



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:35 PM GMT

PDB ID : 1KSW
Title : Structure of Human c-Src Tyrosine Kinase (Thr338Gly Mutant) in Complex with N6-benzyl ADP
Authors : Witucki, L.A.; Huang, X.; Shah, K.; Liu, Y.; Kyin, S.; Eck, M.J.; Shokat, K.M.
Deposited on : 2002-01-14
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

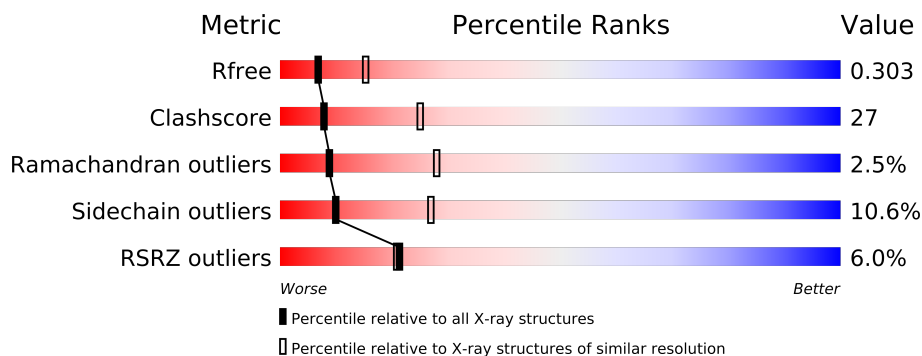
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	452	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3691 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

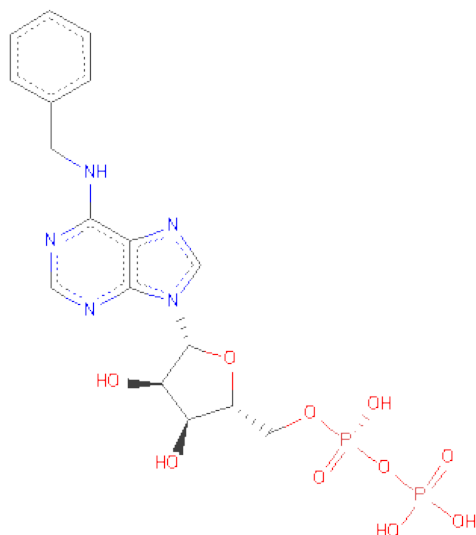
- Molecule 1 is a protein called PROTO-ONCOGENE TYROSINE-PROTEIN KINASE SRC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	450	3611	2294	614	683	1	19	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	MET	-	INITIATING METHIONINE	UNP P12931
A	338	GLY	THR	ENGINEERED	UNP P12931
A	527	PTR	TYR	MODIFIED RESIDUE	UNP P12931

- Molecule 2 is N6-BENZYL ADENOSINE-5'-DIPHOSPHATE (three-letter code: NBS) (formula: C₁₇H₂₁N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	34	17	5	10	2	0	0

