:HG22	2:B:443:GLU:H	1.77	0.49
1:C:7:THR:HG21	1:C:314:PRO:HG3	1.94	0.49
2:D:351:TYR:OH	2:D:426:CYS:O	2.26	0.49
2:B:541:ASN:HD22	2:D:542:GLY:HA2	1.77	0.49
2:B:464:THR:OG1	2:B:464:THR:O	2.23	0.49
2:B:415:ILE:HG12	2:B:424:ALA:HB2	1.94	0.48
2:B:480:VAL:HG12	2:B:481:PRO:HD3	1.96	0.48
2:B:479:ILE:HD11	2:B:488:ARG:HG3	1.95	0.48
1:C:73:ARG:HD2	1:C:112:ARG:HA	1.95	0.48
2:D:313:LYS:O	2:D:317:ASN:HB2	2.14	0.48
2:D:377:THR:O	2:D:378:ASN:HB2	2.14	0.48
2:D:329:ASN:HA	2:D:422:ARG:HG2	1.95	0.48
1:C:46:GLY:O	1:C:64:ILE:HG13	2.14	0.48
1:C:34:ASN:HB3	1:C:294:ARG:CZ	2.43	0.48
1:C:187:ALA:O	1:C:224:LYS:HG3	2.13	0.48
1:A:73:ARG:HD2	1:A:112:ARG:HA	1.96	0.48
1:A:261:GLN:HB3	1:A:286:VAL:HG13	1.96	0.47
1:C:185:TRP:CZ2	1:C:224:LYS:HB3	2.49	0.47
1:A:58:ARG:HG2	1:A:59:PHE:N	2.30	0.47
2:B:433:HIS:HA	2:B:436:SER:HB2	1.97	0.47
2:D:510:LEU:HD23	2:D:513:ILE:HD11	1.96	0.47
2:D:520:PHE:O	2:D:524:VAL:HG23	2.15	0.47
1:C:167:ASN:HB2	1:C:210:ARG:NH2	2.30	0.47
1:C:228:LEU:HD23	1:C:228:LEU:HA	1.79	0.46
1:A:320:THR:HG22	1:A:321:GLU:H	1.80	0.46
2:B:387:SER:O	2:B:391:GLN:HG3	2.15	0.46
1:C:261:GLN:HB3	1:C:286:VAL:HG13	1.97	0.46
2:D:436:SER:OG	2:D:437:PRO:HD2	2.15	0.46
2:D:486:GLN:O	2:D:490:VAL:HG23	2.15	0.46
2:B:447:GLN:OE1	2:B:504:LYS:HB2	2.16	0.46
1:C:34:ASN:O	1:C:320:THR:HG21	2.16	0.46
2:B:407:ARG:NH1	2:B:430:ASP:OD2	2.49	0.46
2:B:390:CYS:SG	2:B:517:LEU:HD23	2.56	0.46
1:C:272:ASN:ND2	1:C:274:SER:OG	2.49	0.46
2:D:318:VAL:HG11	2:D:430:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:HH12	3:C:1330:MES:H82	1.81	0.45
2:B:309:LEU:HB2	2:B:338:THR:HG21	1.98	0.45
2:D:548:MET:SD	2:D:603:LEU:HD11	2.56	0.45
2:D:433:HIS:HA	2:D:436:SER:HB2	1.98	0.45
2:B:588:ALA:O	2:B:589:ASP:HB2	2.16	0.45
1:A:272:ASN:ND2	1:A:274:SER:OG	2.48	0.45
2:D:476:LEU:O	2:D:479:ILE:HG12	2.17	0.45
1:A:259:VAL:HG22	1:A:265:ILE:HG12	1.99	0.45
2:B:276:ARG:HD3	2:B:285:SER:O	2.17	0.45
1:C:7:THR:CG2	1:C:314:PRO:HG3	2.47	0.45
2:D:409:LEU:O	2:D:456:ILE:HD11	2.16	0.45
2:B:318:VAL:HG12	2:B:322:TRP:HD1	1.82	0.45
1:A:51:PHE:CD2	1:A:58:ARG:HA	2.52	0.44
1:A:34:ASN:O	1:A:320:THR:HG21	2.17	0.44
2:D:309:LEU:HD22	2:D:338:THR:HG21	2.00	0.44
1:A:285:GLY:HA3	1:A:305:LYS:HG2	1.99	0.44
1:A:33:ASP:HB2	1:A:38:LEU:HB2	1.98	0.44
2:D:385:LEU:O	2:D:389:VAL:HG23	2.18	0.44
2:D:407:ARG:HD3	2:D:429:LEU:HB2	1.99	0.44
2:B:556:GLU:HB2	2:D:584:HIS:HE2	1.83	0.44
2:D:327:ASN:HB3	2:D:330:ILE:HB	2.00	0.43
1:C:320:THR:HG22	1:C:321:GLU:H	1.81	0.43
1:C:58:ARG:HG2	1:C:59:PHE:N	2.32	0.43
2:D:464:THR:OG1	2:D:464:THR:O	2.23	0.43
