Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:34 AM GMT

PDB ID	:	3PFQ
Title	:	Crystal Structure and Allosteric Activation of Protein Kinase C beta II
Authors	:	Leonard, T.A.; Rozycki, B.; Saidi, L.F.; Hummer, G.; Hurley, J.H.
Deposited on	:	2010-10-28
Resolution	:	4.00 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:

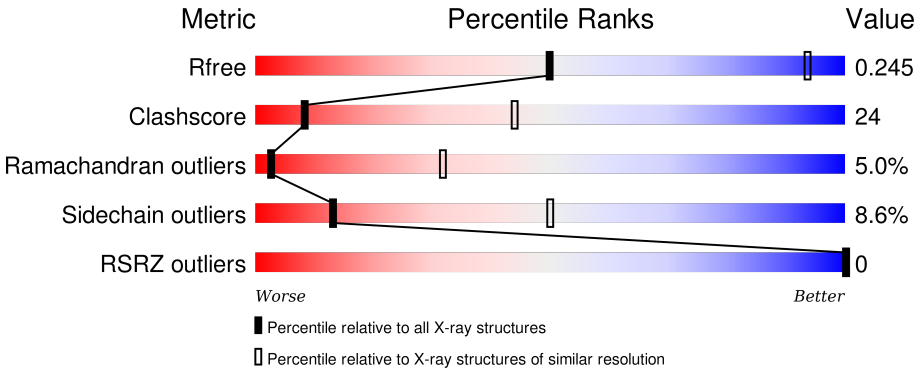
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.00 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	674	39% 33% 5% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4273 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 Protein kinase C beta type.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	523	4237	2711	708	785	3	30	0	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P68403
A	71	SER	CYS	ENGINEERED MUTATION	UNP P68403
A	217	SER	CYS	ENGINEERED MUTATION	UNP P68403
A	?	-	ARG	ENGINEERED MUTATION	UNP P68403
A	622	SER	ASP	VARIANT	UNP P68403
A	623	GLY	LYS	VARIANT	UNP P68403
A	625	ASN	ASP	VARIANT	UNP P68403
A	626	ALA	THR	VARIANT	UNP P68403
A	627	GLU	SER	VARIANT	UNP P68403
A	631	ARG	LYS	VARIANT	UNP P68403
A	632	PHE	GLU	VARIANT	UNP P68403
A	636	HIS	GLN	VARIANT	UNP P68403
A	638	PRO	VAL	VARIANT	UNP P68403
A	639	VAL	GLU	VARIANT	UNP P68403
A	643	PRO	THR	VARIANT	UNP P68403
A	645	GLN	LYS	VARIANT	UNP P68403
A	646	GLU	LEU	VARIANT	UNP P68403
A	647	VAL	PHE	VARIANT	UNP P68403
A	649	ARG	MET	VARIANT	UNP P68403
A	651	ILE	LEU	VARIANT	UNP P68403
A	654	SER	ASN	VARIANT	UNP P68403
A	657	GLU	ALA	VARIANT	UNP P68403
A	661	PHE	TYR	VARIANT	UNP P68403
A	662	VAL	THR	VARIANT	UNP P68403
A	664	SER	PRO	VARIANT	UNP P68403
A	667	LEU	-	VARIANT	UNP P68403
A	668	LYS	-	VARIANT	UNP P68403

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Chain	Residue	Modelled	Actual	Comment	Reference
A	669	PRO	-	VARIANT	UNP P68403
A	670	GLU	-	VARIANT	UNP P68403
A	672	LYS	-	VARIANT	UNP P68403
A	673	SER	-	VARIANT	UNP P68403