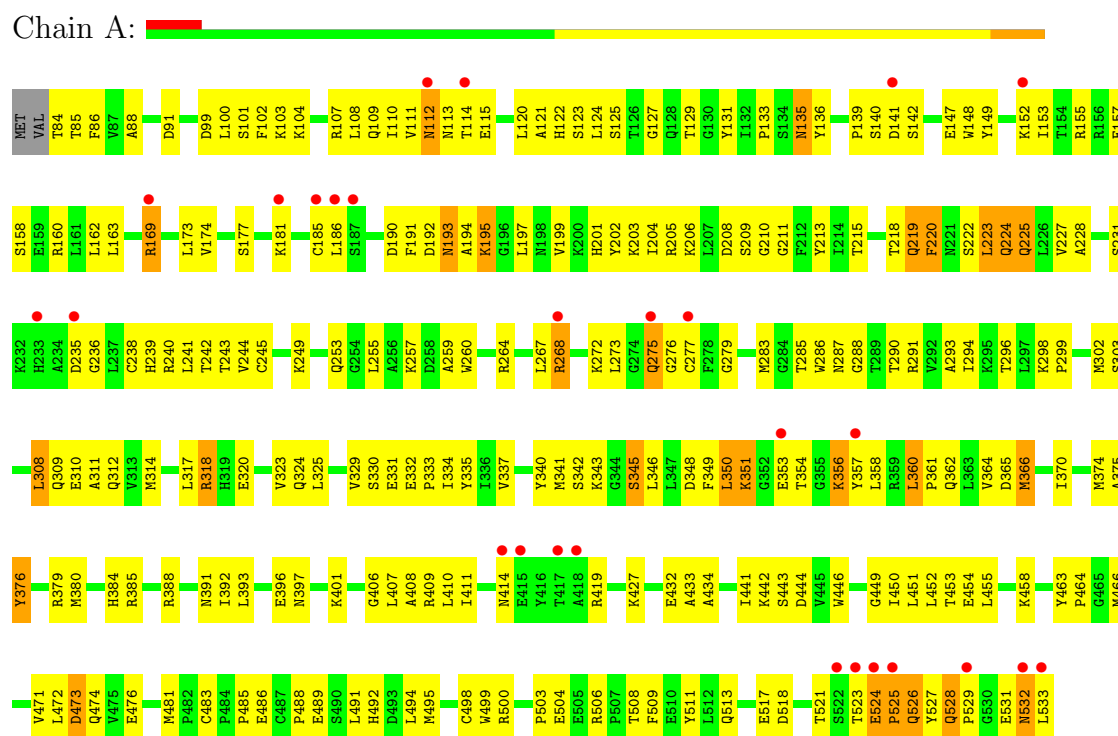
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE SRC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.81Å 87.68Å 106.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 21.53 – 2.43	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 93.9 (21.53-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.44Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.231 , 0.294 0.236 , 0.303	Depositor DCC
R_{free} test set	610 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 17286 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3691	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NBS, PTR

