



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:32 AM GMT

PDB ID : 2C0O
Title : SRC FAMILY KINASE HCK WITH BOUND INHIBITOR A-770041
Authors : Borhani, D.W.; Burchat, A.; Calderwood, D.J.; Hirst, G.C.; Li, B.; Loew, A.
Deposited on : 2005-09-06
Resolution : 2.85 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>

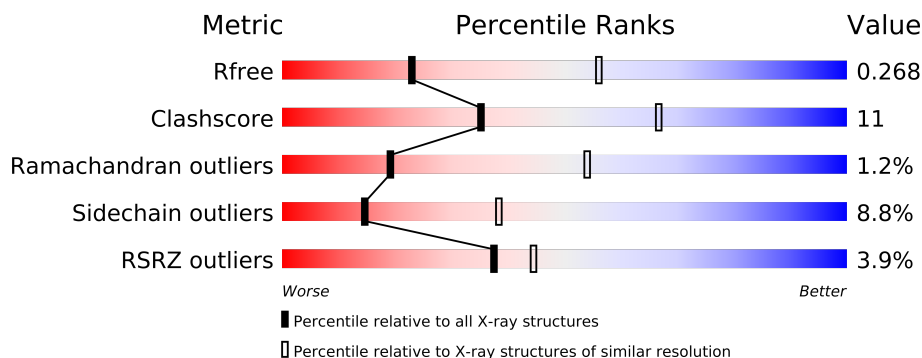
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.85 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	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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	454	
1	B	454	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	B	1507	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7362 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.

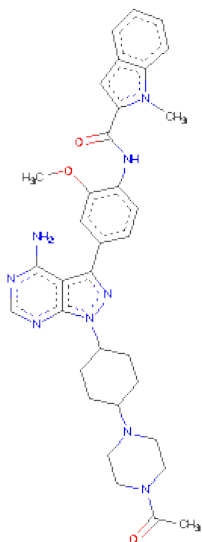
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE HCK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	P	S	0	1	0
			3506	2239	591	655	1	20			
1	B	434	Total	C	N	O	P	S	0	2	0
			3514	2243	593	657	1	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	GLU	GLN	ENGINEERED MUTATION	UNP P08631
A	503	GLU	GLN	ENGINEERED MUTATION	UNP P08631
A	504	ILE	GLN	ENGINEERED MUTATION	UNP P08631
B	502	GLU	GLN	ENGINEERED MUTATION	UNP P08631
B	503	GLU	GLN	ENGINEERED MUTATION	UNP P08631
B	504	ILE	GLN	ENGINEERED MUTATION	UNP P08631

- Molecule 2 is N-(4-{1-[4-(4-ACETYLPYPERAZIN-1-YL)-TRANS-CYCLOHEXYL]-4-AMINO-1H-PYRAZOLO[3,4-D]PYRIMIDIN-3-YL}-2-METHOXYPHENYL)-1-METHYL-1H-INDOLE-2-CARBOXAMIDE (three-letter code: L2G) (formula: C₃₄H₃₉N₉O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			46	34	9	3		
2	B	1	Total	C	N	O	0	0
			46	34	9	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

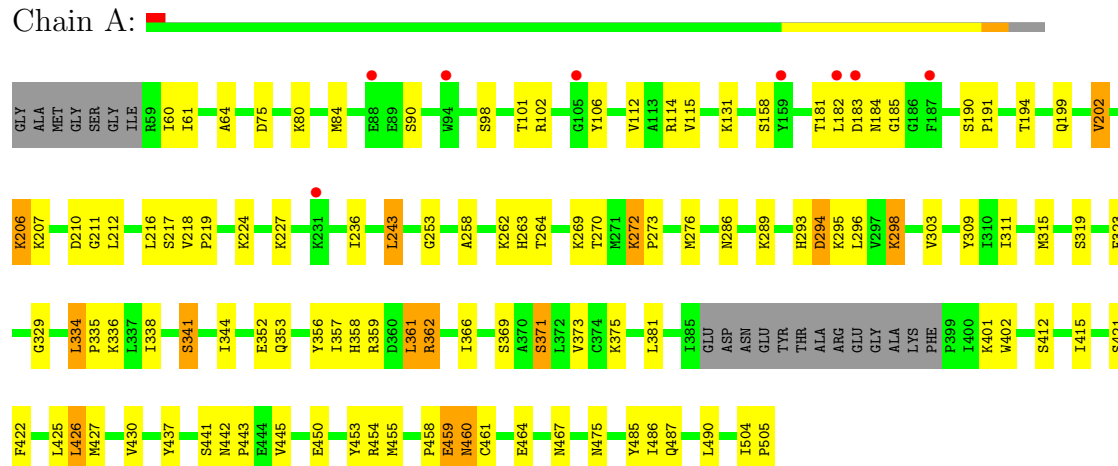
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	89	Total	O	0	0
			89	89		

