



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:10 AM GMT

PDB ID : 2G2F
Title : A Src-like Inactive Conformation in the Abl Tyrosine Kinase Domain
Authors : Levinson, N.M.; Kuchment, O.
Deposited on : 2006-02-15
Resolution : 2.70 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>

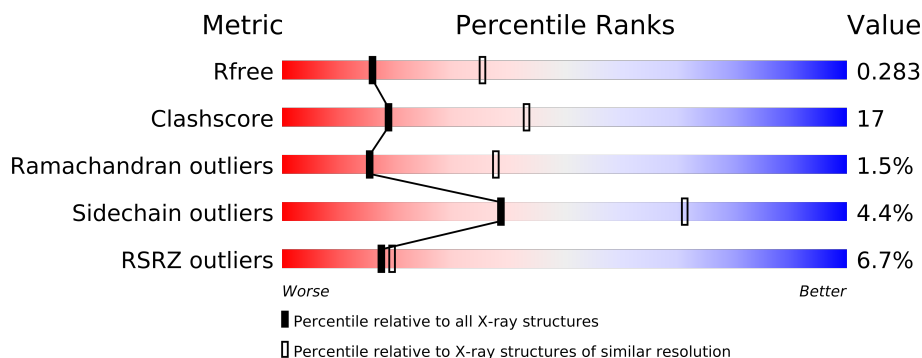
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	287	
1	B	287	
2	C	11	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4586 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 Abl Kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2228	1435	361	415	17			
1	B	264	Total	C	N	O	S	0	0	0
			2150	1388	349	396	17			

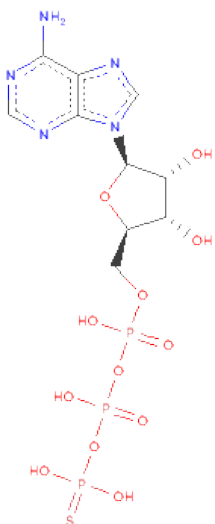
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLY	-	CLONING ARTIFACT	UNP P00519
A	227	HIS	-	CLONING ARTIFACT	UNP P00519
A	228	MET	-	CLONING ARTIFACT	UNP P00519
A	396	PRO	HIS	ENGINEERED	UNP P00519
B	226	GLY	-	CLONING ARTIFACT	UNP P00519
B	227	HIS	-	CLONING ARTIFACT	UNP P00519
B	228	MET	-	CLONING ARTIFACT	UNP P00519
B	396	PRO	HIS	ENGINEERED	UNP P00519

- Molecule 2 is a protein called ATP-Peptide Conjugate.

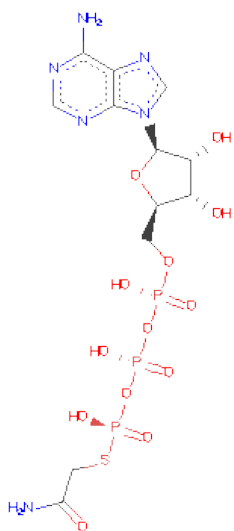
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			57	41	8	8			

- Molecule 3 is PHOSPHOTHIOPHOSPHORICACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	B	1	31	10	5	12	3	1	0	0

- Molecule 4 is THIOPHOSPHORIC ACID O-((ADENOSYL-PHOSPHO)PHOSPHO)-S-AC ETAMIDYL-DIESTER (three-letter code: 112) (formula: C₁₂H₁₉N₆O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	C	1	35	12	6	13	3	1	0	0

- Molecule 5 is water.