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	0.61	0/3679	0.79	0/4984

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3611	0	3539	195	0
2	A	34	0	18	5	0
3	A	46	0	0	2	0
All	All	3691	0	3557	195	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (195) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:TRP:HB3	1:A:244:VAL:HG22	1.55	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:GLU:HG2	1:A:257:LYS:NZ	1.90	0.87
1:A:466:MET:HE2	1:A:471:VAL:HG22	1.62	0.81
1:A:340:TYR:OH	1:A:342:SER:HA	1.84	0.77
1:A:524:GLU:N	1:A:525:PRO:HD3	2.02	0.75
1:A:147:GLU:HG2	1:A:244:VAL:HG11	1.68	0.75
1:A:340:TYR:CZ	1:A:342:SER:HA	2.21	0.75
1:A:310:GLU:HG2	1:A:410:LEU:HD11	1.69	0.75
1:A:222:SER:OG	1:A:224:GLN:HG2	1.87	0.74
1:A:206:LYS:HE2	1:A:210:GLY:HA2	1.71	0.73
1:A:135:ASN:HD22	1:A:135:ASN:H	1.33	0.72
1:A:222:SER:HB2	1:A:224:GLN:HE21	1.55	0.71
1:A:329:VAL:HB	1:A:335:TYR:HB2	1.71	0.71
1:A:115:GLU:HG2	1:A:257:LYS:HZ1	1.56	0.70
1:A:194:ALA:O	1:A:195:LYS:HB2	1.91	0.69
1:A:205:ARG:HB2	1:A:213:TYR:CE1	2.26	0.69
1:A:346:LEU:O	1:A:350:LEU:HB2	1.94	0.68
1:A:268:ARG:NH1	1:A:288:GLY:H	1.92	0.67
1:A:115:GLU:HG2	1:A:257:LYS:HZ3	1.57	0.66
1:A:135:ASN:N	1:A:135:ASN:HD22	1.94	0.66
1:A:500:ARG:O	1:A:506:ARG:HD2	1.95	0.65
1:A:111:VAL:O	1:A:112:ASN:HB2	1.96	0.65
1:A:123:SER:O	1:A:127:GLY:HA2	1.96	0.65
1:A:483:CYS:HA	1:A:492:HIS:CD2	2.32	0.65
1:A:206:LYS:HA	1:A:211:GLY:O	1.98	0.64
1:A:268:ARG:HH12	1:A:287:ASN:N	1.98	0.62
1:A:443:SER:O	1:A:446:TRP:HB3	2.00	0.61
1:A:317:LEU:HA	1:A:376:TYR:OH	2.00	0.61
1:A:91:ASP:OD1	1:A:103:LYS:HA	2.00	0.61
1:A:466:MET:CE	1:A:471:VAL:HA	2.31	0.61
1:A:267:LEU:HD11	1:A:337:VAL:HG21	1.83	0.61
1:A:466:MET:HE1	1:A:471:VAL:HA	1.83	0.60
1:A:222:SER:HB2	1:A:224:GLN:NE2	2.15	0.60
1:A:523:THR:OG1	1:A:525:PRO:HG3	2.02	0.60
1:A:273:LEU:HD11	1:A:283:MET:HB2	1.84	0.60
1:A:345:SER:HA	1:A:393:LEU:HD23	1.85	0.59
1:A:103:LYS:HG3	1:A:104:LYS:O	2.03	0.58
1:A:177:SER:OG	1:A:203:LYS:HE2	2.04	0.57
1:A:206:LYS:CE	1:A:210:GLY:HA2	2.34	0.57
1:A:192:ASP:HB3	1:A:195:LYS:HB3	1.87	0.57
1:A:108:LEU:HD23	1:A:123:SER:HA	1.87	0.57
1:A:276:GLY:HA2	2:A:1:NBS:O4P	2.05	0.56
1:A:442:LYS:HE3	1:A:504:GLU:HA	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:ARG:HG2	1:A:409:ARG:O	2.03	0.56