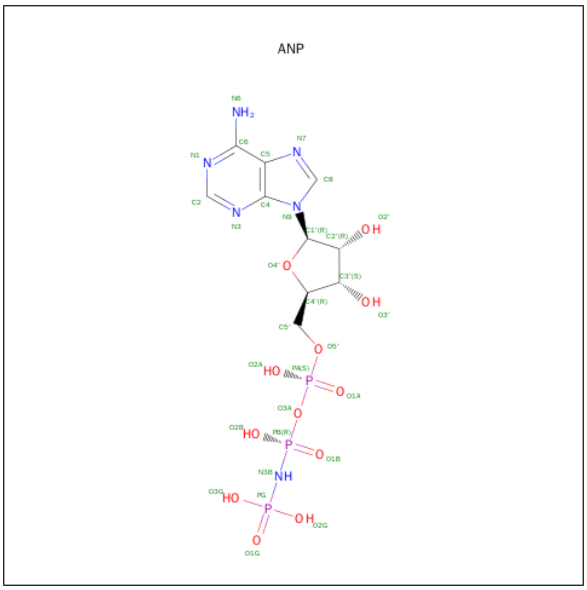
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0

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



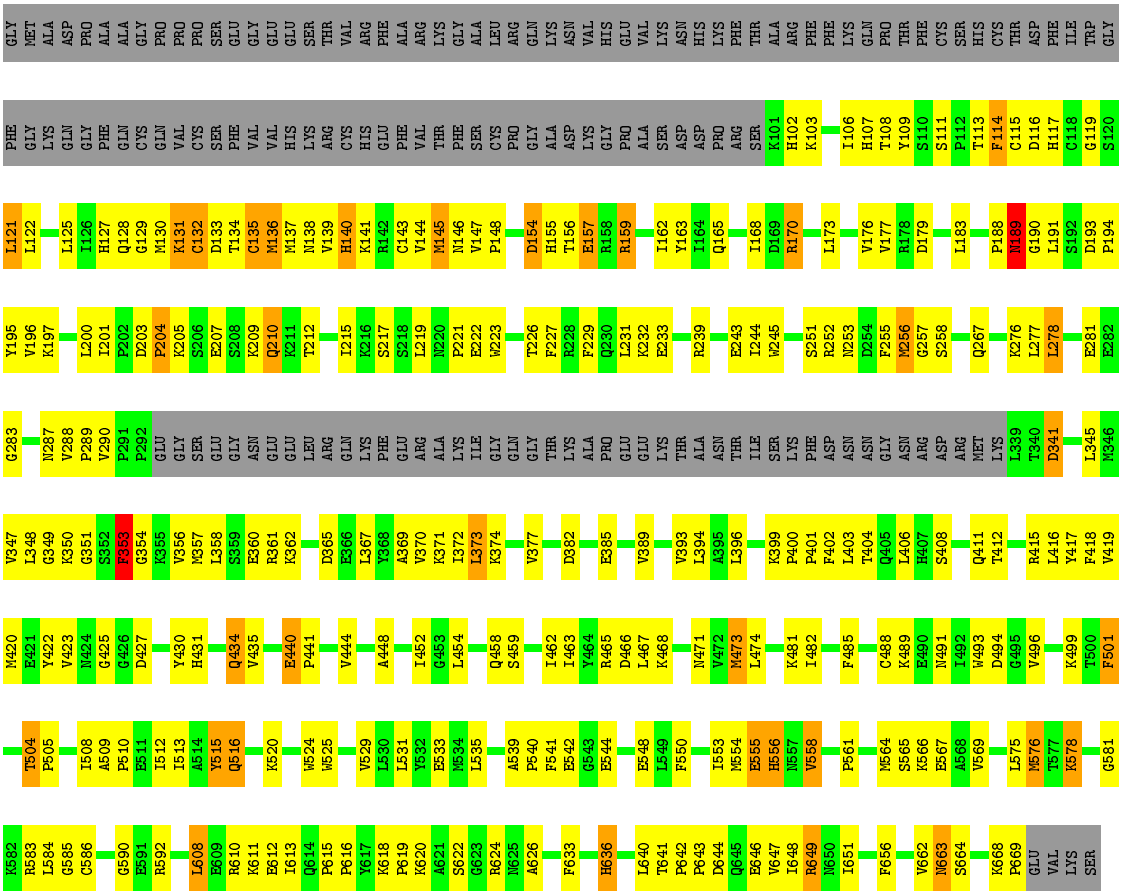
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 10 6 12 3	0	0