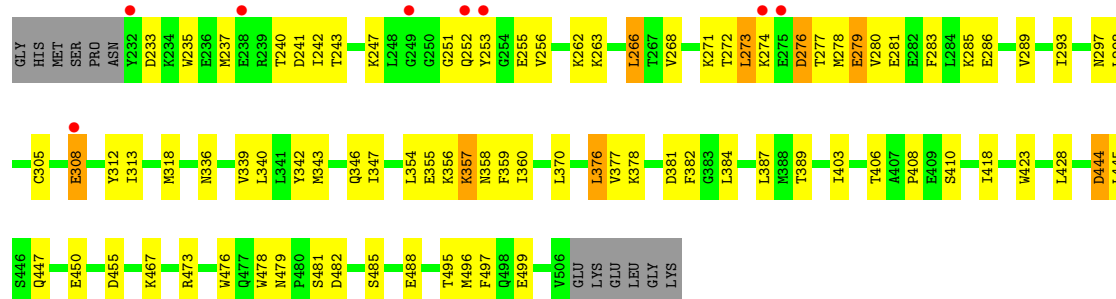
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	30	Total 30	O 30	0	0
5	C	2	Total 2	O 2	0	0

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.

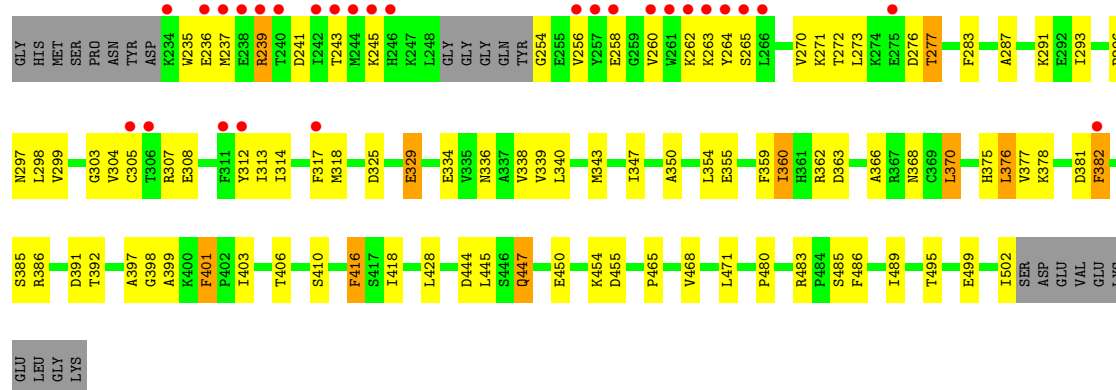
• Molecule 1: Abl Kinase

Chain A: 



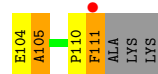
• Molecule 1: Abl Kinase

Chain B: 



• Molecule 2: ATP-Peptide Conjugate

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.67Å 133.32Å 56.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.88 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 97.5 (49.88-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.286 0.231 , 0.283	Depositor DCC
R_{free} test set	1115 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27408 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4586	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: AGS, 112

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	0.42	0/2285	0.66	0/3094
1	B	0.38	0/2204	0.61	0/2983
2	C	0.64	0/59	0.60	0/80
All	All	0.40	0/4548	0.63	0/6157

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	2228	0	2174	69	0
1	B	2150	0	2119	73	0
2	C	57	0	52	3	0
3	B	31	0	12	1	0
4	C	35	0	14	5	0
5	A	53	0	0	1	0
5	B	30	0	0	0	0
5	C	2	0	0	0	0
All	All	4586	0	4371	147	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 17.