1:A:272:LYS:NZ	1:A:275:GLN:HG3	2.20	0.56
1:A:255:LEU:HD13	1:A:286:TRP:CD2	2.41	0.56
1:A:332:GLU:HA	1:A:334:ILE:N	2.21	0.56
1:A:85:THR:CG2	1:A:124:LEU:HD11	2.36	0.56
1:A:264:ARG:NH1	1:A:333:PRO:HD2	2.20	0.56
1:A:388:ARG:HA	1:A:451:LEU:HD12	1.88	0.55
1:A:360:LEU:HD11	1:A:488:PRO:HG3	1.88	0.55
1:A:157:GLU:O	1:A:160:ARG:HB3	2.06	0.55
1:A:190:ASP:O	1:A:197:LEU:HD12	2.07	0.55
1:A:260:TRP:HE1	1:A:312:GLN:HE22	1.55	0.54
1:A:186:LEU:HD21	1:A:241:LEU:HD21	1.90	0.54
1:A:169:ARG:HD3	1:A:191:PHE:HB3	1.88	0.54
1:A:109:GLN:O	1:A:111:VAL:HG13	2.08	0.54
1:A:202:TYR:OH	1:A:238:CYS:SG	2.64	0.54
1:A:463:TYR:CE1	1:A:481:MET:HG3	2.42	0.54
1:A:264:ARG:CZ	1:A:333:PRO:HD2	2.38	0.53
1:A:309:GLN:O	1:A:312:GLN:HB2	2.08	0.53
1:A:268:ARG:HH12	1:A:287:ASN:H	1.55	0.53
1:A:528:GLN:HA	1:A:528:GLN:NE2	2.23	0.53
1:A:99:ASP:HA	1:A:131:TYR:H	1.72	0.53
1:A:239:HIS:ND1	1:A:240:ARG:N	2.56	0.53
1:A:366:MET:O	1:A:370:ILE:HG13	2.08	0.53
1:A:109:GLN:OE1	1:A:109:GLN:HA	2.09	0.52
1:A:449:GLY:O	1:A:452:LEU:HB2	2.09	0.52
1:A:508:THR:O	1:A:511:TYR:HB3	2.09	0.52
1:A:133:PRO:HG2	1:A:136:TYR:HB2	1.92	0.52
1:A:524:GLU:N	1:A:525:PRO:CD	2.73	0.52
1:A:453:THR:HG22	1:A:495:MET:SD	2.50	0.51
1:A:255:LEU:HB3	1:A:286:TRP:CZ3	2.46	0.51
1:A:396:GLU:O	1:A:397:ASN:HB2	2.10	0.51
1:A:242:THR:OG1	1:A:243:THR:N	2.43	0.51
1:A:267:LEU:HD11	1:A:337:VAL:CG2	2.41	0.51
1:A:310:GLU:O	1:A:314:MET:HG3	2.11	0.51
1:A:139:PRO:HB2	1:A:142:SER:HB3	1.93	0.51
1:A:220:PHE:CD1	1:A:220:PHE:N	2.78	0.51
1:A:446:TRP:CE3	1:A:499:TRP:HA	2.46	0.50
1:A:133:PRO:O	1:A:136:TYR:HB2	2.12	0.50
1:A:86:PHE:CD1	1:A:110:ILE:HG12	2.47	0.49
1:A:112:ASN:HB3	1:A:120:LEU:HB3	1.95	0.49
1:A:136:TYR:OH	1:A:249:LYS:HB3	2.13	0.48
1:A:330:SER:O	1:A:334:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:432:GLU:HG2	1:A:433:ALA:N	2.28	0.48
1:A:202:TYR:HH	1:A:238:CYS:HG	1.57	0.48
1:A:122:HIS:HB3	3:A:569:HOH:O	2.12	0.48
1:A:115:GLU:OE2	1:A:131:TYR:HE1	1.97	0.48
1:A:205:ARG:HB2	1:A:213:TYR:CZ	2.49	0.47
1:A:384:HIS:O	1:A:385:ARG:HB2	2.14	0.47
1:A:406:GLY:O	1:A:408:ALA:N	2.47	0.47
1:A:302:MET:HE2	1:A:410:LEU:HB2	1.96	0.47
1:A:308:LEU:O	1:A:312:GLN:HG2	2.14	0.47
1:A:376:TYR:HB2	1:A:379:ARG:NH2	2.28	0.47
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.70	0.47
1:A:285:THR:HA	1:A:290:THR:O	2.15	0.47