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.

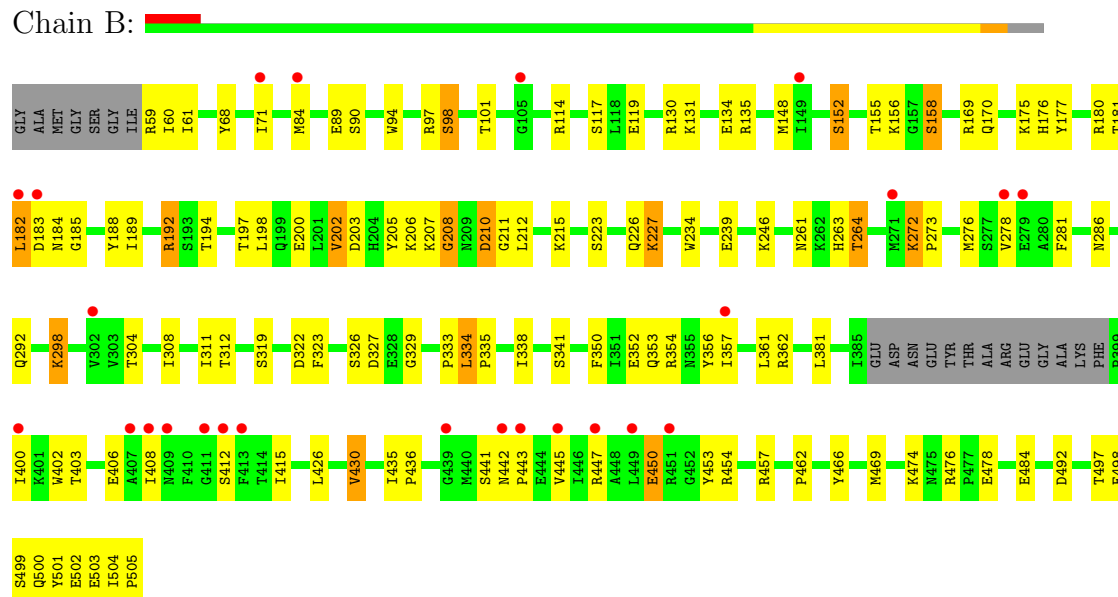
• Molecule 1: TYROSINE-PROTEIN KINASE HCK

Chain A:



• Molecule 1: TYROSINE-PROTEIN KINASE HCK

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.02Å 73.18Å 180.17Å 90.00° 95.52° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85 48.79 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.2 (40.00-2.85) 95.6 (48.79-2.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.273 0.199 , 0.268	Depositor DCC
R_{free} test set	1443 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.1	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 28905 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7362	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 10.98% 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: CA, PTR, L2G

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	0.75	0/3573	0.81	4/4823 (0.1%)
1	B	0.71	2/3581 (0.1%)	0.79	4/4834 (0.1%)
All	All	0.73	2/7154 (0.0%)	0.80	8/9657 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	ARG	CZ-NH1	14.56	1.51	1.33
1	B	447	ARG	NE-CZ	6.38	1.41	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	A	243	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	371	SER	CB-CA-C	-6.08	98.54	110.10
1	A	212	LEU	CA-CB-CG	5.87	128.79	115.30
1	B	447	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	148	MET	CG-SD-CE	5.23	108.57	100.20
1	B	210	ASP	N-CA-C	-5.17	97.03	111.00
1	A	425	LEU	CB-CG-CD2	-5.04	102.43	111.00