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: Protein kinase C beta type

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.27Å 114.27Å 170.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.10 – 4.00 57.14 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (57.10-4.00) 93.9 (57.14-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 4.01Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.193 , 0.244 0.198 , 0.245	Depositor DCC
R_{free} test set	508 reflections (4.76%)	DCC
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 102.8	EDS
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 10670 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4273	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: TPO, ZN, ANP, CA, SEP

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	0.26	0/4311	0.44	0/5811

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	4237	0	4156	204	0
2	A	3	0	0	0	0
3	A	2	0	0	0	0
4	A	31	0	13	0	0
All	All	4273	0	4169	204	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 24.

All (204) 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:145:MET:HE2	1:A:146:ASN:H	1.32	0.94
1:A:130:MET:HG2	1:A:141:LYS:HA	1.55	0.87
1:A:162:ILE:HD12	1:A:244:ILE:HD11	1.58	0.83
1:A:372:ILE:HD13	1:A:640:LEU:HD11	1.59	0.83
1:A:189:ASN:HD22	1:A:191:LEU:H	1.27	0.81
1:A:232:LYS:HG2	1:A:233:GLU:H	1.45	0.81
1:A:622:SER:HB3	1:A:626:ALA:HB2	1.66	0.77
1:A:106:ILE:HD11	1:A:127:HIS:HB3	1.67	0.75
1:A:394:LEU:HD13	1:A:406:LEU:HD13	1.68	0.74
1:A:513:ILE:HD11	1:A:554:MET:SD	2.29	0.73
1:A:114:PHE:HA	1:A:121:LEU:HA	1.71	0.73
1:A:108:THR:HG22	1:A:127:HIS:H	1.52	0.72
1:A:510:PRO:HG2	1:A:578:LYS:HA	1.72	0.72
1:A:454:LEU:HD11	1:A:467:LEU:HD13	1.72	0.70
1:A:529:VAL:HG13	1:A:540:PRO:HG3	1.73	0.69
1:A:107:HIS:HB3	1:A:131:LYS:HB2	1.75	0.69
1:A:145:MET:HE2	1:A:146:ASN:N	2.08	0.68
1:A:176:VAL:HG22	1:A:226:THR:HG23	1.74	0.68
1:A:440:GLU:HB3	1:A:441:PRO:HD3	1.75	0.68
1:A:129:GLY:HA2	1:A:141:LYS:HG3	1.77	0.67
1:A:515:TYR:O	1:A:516:GLN:HG2	1.96	0.66
1:A:143:CYS:HA	1:A:145:MET:HE1	1.78	0.65
1:A:278:LEU:H	1:A:278:LEU:HD12	1.60	0.65
1:A:356:VAL:HG22	1:A:371:LYS:HG3	1.79	0.64
1:A:177:VAL:HG11	1:A:196:VAL:HG21	1.80	0.62
1:A:130:MET:CG	1:A:141:LYS:HA	2.30	0.61
1:A:501:PHE:HA	1:A:512:ILE:HD11	1.81	0.61
1:A:663:ASN:HD22	1:A:664:SER:H	1.49	0.60
1:A:441:PRO:O	1:A:444:VAL:HG12	2.02	0.60
1:A:550:PHE:HA	1:A:553:ILE:HD12	1.83	0.60
1:A:553:ILE:O	1:A:578:LYS:HE3	2.02	0.60
1:A:585:GLY:HA2	1:A:590:GLY:HA2	1.82	0.59