1:A:267:LEU:HD13	1:A:294:ILE:HG12	1.95	0.47
1:A:350:LEU:HD21	1:A:455:LEU:HA	1.97	0.47
1:A:85:THR:HG22	1:A:124:LEU:HD11	1.97	0.47
1:A:140:SER:O	1:A:141:ASP:HB2	2.15	0.47
1:A:268:ARG:HH11	1:A:268:ARG:HG2	1.80	0.46
1:A:353:GLU:HG3	1:A:354:THR:N	2.31	0.46
1:A:356:LYS:HG3	1:A:357:TYR:N	2.30	0.46
1:A:257:LYS:C	1:A:259:ALA:H	2.19	0.46
1:A:463:TYR:N	1:A:464:PRO:CD	2.78	0.46
1:A:349:PHE:CD2	1:A:349:PHE:C	2.89	0.46
1:A:85:THR:HG21	1:A:124:LEU:HD11	1.96	0.46
1:A:513:GLN:O	1:A:517:GLU:HB2	2.15	0.46
1:A:523:THR:C	1:A:525:PRO:HD3	2.36	0.46
1:A:503:PRO:O	1:A:506:ARG:HB2	2.16	0.46
1:A:110:ILE:HD13	1:A:121:ALA:HB2	1.97	0.46
1:A:272:LYS:HZ1	1:A:275:GLN:HG3	1.80	0.45
1:A:213:TYR:HB3	1:A:219:GLN:HB3	1.99	0.45
1:A:391:ASN:O	1:A:392:ILE:HD13	2.16	0.45
1:A:446:TRP:HA	1:A:498:CYS:O	2.16	0.45
1:A:385:ARG:HD3	1:A:409:ARG:HB2	1.98	0.45
1:A:239:HIS:HD1	1:A:240:ARG:N	2.15	0.45
1:A:348:ASP:O	1:A:351:LYS:HG2	2.16	0.45
1:A:427:LYS:HD3	1:A:463:TYR:HB2	1.99	0.45
1:A:149:TYR:HD1	1:A:174:VAL:HG12	1.81	0.45
1:A:253:GLN:HA	1:A:324:GLN:HE22	1.81	0.45
1:A:324:GLN:HG2	1:A:325:LEU:N	2.31	0.45
1:A:228:ALA:O	1:A:231:SER:HB2	2.16	0.45
1:A:331:GLU:HG3	1:A:331:GLU:H	1.65	0.45
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.81	0.45
1:A:452:LEU:HD11	1:A:494:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:451:LEU:O	1:A:454:GLU:HB2	2.17	0.45
1:A:279:GLY:HA3	1:A:296:THR:O	2.17	0.45
1:A:302:MET:CE	1:A:410:LEU:HB2	2.47	0.44
1:A:268:ARG:HG2	1:A:268:ARG:NH1	2.33	0.44
1:A:318:ARG:N	1:A:376:TYR:OH	2.51	0.44
1:A:485:PRO:O	1:A:486:GLU:HB2	2.17	0.44
1:A:103:LYS:HG3	1:A:104:LYS:N	2.31	0.44
1:A:374:MET:HB3	1:A:509:PHE:CD2	2.52	0.44
1:A:162:LEU:HD12	1:A:199:VAL:HG11	1.98	0.44
1:A:131:TYR:CE1	1:A:257:LYS:HD2	2.52	0.44
1:A:155:ARG:HG3	1:A:201:HIS:CE1	2.52	0.44
1:A:202:TYR:CE2	1:A:528:GLN:CB	3.00	0.44
1:A:122:HIS:CD2	1:A:129:THR:HG22	2.53	0.44
1:A:446:TRP:O	1:A:449:GLY:N	2.50	0.44
1:A:466:MET:CE	1:A:474:GLN:HG3	2.48	0.44
1:A:376:TYR:O	1:A:380:MET:HG2	2.18	0.44
1:A:158:SER:HB2	1:A:173:LEU:HD21	2.00	0.43
1:A:148:TRP:O	1:A:148:TRP:HE3	2.01	0.43
1:A:495:MET:O	1:A:498:CYS:HB2	2.18	0.43
1:A:442:LYS:HG3	1:A:504:GLU:HG2	2.01	0.43
1:A:162:LEU:HD23	1:A:245:CYS:SG	2.58	0.43
1:A:185:CYS:SG	1:A:527:PTR:HE1	2.58	0.43