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	3506	0	3461	65	0
1	B	3514	0	3466	84	0
2	A	46	0	39	4	0
2	B	46	0	39	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	159	0	0	8	0
4	B	89	0	0	12	0
All	All	7362	0	7005	150	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 11.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263[B]:HIS:HD2	1:B:264:THR:OG1	1.40	1.04
1:B:263[B]:HIS:CD2	1:B:264:THR:OG1	2.18	0.94
1:B:68:TYR:HE1	1:B:227:LYS:HE3	1.47	0.78
1:B:68:TYR:CE1	1:B:227:LYS:HE3	2.19	0.77
1:B:441:SER:O	1:B:445:VAL:HG23	1.87	0.74
1:B:182:LEU:HD23	1:B:183:ASP:H	1.57	0.69
1:A:263[B]:HIS:ND1	1:A:264:THR:OG1	2.23	0.68
1:B:503:GLU:OE1	4:B:2088:HOH:O	2.13	0.66
1:B:234:TRP:HE1	1:B:286:ASN:HD21	1.43	0.66
1:A:352:GLU:HG3	1:A:415:ILE:HG12	1.76	0.66
1:B:457:ARG:HG3	1:B:466:TYR:CG	2.29	0.66
1:B:499:SER:O	4:B:2084:HOH:O	2.12	0.66
1:A:467:ASN:CB	4:A:2132:HOH:O	2.44	0.66
1:A:467:ASN:HB3	4:A:2132:HOH:O	1.97	0.64
1:B:442:ASN:HB2	1:B:443:PRO:HD3	1.78	0.63
1:B:263[B]:HIS:CE1	4:B:2003:HOH:O	2.51	0.63
1:A:303:VAL:HB	1:A:309:TYR:HB2	1.81	0.62
1:A:358:HIS:O	1:A:359:ARG:HB2	1.97	0.62
1:A:341:SER:HB3	1:A:490:LEU:HD13	1.82	0.61
1:B:263[B]:HIS:HE1	4:B:2003:HOH:O	1.84	0.61
1:A:323:PHE:O	1:A:329:GLY:HA3	1.99	0.61
1:B:426:LEU:O	1:B:430:VAL:HG22	2.00	0.61
1:B:498:GLU:HB3	4:B:2082:HOH:O	1.99	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:442:ASN:HB2	1:A:443:PRO:HD3	1.83	0.60
1:B:400:ILE:HD11	1:B:442:ASN:HB3	1.83	0.60
1:B:210:ASP:O	1:B:212:LEU:N	2.32	0.59
1:B:239:GLU:CD	1:B:239:GLU:H	2.06	0.59
1:B:403:THR:HG22	1:B:408:ILE:HG13	1.84	0.59
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.67	0.58
1:A:441:SER:O	1:A:445:VAL:HG23	2.04	0.58
1:B:152:SER:HB2	4:B:2019:HOH:O	2.03	0.58
1:B:206:LYS:O	1:B:208:GLY:N	2.36	0.57
1:B:182:LEU:HD23	1:B:183:ASP:N	2.19	0.57
1:A:422:PHE:CE2	1:A:426:LEU:HD22	2.40	0.56
1:B:502:GLU:OE2	4:B:2084:HOH:O	2.18	0.56
1:B:323:PHE:O	1:B:329:GLY:HA3	2.06	0.56
1:B:261:ASN:HB2	1:B:263[B]:HIS:CE1	2.41	0.56
1:B:175:LYS:HD2	1:B:502:GLU:OE2	2.07	0.55
1:B:60:ILE:HD13	1:B:114:ARG:NH2	2.21	0.55
1:A:464:GLU:HG2	1:B:497:THR:O	2.06	0.55
1:B:357:ILE:HD12	4:B:2052:HOH:O	2.06	0.54
1:B:442:ASN:HB2	1:B:443:PRO:CD	2.37	0.54
1:A:253:GLY:HA3	1:A:270:THR:O	2.08	0.54
1:B:272:LYS:HE3	1:B:273:PRO:HD2	1.90	0.54
1:A:211:GLY:HA3	1:A:504:ILE:HD11	1.90	0.54
1:B:319:SER:HB3	2:B:1506:L2G:H161	1.90	0.54
1:A:64:ALA:HA	1:A:112:VAL:HG12	1.89	0.54