All (147) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:239:ARG:HH12	1:B:308:GLU:HB2	1.42	0.84
1:A:293:ILE:HD13	1:A:384:LEU:HD11	1.58	0.83
1:A:358:ASN:OD1	1:A:389:THR:HG22	1.78	0.82
1:A:247:LYS:HE3	1:A:255:GLU:HB3	1.63	0.81
1:A:274:LYS:C	1:A:276:ASP:H	1.86	0.80
1:B:237:MET:HE1	1:B:314:ILE:HG13	1.70	0.73
1:A:403:ILE:HB	1:A:445:LEU:HD22	1.69	0.73
1:A:253:TYR:HA	1:A:277:THR:OG1	1.90	0.72
1:B:298:LEU:HD11	1:B:354:LEU:HD11	1.72	0.70
1:A:293:ILE:HD13	1:A:384:LEU:CD1	2.22	0.70
1:A:279:GLU:OE2	1:A:281:GLU:HB2	1.92	0.70
1:B:276:ASP:O	1:B:277:THR:HG23	1.92	0.69
1:A:271:LYS:HB3	1:A:313:ILE:HB	1.75	0.69
1:A:340:LEU:HA	1:A:343:MET:HE2	1.75	0.68
1:B:258:GLU:HG3	1:B:317:PHE:CE1	2.29	0.67
1:B:391:ASP:OD1	1:B:392:THR:HG23	1.95	0.66
1:B:340:LEU:HA	1:B:343:MET:HE2	1.78	0.64
1:A:318:MET:HG3	1:A:370:LEU:CB	2.26	0.64
1:B:360:ILE:CD1	1:B:385:SER:HB2	2.28	0.64
1:A:272:THR:HG22	1:A:273:LEU:N	2.13	0.64
1:B:495:THR:O	1:B:499:GLU:HG2	1.98	0.63
1:A:485:SER:OG	1:A:488:GLU:HG3	1.97	0.63
1:A:251:GLY:C	1:A:253:TYR:H	2.02	0.62
1:A:479:ASN:HB3	1:A:482:ASP:OD2	2.00	0.61
1:A:243:THR:OG1	1:A:262:LYS:HE2	1.99	0.61
1:A:298:LEU:HD11	1:A:354:LEU:HD13	1.82	0.61
1:B:296:PRO:O	1:B:378:LYS:HE2	2.01	0.61
1:A:336:ASN:OD1	1:A:339:VAL:HG23	2.01	0.60
1:B:293:ILE:HD12	1:B:293:ILE:O	2.00	0.60
1:B:350:ALA:O	1:B:354:LEU:HD13	2.02	0.60
1:A:406:THR:CG2	1:A:410:SER:HB2	2.31	0.60
1:B:360:ILE:HD13	1:B:385:SER:HB2	1.84	0.59
1:B:450:GLU:OE2	1:B:454:LYS:HE3	2.02	0.59
1:A:251:GLY:HA2	4:C:201:112:O2G	2.02	0.59
1:B:485:SER:O	1:B:489:ILE:HG13	2.01	0.59
1:A:305:CYS:HB2	1:A:312:TYR:HB2	1.84	0.59
2:C:111:PHE:N	2:C:111:PHE:CD1	2.71	0.58
1:B:325:ASP:O	1:B:329:GLU:HG3	2.03	0.58
1:B:270:VAL:HG22	1:B:314:ILE:CD1	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:270:VAL:HG22	1:B:314:ILE:HD12	1.86	0.57
1:A:256:VAL:CG1	4:C:201:112:H5'1	2.34	0.57
1:A:274:LYS:C	1:A:276:ASP:N	2.57	0.56
3:B:601:AGS:H3'	3:B:601:AGS:O2B	2.05	0.56
4:C:201:112:H5'2	4:C:201:112:O2B	2.05	0.56
1:B:471:LEU:O	1:B:471:LEU:HD23	2.06	0.56
1:A:318:MET:HG3	1:A:370:LEU:HB3	1.87	0.54
1:B:376:LEU:HD11	1:B:378:LYS:HE3	1.90	0.54
1:B:239:ARG:NH1	1:B:308:GLU:HB2	2.18	0.54
1:A:273:LEU:CD1	1:A:278:MET:HB2	2.37	0.54
1:A:237:MET:HE1	1:A:242:ILE:HD13	1.89	0.54
1:B:447:GLN:CA	1:B:447:GLN:HE21	2.21	0.53
1:A:376:LEU:HD11	1:A:378:LYS:HE3	1.91	0.53
1:B:343:MET:O	1:B:347:ILE:HG12	2.08	0.53
1:B:303:GLY:H	1:B:314:ILE:HB	1.74	0.53