2:B:476:LEU:O	2:B:479:ILE:HG12	2.18	0.43
2:B:467:LEU:HD12	2:B:467:LEU:HA	1.81	0.43
2:D:410:GLU:OE2	2:D:455:ARG:NH1	2.52	0.43
2:B:280:CYS:SG	2:B:410:GLU:HG3	2.59	0.43
2:B:469:PHE:HA	2:B:472:ILE:HG23	2.01	0.43
2:B:464:THR:HA	2:B:465:PRO:HD2	1.77	0.43
2:B:412:SER:O	2:B:413:LYS:NZ	2.52	0.43
2:B:410:GLU:CD	2:B:455:ARG:HH22	2.22	0.43
2:B:502:GLU:O	2:B:503:THR:OG1	2.28	0.43
2:B:361:TYR:CE2	2:B:465:PRO:HB2	2.54	0.42
2:D:278:SER:OG	2:D:283:TYR:O	2.26	0.42
2:B:511:GLY:O	2:B:514:THR:HG23	2.20	0.42
1:C:155:PHE:HB2	1:C:165:ALA:HB3	2.01	0.42
2:D:331:VAL:HG21	2:D:415:ILE:HD11	2.00	0.42
2:B:309:LEU:HD12	2:B:309:LEU:HA	1.83	0.42
2:D:452:LYS:O	2:D:456:ILE:HG13	2.20	0.42
2:B:526:GLN:HG3	2:D:328:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:THR:HB	2:D:352:ASP:OD2	2.20	0.42
2:D:480:VAL:HG12	2:D:481:PRO:HD3	2.02	0.42
1:C:295:THR:OG1	1:C:318:GLN:O	2.29	0.41
2:D:244:LYS:HB2	2:D:356:LEU:HD11	2.02	0.41
2:B:244:LYS:HB2	2:B:356:LEU:HD11	2.02	0.41
2:D:428:ILE:O	2:D:432:LEU:HG	2.20	0.41
2:B:543:ARG:NH2	2:B:607:ASP:OD1	2.53	0.41
1:A:254:THR:HG21	1:A:271:LEU:HD11	2.01	0.41
2:B:409:LEU:O	2:B:456:ILE:HD11	2.21	0.41
2:B:407:ARG:HD2	2:B:430:ASP:CG	2.40	0.41
1:C:100:ILE:HG22	1:C:101:TRP:CD1	2.55	0.41
1:A:64:ILE:HG21	1:A:84:PHE:CG	2.56	0.41
2:B:595:ASP:HB3	2:B:598:HIS:HB3	2.03	0.41
2:B:358:GLU:HA	4:B:1650:ANP:O2'	2.21	0.40
2:D:447:GLN:OE1	2:D:504:LYS:HB2	2.22	0.40
2:B:356:LEU:HD23	2:B:356:LEU:HA	1.88	0.40
1:C:224:LYS:HD3	1:C:236:PRO:HB3	2.03	0.40
1:C:52:ILE:HG13	1:C:59:PHE:HB2	2.02	0.40
2:D:464:THR:OG1	2:D:467:LEU:HD13	2.21	0.40
2:B:331:VAL:HG21	2:B:415:ILE:HD11	2.03	0.40
2:D:440:LYS:HB3	2:D:444:GLU:OE2	2.21	0.40
2:B:367:PRO:O	2:B:368:ASN:HB2	2.21	0.40
2:B:486:GLN:O	2:B:490:VAL:HG23	2.22	0.40
1:A:191:PHE:CG	3:A:1330:MES:H32	2.56	0.40
2:D:354:HIS:HA	2:D:355:PRO:HD2	1.89	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	321/354 (91%)	311 (97%)	9 (3%)	1 (0%)	46 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	321/354 (91%)	310 (97%)	10 (3%)	1 (0%)	46 82
2	B	397/429 (92%)	381 (96%)	16 (4%)	0	100 100
2	D	397/429 (92%)	378 (95%)	19 (5%)	0	100 100
All	All	1436/1566 (92%)	1380 (96%)	54 (4%)	2 (0%)	56 89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	LYS
1	C	316	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	273/308 (89%)	270 (99%)	3 (1%)	80 92
1	C	275/308 (89%)	271 (98%)	4 (2%)	72 90
2	B	355/380 (93%)	353 (99%)	2 (1%)	90 96
2	D	353/380 (93%)	351 (99%)	2 (1%)	90 96
All	All	1256/1376 (91%)	1245 (99%)	11 (1%)	84 94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	PHE