1:A:272:LYS:HD2	1:A:273:PRO:HD2	1.91	0.53
1:A:341:SER:OG	1:A:426:LEU:HD13	2.09	0.53
1:A:401:LYS:HE2	1:A:437:TYR:HB2	1.91	0.53
1:B:189:ILE:HG22	1:B:504:ILE:HG21	1.89	0.52
1:A:336:LYS:HE3	4:A:2091:HOH:O	2.10	0.52
1:B:130:ARG:NH2	1:B:500:GLN:HG2	2.25	0.52
1:B:334:LEU:HB3	1:B:335:PRO:HD3	1.91	0.52
1:B:155:THR:HG22	1:B:158:SER:HB2	1.93	0.51
1:A:98:SER:HB3	1:A:101:THR:OG1	2.11	0.51
1:A:362:ARG:HB3	1:A:402:TRP:CD1	2.46	0.51
1:A:319:SER:HB3	2:A:1506:L2G:H161	1.91	0.51
1:B:334:LEU:HD21	1:B:462:PRO:HD3	1.93	0.51
1:A:218:VAL:HG23	1:A:219:PRO:HD2	1.92	0.50
1:B:205:TYR:HE1	1:B:210:ASP:HB2	1.76	0.50
1:B:356:TYR:C	1:B:357:ILE:HG13	2.31	0.50
1:A:344:ILE:HG12	1:A:366:ILE:HD12	1.93	0.50
1:B:234:TRP:HE1	1:B:286:ASN:ND2	2.09	0.49
1:B:261:ASN:O	1:B:263[B]:HIS:ND1	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:239:GLU:CD	1:B:239:GLU:N	2.66	0.49
2:B:1506:L2G:H5N1	2:B:1506:L2G:C6	2.26	0.49
1:B:484:GLU:HB3	4:B:2070:HOH:O	2.12	0.49
1:B:177:TYR:CE2	1:B:502:GLU:HB2	2.48	0.48
1:A:206:LYS:HG3	1:A:216:LEU:O	2.13	0.48
1:B:474:LYS:HE3	4:B:2067:HOH:O	2.12	0.48
1:A:334:LEU:HB3	1:A:335:PRO:HD3	1.96	0.48
1:A:102:ARG:HD3	4:A:2018:HOH:O	2.14	0.48
1:A:84:MET:HE3	1:A:98:SER:HA	1.96	0.47
1:A:182:LEU:HD23	1:A:183:ASP:N	2.29	0.47
1:B:352:GLU:HG3	1:B:415:ILE:HG12	1.95	0.47
1:B:450:GLU:HA	1:B:450:GLU:OE2	2.15	0.47
1:B:435:ILE:HG22	1:B:436:PRO:O	2.14	0.47
1:A:460:ASN:N	1:A:460:ASN:OD1	2.47	0.47
1:A:369:SER:CB	4:A:2104:HOH:O	2.61	0.47
1:B:503:GLU:O	1:B:504:ILE:HB	2.15	0.47
1:B:333:PRO:HB2	1:B:335:PRO:HD2	1.97	0.47
1:A:276:MET:O	1:A:276:MET:SD	2.73	0.47
1:B:114:ARG:HG3	1:B:114:ARG:HH11	1.79	0.47
2:A:1506:L2G:H5N1	2:A:1506:L2G:C6	2.28	0.47
1:A:236:ILE:O	1:A:303:VAL:HG22	2.15	0.47
1:B:182:LEU:CD2	1:B:183:ASP:H	2.25	0.47
1:B:362:ARG:HB3	1:B:402:TRP:CD1	2.49	0.47
1:A:61:ILE:HG22	1:A:115:VAL:HG21	1.96	0.46
1:B:312:THR:OG1	2:B:1506:L2G:H153	2.15	0.46
1:B:292:GLN:NE2	1:B:298:LYS:HZ1	2.13	0.46
1:A:338:ILE:O	1:A:341:SER:HB2	2.14	0.46
1:B:183:ASP:O	1:B:185:GLY:N	2.41	0.46
1:B:272:LYS:HD2	1:B:272:LYS:HA	1.80	0.46
1:B:338:ILE:O	1:B:341:SER:HB2	2.16	0.45
1:A:293:HIS:HB3	1:A:296:LEU:HG	1.97	0.45
1:B:131:LYS:NZ	1:B:134:GLU:OE1	2.42	0.45
1:B:180:ARG:HG3	1:B:188:TYR:CE2	2.52	0.45
1:B:71:ILE:HD12	1:B:263[B]:HIS:CD2	2.52	0.45
1:A:356:TYR:O	1:A:357:ILE:HG13	2.16	0.45
1:A:80:LYS:HD2	4:A:2001:HOH:O	2.17	0.45
1:B:198:LEU:O	1:B:202:VAL:HG13	2.17	0.45
1:B:98:SER:HG	1:B:101:THR:H	1.63	0.44