1:A:431:HIS:O	1:A:434:GLN:HG3	2.02	0.59
1:A:561:PRO:HG2	1:A:564:MET:HG2	1.85	0.59
1:A:194:PRO:HA	1:A:245:TRP:O	2.02	0.59
1:A:345:LEU:HD11	1:A:360:GLU:HB2	1.84	0.59
1:A:103:LYS:HB2	1:A:133:ASP:HB2	1.85	0.59
1:A:354:GLY:HA3	1:A:373:LEU:HB3	1.83	0.58
1:A:131:LYS:HD2	1:A:132:CYS:H	1.68	0.58
1:A:341:ASP:HA	1:A:362:LYS:HE3	1.84	0.58
1:A:525:TRP:O	1:A:529:VAL:HG23	2.02	0.58
1:A:197:LYS:HD3	1:A:209:LYS:NZ	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:THR:HG22	1:A:227:PHE:CZ	2.39	0.58
1:A:558:VAL:HG11	1:A:576:MET:HE3	1.84	0.58
1:A:425:GLY:HA3	1:A:474:LEU:O	2.04	0.58
1:A:385:GLU:O	1:A:389:VAL:HG23	2.04	0.57
1:A:147:VAL:HG22	1:A:148:PRO:HD2	1.86	0.57
1:A:402:PHE:O	1:A:482:ILE:HD12	2.04	0.57
1:A:531:LEU:O	1:A:535:LEU:HD23	2.04	0.57
1:A:608:LEU:HA	1:A:613:ILE:HD13	1.86	0.57
1:A:458:GLN:OE1	1:A:520:LYS:HD2	2.04	0.56
1:A:122:LEU:HB3	1:A:128:GLN:HB3	1.86	0.56
1:A:243:GLU:HB2	1:A:245:TRP:HE1	1.71	0.56
1:A:370:VAL:HG22	1:A:419:VAL:HA	1.87	0.56
1:A:647:VAL:O	1:A:651:ILE:HG13	2.06	0.55
1:A:508:ILE:HG21	1:A:550:PHE:CE1	2.41	0.55
1:A:347:VAL:HA	1:A:357:MET:HB3	1.88	0.55
1:A:137:MET:HG3	1:A:137:MET:O	2.07	0.55
1:A:374:LYS:H	1:A:374:LYS:HD2	1.72	0.55
1:A:406:LEU:O	1:A:663:ASN:HB2	2.07	0.55
1:A:567:GLU:H	1:A:567:GLU:CD	2.11	0.54
1:A:183:LEU:HB2	1:A:219:LEU:O	2.08	0.54
1:A:427:ASP:HA	1:A:473:MET:HA	1.89	0.54
1:A:173:LEU:HB3	1:A:229:PHE:HB2	1.89	0.54
1:A:179:ASP:HB3	1:A:222:GLU:HG3	1.90	0.54
1:A:400:PRO:HD2	1:A:403:LEU:HD12	1.89	0.53
1:A:204:PRO:HG2	1:A:205:LYS:H	1.73	0.53
1:A:201:ILE:HG13	1:A:239:ARG:HB2	1.89	0.53
1:A:215:ILE:HD12	1:A:215:ILE:H	1.72	0.53
1:A:121:LEU:HD13	1:A:620:LYS:NZ	2.24	0.53
1:A:448:ALA:O	1:A:452:ILE:HG13	2.09	0.52
1:A:287:ASN:O	1:A:289:PRO:HD3	2.09	0.52
1:A:415:ARG:NH1	1:A:640:LEU:HD22	2.24	0.52
1:A:191:LEU:HA	1:A:219:LEU:HD21	1.91	0.52
1:A:465:ARG:NH2	1:A:489:LYS:HB2	2.24	0.52
1:A:215:ILE:HD12	1:A:215:ILE:N	2.23	0.52
1:A:370:VAL:HA	1:A:418:PHE:O	2.10	0.52
1:A:109:TYR:OH	1:A:138:ASN:HB3	2.10	0.51
1:A:196:VAL:HG22	1:A:244:ILE:HG12	1.92	0.51
1:A:232:LYS:HG2	1:A:233:GLU:N	2.21	0.51
1:A:196:VAL:HG12	1:A:197:LYS:H	1.74	0.51
1:A:668:LYS:HB2	1:A:669:PRO:HD2	1.91	0.51
1:A:592:ARG:HH11	1:A:592:ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HG12	1:A:197:LYS:N	2.25	0.51
1:A:115:CYS:SG	1:A:139:VAL:HG23	2.51	0.51
1:A:644:ASP:OD1	1:A:646:GLU:HB3	2.11	0.51
1:A:663:ASN:HD22	1:A:664:SER:N	2.09	0.51
1:A:468:LYS:HE2	1:A:504:THR:OG1	2.09	0.51
1:A:147:VAL:CG2	1:A:148:PRO:HD2	2.40	0.50
1:A:454:LEU:HD11	1:A:467:LEU:CD1	2.40	0.50