1:A:101:SER:O	1:A:102:PHE:HB3	2.18	0.43
1:A:311:ALA:HA	1:A:314:MET:CE	2.48	0.43
1:A:173:LEU:O	1:A:186:LEU:HD12	2.18	0.43
1:A:323:VAL:HG11	2:A:1:NBS:HB3	2.00	0.43
1:A:152:LYS:O	1:A:152:LYS:HD3	2.19	0.43
1:A:350:LEU:HD21	1:A:455:LEU:HD23	2.00	0.43
1:A:139:PRO:HD2	1:A:142:SER:OG	2.18	0.43
1:A:86:PHE:CD1	1:A:110:ILE:CG1	3.02	0.43
1:A:298:LYS:HG3	1:A:299:PRO:HD2	2.01	0.43
1:A:186:LEU:HB2	1:A:204:ILE:HD11	2.00	0.42
1:A:169:ARG:HD3	1:A:191:PHE:CB	2.48	0.42
1:A:169:ARG:NH1	1:A:191:PHE:CG	2.87	0.42
1:A:317:LEU:HD22	1:A:376:TYR:CE2	2.54	0.42
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.84	0.42
1:A:473:ASP:O	1:A:476:GLU:HB3	2.19	0.42
1:A:323:VAL:CG1	2:A:1:NBS:HB3	2.49	0.42
1:A:255:LEU:HB3	1:A:286:TRP:CE3	2.54	0.42
1:A:450:ILE:HD13	1:A:499:TRP:NE1	2.33	0.42
1:A:213:TYR:HD2	1:A:215:THR:C	2.23	0.42
1:A:341:MET:SD	1:A:401:LYS:HD2	2.59	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:GLY:O	1:A:532:ASN:ND2	2.49	0.42
1:A:310:GLU:HB2	1:A:410:LEU:HD21	2.00	0.41
1:A:360:LEU:HD22	1:A:364:VAL:HG23	2.02	0.41
1:A:115:GLU:CG	1:A:257:LYS:HZ1	2.28	0.41
1:A:452:LEU:HA	1:A:452:LEU:HD23	1.80	0.41
1:A:375:ALA:HB3	3:A:560:HOH:O	2.19	0.41
1:A:100:LEU:O	1:A:100:LEU:HG	2.20	0.41
1:A:489:GLU:OE2	1:A:492:HIS:HB3	2.20	0.41
1:A:223:LEU:O	1:A:227:VAL:HG23	2.19	0.41
1:A:388:ARG:CA	1:A:451:LEU:HD12	2.48	0.41
1:A:441:ILE:O	1:A:444:ASP:HB2	2.20	0.41
1:A:225:GLN:HE21	1:A:225:GLN:HB2	1.59	0.41
1:A:192:ASP:HB3	1:A:195:LYS:CB	2.49	0.41
1:A:317:LEU:HD22	1:A:380:MET:HG3	2.02	0.41
1:A:408:ALA:HA	1:A:411:ILE:HG12	2.01	0.41
1:A:88:ALA:HB3	1:A:103:LYS:O	2.20	0.41
1:A:193:ASN:HD22	1:A:194:ALA:H	1.69	0.41
1:A:419:ARG:HG2	1:A:434:ALA:HA	2.02	0.41
1:A:393:LEU:HD11	2:A:1:NBS:C5	2.51	0.41
1:A:360:LEU:HB3	1:A:361:PRO:HD3	2.01	0.40
1:A:135:ASN:H	1:A:135:ASN:ND2	2.09	0.40
1:A:293:ALA:HB1	2:A:1:NBS:CB7	2.51	0.40
1:A:153:ILE:HD11	1:A:158:SER:N	2.36	0.40
1:A:236:GLY:C	1:A:532:ASN:HD22	2.25	0.40
1:A:160:ARG:HH22	1:A:365:ASP:CG	2.24	0.40
1:A:86:PHE:O	1:A:107:ARG:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	447/452 (99%)	384 (86%)	52 (12%)	11 (2%)	9	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	195	LYS
1	A	407	LEU
1	A	525	PRO
1	A	114	THR
1	A	343	LYS
1	A	458	LYS
1	A	521	THR
1	A	526	GLN
1	A	414	ASN
1	A	529	PRO