1:B:336:ASN:ND2	1:B:338:VAL:HG12	2.23	0.52
1:B:416:PHE:CD1	1:B:416:PHE:N	2.77	0.52
1:B:336:ASN:HD21	1:B:502:ILE:HG23	1.73	0.52
1:A:243:THR:OG1	1:A:262:LYS:CE	2.58	0.52
2:C:104:GLU:O	2:C:105:ALA:CB	2.56	0.52
1:A:273:LEU:O	1:A:273:LEU:HD23	2.10	0.51
1:A:355:GLU:HG3	1:A:418:ILE:HG12	1.92	0.51
1:B:237:MET:CE	1:B:314:ILE:HG13	2.38	0.51
1:B:336:ASN:HD21	1:B:338:VAL:HG12	1.76	0.51
1:B:287:ALA:O	1:B:291:LYS:HG3	2.11	0.51
1:A:423:TRP:CE3	1:A:476:TRP:HA	2.46	0.50
1:A:297:ASN:ND2	1:A:346:GLN:HB3	2.26	0.50
1:A:286:GLU:HG2	1:A:382:PHE:CD1	2.47	0.50
1:A:272:THR:HG22	1:A:273:LEU:H	1.75	0.50
1:A:370:LEU:N	1:A:370:LEU:HD22	2.27	0.50
1:A:286:GLU:HG2	1:A:382:PHE:CE1	2.46	0.50
1:B:398:GLY:O	1:B:399:ALA:C	2.50	0.50
1:B:480:PRO:HA	1:B:483:ARG:NE	2.27	0.50
1:A:273:LEU:HD12	1:A:278:MET:HB2	1.93	0.49
1:B:297:ASN:HA	1:B:378:LYS:HG2	1.94	0.49
1:B:366:ALA:N	1:B:428:LEU:HD13	2.27	0.49
1:A:237:MET:O	1:A:305:CYS:SG	2.63	0.49
1:B:355:GLU:HG3	1:B:418:ILE:HG12	1.94	0.49
1:B:376:LEU:HD22	1:B:377:VAL:H	1.77	0.49
1:A:273:LEU:HD13	1:A:283:PHE:CD1	2.48	0.49
1:B:245:LYS:NZ	1:B:260:VAL:HG21	2.28	0.49
1:B:304:VAL:HG12	1:B:313:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:376:LEU:HD22	1:B:377:VAL:N	2.27	0.49
1:B:293:ILE:HD11	1:B:381:ASP:OD1	2.13	0.49
1:A:256:VAL:HG12	4:C:201:112:H5'1	1.95	0.49
1:A:347:ILE:HD11	1:A:377:VAL:CG1	2.43	0.48
1:B:334:GLU:OE2	1:B:375:HIS:HE1	1.97	0.47
1:B:241:ASP:OD1	1:B:263:LYS:HE3	2.14	0.47
1:A:495:THR:O	1:A:499:GLU:HG2	2.14	0.47
1:A:256:VAL:HG11	4:C:201:112:H5'1	1.96	0.47
1:B:454:LYS:O	1:B:455:ASP:HB2	2.14	0.47
1:A:406:THR:HG22	1:A:410:SER:HB2	1.96	0.47
1:B:336:ASN:OD1	1:B:339:VAL:HG23	2.15	0.47
1:B:362:ARG:NH1	1:B:385:SER:OG	2.44	0.47
1:B:502:ILE:O	1:B:502:ILE:HG22	2.15	0.47
1:A:241:ASP:HB3	1:A:263:LYS:HE3	1.96	0.47
1:A:356:LYS:C	1:A:358:ASN:H	2.19	0.46
1:B:447:GLN:NE2	1:B:447:GLN:CA	2.79	0.46
1:A:318:MET:HG3	1:A:370:LEU:HB2	1.97	0.46
1:A:251:GLY:C	1:A:253:TYR:N	2.68	0.46
1:B:318:MET:SD	1:B:378:LYS:HD2	2.56	0.46
2:C:104:GLU:O	2:C:105:ALA:HB3	2.16	0.45
1:A:347:ILE:HD11	1:A:377:VAL:HG11	1.97	0.45
1:B:236:GLU:OE2	1:B:307:ARG:HD2	2.16	0.45
1:A:255:GLU:HG3	1:A:255:GLU:H	1.61	0.45
1:A:237:MET:CE	1:A:242:ILE:HD13	2.47	0.45
1:B:340:LEU:HD23	1:B:343:MET:CE	2.46	0.45
1:B:465:PRO:HG2	1:B:468:VAL:CG2	2.47	0.45
1:A:408:PRO:HB3	1:A:478:TRP:CZ3	2.52	0.45
1:A:357:LYS:HB3	1:A:359:PHE:CE1	2.53	0.44
1:A:272:THR:CG2	1:A:273:LEU:N	2.79	0.44