1:A:524:TRP:CE3	1:A:524:TRP:HA	2.46	0.50
1:A:209:LYS:O	1:A:210:GLN:HB2	2.11	0.50
1:A:491:ASN:HA	1:A:493:TRP:CZ3	2.47	0.50
1:A:508:ILE:HG21	1:A:550:PHE:HE1	1.77	0.50
1:A:278:LEU:HD21	1:A:288:VAL:HG23	1.93	0.50
1:A:106:ILE:HD13	1:A:367:LEU:HD21	1.93	0.49
1:A:610:ARG:HB2	1:A:612:GLU:HG3	1.94	0.49
1:A:411:GLN:O	1:A:411:GLN:HG3	2.12	0.49
1:A:416:LEU:HD11	1:A:656:PHE:CE1	2.47	0.49
1:A:663:ASN:ND2	1:A:664:SER:H	2.11	0.49
1:A:508:ILE:O	1:A:508:ILE:HG23	2.12	0.49
1:A:189:ASN:ND2	1:A:191:LEU:H	2.03	0.49
1:A:423:VAL:HG11	1:A:473:MET:HE3	1.94	0.49
1:A:372:ILE:HG12	1:A:417:TYR:CD2	2.48	0.49
1:A:121:LEU:HD22	1:A:620:LYS:HD2	1.94	0.48
1:A:348:LEU:HD23	1:A:633:PHE:CE1	2.47	0.48
1:A:232:LYS:CG	1:A:233:GLU:H	2.19	0.48
1:A:369:ALA:HB2	1:A:422:TYR:HD1	1.78	0.48
1:A:618:LYS:HE2	1:A:620:LYS:HE3	1.94	0.48
1:A:278:LEU:HD13	1:A:283:GLY:HA2	1.96	0.48
1:A:663:ASN:ND2	1:A:664:SER:N	2.61	0.48
1:A:255:PHE:HZ	1:A:258:SER:HB2	1.79	0.48
1:A:389:VAL:O	1:A:393:VAL:HG23	2.13	0.48
1:A:648:ILE:HA	1:A:651:ILE:HD12	1.95	0.48
1:A:533:GLU:OE2	1:A:539:ALA:HA	2.14	0.47
1:A:644:ASP:OD1	1:A:647:VAL:HG23	2.15	0.47
1:A:350:LYS:HD3	1:A:636:HIS:CD2	2.49	0.47
1:A:188:PRO:C	1:A:190:GLY:H	2.18	0.47
1:A:565:SER:O	1:A:569:VAL:HG23	2.14	0.47
1:A:159:ARG:HG2	1:A:256:MET:O	2.15	0.47
1:A:351:GLY:C	1:A:353:PHE:H	2.17	0.47
1:A:215:ILE:HD13	1:A:221:PRO:HB2	1.97	0.47
1:A:468:LYS:HE3	1:A:471:ASN:ND2	2.29	0.47
1:A:493:TRP:H	1:A:496:VAL:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD13	1:A:620:LYS:HZ2	1.80	0.46
1:A:431:HIS:O	1:A:435:VAL:HG22	2.16	0.46
1:A:115:CYS:HB3	1:A:119:GLY:H	1.81	0.46
1:A:111:SER:O	1:A:113:THR:HG23	2.16	0.46
1:A:165:GLN:HB3	1:A:176:VAL:HB	1.97	0.46
1:A:613:ILE:N	1:A:613:ILE:HD12	2.30	0.46
1:A:252:ARG:O	1:A:253:ASN:C	2.53	0.46
1:A:544:GLU:HG2	1:A:548:GLU:OE2	2.15	0.46
1:A:139:VAL:HG22	1:A:140:HIS:N	2.31	0.46
1:A:258:SER:HB3	1:A:283:GLY:HA3	1.98	0.46
1:A:509:ALA:HA	1:A:525:TRP:CD1	2.51	0.45
1:A:276:LYS:HB2	1:A:290:VAL:CG2	2.46	0.45
1:A:615:PRO:HA	1:A:616:PRO:HD3	1.85	0.45
1:A:358:LEU:HD21	1:A:367:LEU:HD23	1.98	0.45
1:A:200:LEU:HA	1:A:239:ARG:O	2.17	0.45
1:A:373:LEU:HD12	1:A:416:LEU:HB2	1.99	0.45
1:A:125:LEU:HD21	1:A:430:TYR:CE2	2.51	0.45
1:A:205:LYS:HB2	1:A:207:GLU:CD	2.36	0.45
1:A:215:ILE:HD11	1:A:223:TRP:CD1	2.52	0.45
1:A:358:LEU:HD11	1:A:367:LEU:HB3	1.98	0.45
1:A:558:VAL:HG11	1:A:576:MET:CE	2.47	0.45
1:A:122:LEU:HB3	1:A:128:GLN:CB	2.47	0.45
1:A:205:LYS:HB2	1:A:207:GLU:OE1	2.17	0.45
1:A:394:LEU:HB2	1:A:406:LEU:HD22	1.99	0.44
1:A:201:ILE:HD11	1:A:239:ARG:HD3	1.98	0.44