5.3.2 Protein sidechains ⓘ

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	387/390 (99%)	346 (89%)	41 (11%)	10	27

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	A	113	ASN
1	A	125	SER
1	A	135	ASN
1	A	163	LEU
1	A	169	ARG
1	A	181	LYS
1	A	193	ASN
1	A	208	ASP
1	A	209	SER
1	A	218	THR
1	A	219	GLN
1	A	220	PHE
1	A	223	LEU
1	A	224	GLN
1	A	225	GLN

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Mol	Chain	Res	Type
1	A	235	ASP
1	A	268	ARG
1	A	275	GLN
1	A	277	CYS
1	A	291	ARG
1	A	303	SER
1	A	308	LEU
1	A	318	ARG
1	A	320	GLU
1	A	345	SER
1	A	350	LEU
1	A	351	LYS
1	A	356	LYS
1	A	360	LEU
1	A	362	GLN
1	A	366	MET
1	A	376	TYR
1	A	472	LEU
1	A	473	ASP
1	A	518	ASP
1	A	524	GLU
1	A	526	GLN
1	A	528	GLN
1	A	531	GLU
1	A	532	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	164	ASN
1	A	193	ASN
1	A	224	GLN
1	A	225	GLN
1	A	312	GLN
1	A	324	GLN
1	A	532	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PTR	A	527	1	16,16,17	4.52	2 (12%)	20,22,24	3.14	8 (40%)

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	PTR	A	527	1	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	PTR	O-C	17.66	1.23	1.11
1	A	527	PTR	CA-C	2.21	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	PTR	C-CA-N	-11.11	102.74	113.83
1	A	527	PTR	CB-CG-CD1	-4.51	112.05	120.90
1	A	527	PTR	CB-CG-CD2	3.90	128.56	120.90
1	A	527	PTR	CD1-CE1-CZ	-2.34	116.62	119.76
1	A	527	PTR	O3P-P-O2P	2.31	116.61	107.61
1	A	527	PTR	O3P-P-O1P	2.25	117.81	110.44
1	A	527	PTR	O2P-P-O1P	2.22	117.69	110.44
1	A	527	PTR	O3P-P-OH	-2.17	96.75	105.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

1 ligand is 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$
2	NBS	A	1	-	37,37,37	1.33	5 (13%)	55,55,55	1.24	6 (10%)

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
2	NBS	A	1	-	-	0/21/37/37	0/2/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NBS	PB-O3P	3.74	1.66	1.60
2	A	1	NBS	C6-N6	3.00	1.40	1.34
2	A	1	NBS	PA-O3P	2.87	1.65	1.59
2	A	1	NBS	O4'-C1'	2.78	1.45	1.41
2	A	1	NBS	C8-N7	-2.17	1.30	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NBS	C2-N1-C6	4.38	119.44	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NBS	C3'-C2'-C1'	3.19	105.90	100.91
2	A	1	NBS	C8-N9-C4	-2.71	104.83	106.90
2	A	1	NBS	PA-O3P-PB	-2.44	124.53	131.68
2	A	1	NBS	O4P-PB-O3P	-2.42	93.64	105.14
2	A	1	NBS	C5-C6-N6	2.28	124.44	120.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	450/452 (99%)	0.04	27 (6%) 21 21	18, 54, 82, 100	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	THR	14.5
1	A	522	SER	9.1
1	A	357	TYR	6.3
1	A	233	HIS	5.2
1	A	533	LEU	5.1
1	A	114	THR	4.9
1	A	532	ASN	4.0
1	A	186	LEU	3.8
1	A	112	ASN	3.5
1	A	275	GLN	3.4
1	A	415	GLU	3.2
1	A	525	PRO	3.1
1	A	169	ARG	2.7
1	A	418	ALA	2.7
1	A	417	THR	2.6
1	A	152	LYS	2.6
1	A	353	GLU	2.6
1	A	524	GLU	2.5
1	A	414	ASN	2.4
1	A	141	ASP	2.3
1	A	277	CYS	2.3
1	A	187	SER	2.2
1	A	181	LYS	2.1
1	A	185	CYS	2.1
1	A	268	ARG	2.1
1	A	529	PRO	2.1
1	A	235	ASP	2.1

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	A	527	16/17	0.15	-1.04	66,69,75,77	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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NBS	A	1	34/34	0.16	-0.45	39,58,93,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.