1	A	65	HIS
1	A	260	ASN
2	B	271	ASP
2	B	533	PHE
1	C	47	PHE
1	C	65	HIS
1	C	260	ASN
1	C	320	THR

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Mol	Chain	Res	Type
2	D	271	ASP
2	D	481	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
2	B	354	HIS
2	B	363	HIS
2	B	433	HIS
2	B	470	ASN
2	B	541	ASN
1	C	23	HIS
1	C	264	GLN
2	D	243	GLN
2	D	298	HIS
2	D	354	HIS

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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	MES	A	1330	-	11,12,12	0.58	0	14,16,16	2.00	3 (21%)
4	ANP	B	1650	5	27,33,33	1.93	8 (29%)	30,52,52	2.19	8 (26%)
3	MES	C	1330	-	11,12,12	0.59	0	14,16,16	1.94	3 (21%)
4	ANP	D	1650	5	27,33,33	2.11	5 (18%)	30,52,52	2.19	8 (26%)

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	MES	A	1330	-	-	0/6/14/14	0/1/1/1
4	ANP	B	1650	5	-	1/12/38/38	0/3/3/3
3	MES	C	1330	-	-	0/6/14/14	0/1/1/1
4	ANP	D	1650	5	-	1/12/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1650	ANP	PG-O2G	-2.12	1.50	1.56
4	B	1650	ANP	PG-O3G	-2.07	1.50	1.56
4	B	1650	ANP	PB-O2B	-2.01	1.51	1.56
4	B	1650	ANP	C5-C4	2.75	1.46	1.40
4	D	1650	ANP	C5-C4	3.13	1.47	1.40
4	B	1650	ANP	PG-N3B	4.09	1.74	1.63
4	B	1650	ANP	PB-N3B	4.16	1.74	1.63
4	B	1650	ANP	PB-O1B	4.19	1.50	1.46
4	B	1650	ANP	PG-O1G	4.21	1.50	1.46
4	D	1650	ANP	PB-N3B	4.57	1.75	1.63
4	D	1650	ANP	PG-N3B	4.57	1.75	1.63
4	D	1650	ANP	PG-O1G	4.64	1.51	1.46
4	D	1650	ANP	PB-O1B	4.68	1.51	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1650	ANP	N3-C2-N1	-6.79	123.70	128.89
4	D	1650	ANP	N3-C2-N1	-6.69	123.78	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1650	ANP	O1G-PG-N3B	-4.71	104.68	111.90
4	B	1650	ANP	PA-O3A-PB	-4.61	117.22	132.67
4	B	1650	ANP	O1G-PG-N3B	-4.10	105.61	111.90
4	D	1650	ANP	PA-O3A-PB	-3.63	120.51	132.67
4	D	1650	ANP	C4-C5-N7	-3.14	106.59	109.48
4	B	1650	ANP	C4-C5-N7	-3.04	106.68	109.48
4	D	1650	ANP	C2'-C1'-N9	-3.03	109.67	114.29
4	B	1650	ANP	C2'-C1'-N9	-2.99	109.73	114.29
4	B	1650	ANP	O1B-PB-N3B	-2.52	108.03	111.90
4	D	1650	ANP	O1B-PB-N3B	-2.50	108.06	111.90
3	A	1330	MES	C6-C5-N4	-2.11	106.92	110.12
4	D	1650	ANP	O3G-PG-O2G	2.11	113.82	107.58
3	C	1330	MES	O1S-S-C8	2.25	108.83	106.91
4	B	1650	ANP	O3G-PG-O2G	2.36	114.57	107.58
3	C	1330	MES	O2S-S-C8	3.17	109.61	106.91
3	A	1330	MES	O2S-S-C8	3.62	109.99	106.91
4	D	1650	ANP	O2B-PB-O1B	4.05	118.46	110.00
4	B	1650	ANP	O2B-PB-O1B	4.30	118.97	110.00
3	A	1330	MES	C5-N4-C3	4.92	119.55	108.90