1:B:305:CYS:HB2	1:B:312:TYR:HB2	1.99	0.44
1:B:256:VAL:HG22	1:B:271:LYS:HG3	2.00	0.44
1:B:401:PHE:CD1	1:B:401:PHE:N	2.84	0.44
1:B:243:THR:OG1	1:B:262:LYS:HE3	2.17	0.44
1:B:235:TRP:O	1:B:236:GLU:C	2.56	0.44
1:B:283:PHE:CZ	1:B:313:ILE:HG12	2.53	0.43
1:A:285:LYS:O	1:A:289:VAL:HG23	2.18	0.43
1:B:376:LEU:CD1	1:B:378:LYS:HE3	2.48	0.43
1:B:406:THR:HG22	1:B:410:SER:HB2	2.00	0.43
1:B:273:LEU:HD22	1:B:283:PHE:HB2	2.00	0.43
1:B:486:PHE:CD1	1:B:489:ILE:HD12	2.54	0.42
1:A:276:ASP:CG	1:A:277:THR:H	2.22	0.42
1:A:342:TYR:HB2	1:A:497:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:467:LYS:HD3	1:A:496:MET:SD	2.59	0.42
1:A:473:ARG:HD2	5:A:601:HOH:O	2.18	0.42
1:B:381:ASP:O	1:B:382:PHE:C	2.57	0.42
1:B:450:GLU:O	1:B:454:LYS:HG2	2.19	0.42
1:B:403:ILE:HB	1:B:445:LEU:HD22	2.01	0.42
1:A:308:GLU:N	1:A:308:GLU:OE2	2.52	0.42
1:B:359:PHE:CZ	1:B:386:ARG:HD2	2.55	0.42
1:B:416:PHE:HD1	1:B:416:PHE:N	2.16	0.42
1:A:428:LEU:O	1:A:428:LEU:HD12	2.20	0.41
1:B:299:VAL:HG21	1:B:370:LEU:HD23	2.02	0.41
1:B:264:TYR:O	1:B:265:SER:C	2.59	0.41
1:A:293:ILE:HD11	1:A:381:ASP:HB2	2.01	0.41
1:A:360:ILE:HG21	1:A:387:LEU:HD23	2.01	0.41
1:A:266:LEU:HD13	1:A:268:VAL:CG1	2.51	0.41
1:B:363:ASP:OD2	1:B:368:ASN:ND2	2.54	0.41
1:B:293:ILE:HD12	1:B:293:ILE:C	2.41	0.41
1:B:263:LYS:O	1:B:264:TYR:HB2	2.21	0.41
1:B:254:GLY:HA3	1:B:272:THR:O	2.21	0.41
1:A:233:ASP:OD1	1:A:235:TRP:HD1	2.05	0.40
1:A:444:ASP:OD2	1:A:447:GLN:HG3	2.20	0.40
1:A:357:LYS:HB3	1:A:359:PHE:HE1	1.87	0.40
1:A:251:GLY:O	1:A:253:TYR:N	2.55	0.40
1:A:272:THR:CG2	1:A:273:LEU:H	2.34	0.40
1:B:406:THR:CG2	1:B:410:SER:HB2	2.52	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	273/287 (95%)	247 (90%)	22 (8%)	4 (2%)	15	38
1	B	260/287 (91%)	232 (89%)	26 (10%)	2 (1%)	27	58
2	C	6/11 (54%)	4 (67%)	0	2 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	539/585 (92%)	483 (90%)	48 (9%)	8 (2%)	15	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	ASP
1	B	382	PHE
1	B	397	ALA
2	C	105	ALA
1	A	280	VAL
1	A	252	GLN
1	A	357	LYS
2	C	110	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	238/251 (95%)	228 (96%)	10 (4%)	40	73
1	B	232/251 (92%)	222 (96%)	10 (4%)	40	72
2	C	4/7 (57%)	3 (75%)	1 (25%)	1	2
All	All	474/509 (93%)	453 (96%)	21 (4%)	39	71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	THR
1	A	266	LEU
1	A	273	LEU
1	A	279	GLU
1	A	308	GLU
1	A	376	LEU
1	A	444	ASP
1	A	450	GLU
1	A	455	ASP
1	A	481	SER