1:A:575:LEU:HG	1:A:584:LEU:HD23	1.99	0.44
1:A:403:LEU:HD22	1:A:485:PHE:HZ	1.82	0.44
1:A:531:LEU:HD23	1:A:535:LEU:HD23	1.98	0.44
1:A:201:ILE:CG1	1:A:239:ARG:HB2	2.46	0.44
1:A:415:ARG:HD3	1:A:640:LEU:HD13	1.98	0.44
1:A:510:PRO:O	1:A:513:ILE:HG12	2.17	0.44
1:A:541:PHE:CD1	1:A:553:ILE:HA	2.53	0.43
1:A:212:THR:HG22	1:A:227:PHE:CE1	2.53	0.43
1:A:349:GLY:O	1:A:350:LYS:HG2	2.18	0.43
1:A:141:LYS:HE3	1:A:367:LEU:HD22	2.00	0.43
1:A:244:ILE:O	1:A:256:MET:HB2	2.18	0.43
1:A:592:ARG:NH1	1:A:592:ARG:HG2	2.34	0.43
1:A:135:CYS:O	1:A:136:MET:HB2	2.18	0.43
1:A:555:GLU:O	1:A:556:HIS:C	2.56	0.43
1:A:361:ARG:HG3	1:A:362:LYS:N	2.33	0.43
1:A:504:THR:HG22	1:A:505:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:ARG:HH11	1:A:649:ARG:HB2	1.84	0.43
1:A:109:TYR:CE2	1:A:122:LEU:HD13	2.53	0.43
1:A:374:LYS:HB2	1:A:377:VAL:CG2	2.48	0.43
1:A:394:LEU:HB3	1:A:406:LEU:HB2	2.00	0.43
1:A:431:HIS:CE1	1:A:474:LEU:HD12	2.54	0.42
1:A:239:ARG:HH11	1:A:239:ARG:HG2	1.84	0.42
1:A:212:THR:HG22	1:A:227:PHE:HZ	1.80	0.42
1:A:463:ILE:HG21	1:A:520:LYS:HA	2.00	0.42
1:A:276:LYS:HB3	1:A:288:VAL:HB	2.00	0.42
1:A:516:GLN:HE21	1:A:516:GLN:HB3	1.54	0.42
1:A:644:ASP:O	1:A:648:ILE:HG13	2.19	0.42
1:A:205:LYS:HB2	1:A:207:GLU:CG	2.50	0.42
1:A:348:LEU:HD11	1:A:358:LEU:HB2	2.00	0.42
1:A:583:ARG:HB3	1:A:586:CYS:SG	2.60	0.42
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.84	0.42
1:A:510:PRO:HB2	1:A:578:LYS:O	2.20	0.42
1:A:351:GLY:C	1:A:353:PHE:N	2.73	0.42
1:A:401:PRO:HB2	1:A:611:LYS:HE3	2.01	0.42
1:A:145:MET:C	1:A:147:VAL:H	2.24	0.42
1:A:119:GLY:C	1:A:121:LEU:H	2.24	0.42
1:A:608:LEU:CA	1:A:613:ILE:HD13	2.50	0.42
1:A:408:SER:HB3	1:A:662:VAL:HG13	2.01	0.41
1:A:465:ARG:HH21	1:A:489:LYS:HB2	1.85	0.41
1:A:130:MET:HG3	1:A:144:VAL:HG11	2.03	0.41
1:A:510:PRO:HD3	1:A:525:TRP:CE2	2.56	0.41
1:A:255:PHE:CZ	1:A:258:SER:HB2	2.55	0.41
1:A:420:MET:HE2	1:A:420:MET:HB3	2.00	0.41
1:A:168:ILE:HG12	1:A:231:LEU:HD11	2.01	0.41
1:A:189:ASN:HD22	1:A:189:ASN:C	2.24	0.41
1:A:641:TPO:HG23	1:A:642:PRO:HD2	2.02	0.41
1:A:408:SER:O	1:A:419:VAL:HB	2.20	0.41
1:A:203:ASP:HA	1:A:204:PRO:HD2	1.95	0.41
1:A:257:GLY:HA3	1:A:277:LEU:HD22	2.01	0.41
1:A:462:ILE:HD11	1:A:488:CYS:HB3	2.03	0.40
1:A:396:LEU:O	1:A:399:LYS:HG3	2.21	0.40
1:A:122:LEU:HD22	1:A:129:GLY:HA3	2.02	0.40
1:A:195:TYR:HE2	1:A:253:ASN:HD22	1.68	0.40
1:A:404:THR:HG21	1:A:420:MET:CE	2.52	0.40
1:A:642:PRO:HA	1:A:643:PRO:HD3	1.94	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	516/674 (77%)	412 (80%)	78 (15%)	26 (5%)	3 32