3	C	1330	MES	C5-N4-C3	4.95	119.62	108.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1650	ANP	O1B-PB-N3B-PG
4	D	1650	ANP	O1B-PB-N3B-PG

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1330	MES	1	0
4	B	1650	ANP	7	0
3	C	1330	MES	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	323/354 (91%)	0.56	35 (10%) 8 7	135, 163, 180, 197	0
1	C	323/354 (91%)	0.48	29 (8%) 12 11	131, 156, 182, 203	0
2	B	403/429 (93%)	0.35	12 (2%) 54 49	91, 122, 167, 191	0
2	D	403/429 (93%)	0.33	8 (1%) 68 62	91, 121, 167, 199	0
All	All	1452/1566 (92%)	0.42	84 (5%) 26 24	91, 147, 177, 203	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	ILE	5.2
1	C	299	LYS	4.4
1	A	202	ILE	4.4
1	C	280	TYR	4.1
2	B	616	LEU	4.1
1	A	183	LYS	4.1
1	A	172	ASN	4.0
1	A	9	LEU	4.0
1	A	145	LYS	3.9
1	A	201	PHE	3.9
2	D	275	THR	3.8
1	C	203	VAL	3.7
1	C	256	ALA	3.7
1	C	270	LEU	3.6
1	C	257	ILE	3.5
1	C	202	ILE	3.5
1	C	266	HIS	3.2
1	C	117	THR	3.2
1	A	127	ALA	3.2
1	C	6	TRP	3.1
1	A	133	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	626	VAL	3.0
2	B	625	PHE	3.0
1	A	171	VAL	2.9
1	A	310	VAL	2.9
1	A	81	GLY	2.8
2	B	614	ILE	2.8
1	C	176	PRO	2.8
2	B	275	THR	2.7
1	A	257	ILE	2.7
1	A	82	VAL	2.7
1	C	133	MET	2.7
2	D	418	ASN	2.7
1	C	123	GLU	2.6
1	A	12	VAL	2.6
2	B	615	LEU	2.6
1	C	83	ILE	2.6
1	C	179	PHE	2.6
2	B	261	LEU	2.6
1	A	196	ASP	2.5
2	B	309	LEU	2.5
2	D	583	PHE	2.5
1	A	153	TYR	2.4
1	C	118	SER	2.4
1	C	0	MET	2.4
1	A	170	THR	2.4
1	C	290	PHE	2.4
2	B	574	LEU	2.4
1	C	228	LEU	2.4
2	D	625	PHE	2.4
1	A	162	ILE	2.3
1	C	275	ASN	2.3
2	D	390	CYS	2.3
1	A	6	TRP	2.3
1	A	203	VAL	2.3
1	C	-1	HIS	2.3
1	C	59	PHE	2.3
1	C	278	VAL	2.3
1	A	146	GLU	2.3
1	C	171	VAL	2.3
1	A	147	LEU	2.2
1	A	83	ILE	2.2
1	A	301	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	116	PHE	2.2
2	D	376	ASN	2.2
1	A	319	PHE	2.1
2	D	369	ASN	2.1
1	A	108	MET	2.1
1	A	290	PHE	2.1
1	A	10	GLY	2.1
1	A	179	PHE	2.1
1	C	107	SER	2.1
1	A	249	HIS	2.1
1	C	124	ILE	2.1
2	B	578	PHE	2.1
1	A	164	ALA	2.1
1	A	270	LEU	2.0
2	B	368	ASN	2.0
2	D	299	PHE	2.0
2	B	592	ALA	2.0
1	A	59	PHE	2.0
1	A	49	GLY	2.0
1	C	243	ALA	2.0
1	C	254	THR	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	MES	C	1330	12/12	0.83	0.37	1.55	130,152,164,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MES	A	1330	12/12	0.88	0.31	0.74	129,146,176,177	0
4	ANP	D	1650	31/31	0.90	0.25	-0.38	90,111,136,153	0
4	ANP	B	1650	31/31	0.92	0.25	-0.42	90,111,143,159	0
5	MG	B	1651	1/1	0.98	0.25	-	106,106,106,106	0
5	MG	D	1651	1/1	0.98	0.30	-	111,111,111,111	0

6.5 Other polymers

There are no such residues in this entry.