1:B:354:ARG:HD3	1:B:354:ARG:HA	1.63	0.44
1:B:130:ARG:NH2	1:B:492:ASP:OD1	2.51	0.44
1:B:453:TYR:O	1:B:454:ARG:HD3	2.18	0.44
1:B:89:GLU:HG2	1:B:94:TRP:CE2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:487:GLN:OE1	4:A:2143:HOH:O	2.21	0.43
1:A:269:LYS:HB2	1:A:269:LYS:HE3	1.70	0.43
1:A:458:PRO:HG2	1:A:461:CYS:HB2	2.00	0.43
1:B:131:LYS:O	1:B:134:GLU:HB3	2.19	0.43
1:B:453:TYR:O	1:B:454:ARG:CD	2.66	0.43
1:B:246:LYS:NZ	4:B:2034:HOH:O	2.51	0.43
1:B:476:ARG:HB3	1:B:478:GLU:OE1	2.18	0.43
1:B:281:PHE:CE2	1:B:308:ILE:HG21	2.53	0.43
1:A:485:TYR:O	1:A:486:ILE:C	2.54	0.43
1:A:459:GLU:OE1	1:A:459:GLU:HA	2.18	0.43
1:B:322:ASP:OD2	2:B:1506:L2G:H271	2.19	0.43
1:A:341:SER:OG	1:A:426:LEU:CD1	2.66	0.42
1:A:311:ILE:N	1:A:311:ILE:HD12	2.34	0.42
1:A:361:LEU:HD23	1:A:361:LEU:HA	1.54	0.42
1:A:371:SER:HB2	1:A:373:VAL:HG23	2.00	0.42
1:A:60:ILE:HG22	1:A:60:ILE:O	2.19	0.42
1:A:75:ASP:HA	1:A:106:TYR:H	1.85	0.42
1:B:234:TRP:NE1	1:B:286:ASN:ND2	2.68	0.42
1:A:315:MET:H	2:A:1506:L2G:C11	2.33	0.42
1:A:183:ASP:O	1:A:185:GLY:N	2.51	0.42
1:A:453:TYR:O	1:A:454:ARG:HD3	2.19	0.42
1:A:298:LYS:HG2	4:A:2077:HOH:O	2.20	0.41
1:B:59:ARG:HE	1:B:61:ILE:HD11	1.85	0.41
1:B:504:ILE:HA	1:B:505:PRO:HD2	1.60	0.41
1:A:243:LEU:HA	1:A:258:ALA:HB2	2.01	0.41
1:B:292:GLN:NE2	1:B:298:LYS:NZ	2.68	0.41
1:B:197:THR:OG1	1:B:200:GLU:HG3	2.21	0.41
1:A:295:LYS:O	1:A:375:LYS:HA	2.21	0.41
1:B:311:ILE:HD12	1:B:311:ILE:N	2.36	0.41
1:B:400:ILE:HD11	1:B:442:ASN:CB	2.49	0.41
1:A:381:LEU:HB2	2:A:1506:L2G:C26	2.51	0.41
1:B:176:HIS:HB3	1:B:501:PTR:CE1	2.51	0.41
1:B:426:LEU:HD23	1:B:469:MET:HG2	2.03	0.41
1:A:218:VAL:CG2	1:A:219:PRO:HD2	2.50	0.41
1:A:190:SER:HA	1:A:191:PRO:HD3	1.82	0.41
1:A:294:ASP:N	1:A:294:ASP:OD1	2.54	0.41
1:A:272:LYS:HD2	1:A:273:PRO:CD	2.51	0.40
1:A:504:ILE:HA	1:A:505:PRO:HD2	1.39	0.40
1:A:315:MET:HE2	1:A:375:LYS:HB2	2.01	0.40
1:A:182:LEU:HD23	1:A:183:ASP:H	1.86	0.40
1:A:427:MET:HG2	1:A:455:MET:CE	2.52	0.40
1:B:350:PHE:HA	4:B:2049:HOH:O	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:VAL:O	1:A:206:LYS:HB2	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	430/454 (95%)	398 (93%)	27 (6%)	5 (1%)	19	54
1	B	431/454 (95%)	398 (92%)	28 (6%)	5 (1%)	19	54
All	All	861/908 (95%)	796 (92%)	55 (6%)	10 (1%)	19	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	211	GLY
1	A	184	ASN
1	A	459	GLU
1	B	182	LEU
1	B	184	ASN
1	B	207	LYS
1	A	460	ASN
1	A	217	SER
1	A	362	ARG
1	B	208	GLY