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	135	CYS
1	A	136	MET
1	A	217	SER
1	A	353	PHE
1	A	412	THR
1	A	466	ASP
1	A	556	HIS
1	A	558	VAL
1	A	114	PHE
1	A	117	HIS
1	A	134	THR
1	A	140	HIS
1	A	154	ASP
1	A	210	GLN
1	A	157	GLU
1	A	189	ASN
1	A	251	SER
1	A	515	TYR
1	A	636	HIS
1	A	170	ARG
1	A	204	PRO
1	A	555	GLU
1	A	619	PRO
1	A	578	LYS
1	A	581	GLY

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	463/589 (79%)	423 (91%)	40 (9%)	13 50

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	116	ASP
1	A	121	LEU
1	A	132	CYS
1	A	145	MET
1	A	154	ASP
1	A	155	HIS
1	A	156	THR
1	A	157	GLU
1	A	159	ARG
1	A	163	TYR
1	A	170	ARG
1	A	189	ASN
1	A	193	ASP
1	A	256	MET
1	A	267	GLN
1	A	278	LEU
1	A	281	GLU
1	A	341	ASP
1	A	353	PHE
1	A	365	ASP
1	A	373	LEU
1	A	382	ASP
1	A	434	GLN
1	A	440	GLU
1	A	459	SER
1	A	473	MET
1	A	481	LYS
1	A	494	ASP
1	A	499	LYS