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Mol	Chain	Res	Type
1	B	239	ARG
1	B	277	THR
1	B	329	GLU
1	B	360	ILE
1	B	370	LEU
1	B	376	LEU
1	B	401	PHE
1	B	416	PHE
1	B	444	ASP
1	B	447	GLN
2	C	111	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	375	HIS
1	B	447	GLN
1	B	490	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	$\# Z > 2$
3	AGS	B	601	-	33,33,33	2.32	15 (45%)	52,52,52	2.50	16 (30%)
4	112	C	201	2	37,37,37	3.34	12 (32%)	55,57,57	2.32	14 (25%)

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	AGS	B	601	-	-	0/21/38/38	0/1/3/3
4	112	C	201	2	-	0/26/44/44	0/1/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	112	C1S-S1G	-12.21	1.69	1.83
4	C	201	112	PG-S1G	-8.70	1.85	2.08
4	C	201	112	PA-O3A	7.69	1.73	1.59
4	C	201	112	C2'-C1'	5.21	1.60	1.53
3	B	601	AGS	PA-O3A	4.84	1.68	1.59
3	B	601	AGS	C8-N9	4.49	1.43	1.36
3	B	601	AGS	C4-N3	4.42	1.42	1.35
3	B	601	AGS	C2-N3	4.41	1.40	1.32
4	C	201	112	C4-N3	4.40	1.42	1.35
3	B	601	AGS	C2-N1	3.91	1.41	1.33
4	C	201	112	C6-N6	3.54	1.46	1.35
4	C	201	112	PG-O2G	-3.40	1.47	1.55
4	C	201	112	C8-N9	3.22	1.41	1.36
3	B	601	AGS	C5-C4	3.14	1.47	1.40
3	B	601	AGS	C2'-C1'	-2.93	1.49	1.53
3	B	601	AGS	PG-O3B	2.83	1.63	1.60
3	B	601	AGS	C6-N6	2.78	1.44	1.35
4	C	201	112	C2-N1	2.75	1.39	1.33
4	C	201	112	C2-N3	2.71	1.37	1.32
3	B	601	AGS	PB-O1B	2.51	1.61	1.51
3	B	601	AGS	O2'-C2'	2.44	1.48	1.43
3	B	601	AGS	PG-O3G	-2.29	1.51	1.56
4	C	201	112	O4'-C4'	-2.28	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	AGS	PB-O3A	-2.27	1.55	1.59
3	B	601	AGS	PA-O5'	2.24	1.69	1.59
4	C	201	112	C5-C4	2.23	1.45	1.40
3	B	601	AGS	C4-N9	2.13	1.40	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	112	O3A-PB-O3B	9.35	120.67	101.66
3	B	601	AGS	C8-N9-C4	-7.45	101.22	106.90
3	B	601	AGS	O3B-PG-S1G	-7.43	111.23	114.53
3	B	601	AGS	O3A-PB-O3B	6.73	115.35	101.66
4	C	201	112	C8-N9-C4	-5.62	102.61	106.90
4	C	201	112	C1S-C2S-NS	5.55	123.77	115.59
3	B	601	AGS	O2G-PG-S1G	-4.56	107.92	112.73
4	C	201	112	O2G-PG-S1G	4.39	115.40	104.29
3	B	601	AGS	C4-C5-N7	4.36	113.26	109.52
4	C	201	112	N3-C2-N1	-4.29	125.12	128.71
3	B	601	AGS	C2'-C1'-N9	-4.02	102.95	113.27
4	C	201	112	C4-C5-N7	3.93	112.89	109.52
4	C	201	112	PA-O3A-PB	3.62	142.31	131.68
3	B	601	AGS	PA-O3A-PB	3.62	142.31	131.68
3	B	601	AGS	O4'-C1'-N9	3.47	111.66	108.44
4	C	201	112	C4'-O4'-C1'	3.17	113.19	109.75
3	B	601	AGS	N3-C2-N1	-3.13	126.09	128.71
3	B	601	AGS	C8-N9-C1'	3.12	132.53	126.38
3	B	601	AGS	C3'-C2'-C1'	2.88	105.41	100.91
3	B	601	AGS	O3G-PG-S1G	2.77	115.64	112.73
4	C	201	112	C8-N9-C1'	2.61	131.53	126.38
3	B	601	AGS	PB-O3B-PG	-2.59	122.97	131.81
3	B	601	AGS	O3A-PA-O5'	-2.55	92.00	103.41
3	B	601	AGS	O4'-C1'-C2'	2.35	110.38	106.77
4	C	201	112	O2'-C2'-C1'	2.29	118.16	111.23
4	C	201	112	O2S-C2S-NS	-2.26	115.83	122.47
4	C	201	112	O3A-PA-O5'	-2.17	93.70	103.41
3	B	601	AGS	O2A-PA-O5'	2.17	119.43	108.51
4	C	201	112	C2S-C1S-S1G	2.12	117.65	111.24
4	C	201	112	O4'-C4'-C3'	2.01	109.24	105.17