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Mol	Chain	Res	Type
1	A	501	PHE
1	A	504	THR
1	A	516	GLN
1	A	542	GLU
1	A	566	LYS
1	A	576	MET
1	A	608	LEU
1	A	624	ARG
1	A	649	ARG
1	A	663	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	210	GLN
1	A	434	GLN
1	A	471	ASN
1	A	491	ASN
1	A	516	GLN
1	A	557	ASN
1	A	614	GLN
1	A	628	ASN
1	A	663	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	TPO	A	500	1	8,10,11	1.11	0	7,14,16	1.15	1 (14%)
1	TPO	A	641	1	8,10,11	1.24	0	7,14,16	0.97	0
1	SEP	A	660	1	8,9,10	1.05	0	8,12,14	1.14	0

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
1	TPO	A	500	1	-	0/8/11/13	0/0/0/0
1	TPO	A	641	1	-	0/8/11/13	0/0/0/0
1	SEP	A	660	1	-	0/6/8/10	0/0/0/0

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	500	TPO	CG2-CB-CA	-2.10	108.90	113.17

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
1	A	641	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	ANP	A	800	-	27,33,33	3.50	8 (29%)	30,52,52	2.47	10 (33%)

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
4	ANP	A	800	-	-	0/12/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	ANP	PA-O1A	2.03	1.58	1.51
4	A	800	ANP	C5-C4	2.26	1.45	1.40
4	A	800	ANP	PG-N3B	4.24	1.74	1.63
4	A	800	ANP	PB-N3B	4.51	1.75	1.63
4	A	800	ANP	PB-O3A	5.97	1.66	1.59
4	A	800	ANP	C4-N3	6.12	1.44	1.35
4	A	800	ANP	PB-O1B	9.92	1.57	1.46
4	A	800	ANP	PG-O1G	9.96	1.57	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	800	ANP	N3-C2-N1	-8.95	122.04	128.89
4	A	800	ANP	C2'-C1'-N9	-4.41	107.55	114.29
4	A	800	ANP	C4-C5-N7	-4.14	105.67	109.48
4	A	800	ANP	O1B-PB-N3B	-2.55	107.99	111.90
4	A	800	ANP	O2'-C2'-C3'	-2.16	104.80	111.83
4	A	800	ANP	O3'-C3'-C2'	2.06	118.51	111.83
4	A	800	ANP	O4'-C1'-N9	2.07	112.44	108.10
4	A	800	ANP	O3'-C3'-C4'	2.20	117.65	111.05
4	A	800	ANP	C2-N1-C6	2.90	123.96	118.77
4	A	800	ANP	C4'-O4'-C1'	3.90	114.00	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	520/674 (77%)	-0.25	0 100 100	35, 105, 167, 234	0

There are no RSRZ outliers to report.

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

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
1	SEP	A	660	10/11	0.91	0.12	-	128,143,143,143	0
1	TPO	A	641	11/12	0.91	0.18	-	171,171,177,177	0
1	TPO	A	500	11/12	0.87	0.24	-	93,112,112,112	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
4	ANP	A	800	31/31	0.78	0.31	-0.06	78,133,182,200	0
2	CA	A	674	1/1	0.88	0.20	-1.09	76,76,76,76	0
3	ZN	A	751	1/1	0.98	0.13	-1.13	96,96,96,96	0
3	ZN	A	750	1/1	0.99	0.06	-1.90	113,113,113,113	0
2	CA	A	675	1/1	0.95	0.15	-	61,61,61,61	0
2	CA	A	676	1/1	0.94	0.16	-	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.