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	275/287 (95%)	-0.06	8 (2%) 49 55	21, 41, 81, 93	0
1	B	264/287 (91%)	0.28	28 (10%) 7 7	25, 52, 104, 117	0
2	C	8/11 (72%)	0.55	1 (12%) 5 5	49, 55, 63, 66	0
All	All	547/585 (93%)	0.11	37 (6%) 17 19	21, 47, 98, 117	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	LYS	4.8
1	B	237	MET	4.6
1	B	244	MET	4.5
1	B	239	ARG	4.2
1	A	274	LYS	4.1
1	B	245	LYS	3.9
1	B	264	TYR	3.9
1	B	243	THR	3.1
1	A	253	TYR	3.0
1	B	266	LEU	3.0
1	B	306	THR	2.8
1	B	261	TRP	2.8
1	A	232	TYR	2.8
1	B	256	VAL	2.8
1	B	262	LYS	2.7
1	B	317	PHE	2.7
1	B	305	CYS	2.6
1	B	258	GLU	2.6
1	A	275	GLU	2.6
1	B	234	LYS	2.5
1	B	238	GLU	2.5
1	B	242	ILE	2.5
1	B	260	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	240	THR	2.4
1	A	238	GLU	2.2
1	B	382	PHE	2.2
1	B	312	TYR	2.2
1	B	236	GLU	2.2
1	B	246	HIS	2.1
1	A	252	GLN	2.1
1	B	311	PHE	2.1
1	A	308	GLU	2.1
2	C	111	PHE	2.1
1	B	275	GLU	2.1
1	B	257	TYR	2.1
1	A	249	GLY	2.0
1	B	265	SER	2.0

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

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

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
3	AGS	B	601	31/31	0.23	0.44	73,87,107,108	0
4	112	C	201	35/35	0.16	-0.52	30,51,77,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.