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	378/393 (96%)	349 (92%)	29 (8%)	18	46
1	B	379/393 (96%)	342 (90%)	37 (10%)	12	31
All	All	757/786 (96%)	691 (91%)	66 (9%)	14	39

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	114	ARG
1	A	131	LYS
1	A	158	SER
1	A	181	THR
1	A	194	THR
1	A	199	GLN
1	A	202	VAL
1	A	206	LYS
1	A	207	LYS
1	A	210	ASP
1	A	224	LYS
1	A	227	LYS
1	A	262	LYS
1	A	272	LYS
1	A	286	ASN
1	A	289	LYS
1	A	294	ASP
1	A	298	LYS
1	A	334	LEU
1	A	341	SER
1	A	353	GLN
1	A	361	LEU
1	A	412	SER
1	A	421	SER
1	A	426	LEU
1	A	430	VAL
1	A	450	GLU
1	A	475	ASN
1	B	84	MET
1	B	90	SER
1	B	97	ARG
1	B	98	SER
1	B	117	SER
1	B	119	GLU

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Mol	Chain	Res	Type
1	B	135	ARG
1	B	152	SER
1	B	156	LYS
1	B	158	SER
1	B	169	ARG
1	B	170	GLN
1	B	181	THR
1	B	192	ARG
1	B	194	THR
1	B	202	VAL
1	B	203	ASP
1	B	215	LYS
1	B	223	SER
1	B	226	GLN
1	B	227	LYS
1	B	264	THR
1	B	272	LYS
1	B	276	MET
1	B	278	VAL
1	B	298	LYS
1	B	304	THR
1	B	326	SER
1	B	327	ASP
1	B	334	LEU
1	B	353	GLN
1	B	361	LEU
1	B	381	LEU
1	B	406	GLU
1	B	412	SER
1	B	430	VAL
1	B	450	GLU

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	209	ASN
1	A	226	GLN
1	A	261	ASN
1	A	475	ASN
1	B	214	GLN
1	B	286	ASN
1	B	292	GLN

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Mol	Chain	Res	Type
1	B	442	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	PTR	A	501	1,3	16,16,17	4.91	2 (12%)	20,22,24	1.27	1 (5%)
1	PTR	B	501	1,3	16,16,17	5.04	3 (18%)	20,22,24	1.16	3 (15%)

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	501	1,3	-	0/9/11/13	0/1/1/1
1	PTR	B	501	1,3	-	0/9/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	501	PTR	O-C	18.83	1.24	1.11
1	A	501	PTR	O-C	18.42	1.24	1.11
1	A	501	PTR	OH-CZ	-6.38	1.24	1.40
1	B	501	PTR	OH-CZ	-6.20	1.24	1.40
1	B	501	PTR	CA-C	2.78	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	PTR	C-CA-N	-4.61	109.22	113.83
1	B	501	PTR	C-CA-N	-2.68	111.15	113.83
1	B	501	PTR	O2P-P-O1P	2.26	117.82	110.44
1	B	501	PTR	P-OH-CZ	2.20	129.77	123.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	L2G	A	1506	-	52,52,52	1.32	3 (5%)	71,76,76	2.31	13 (18%)
2	L2G	B	1506	-	52,52,52	1.03	3 (5%)	71,76,76	2.37	15 (21%)

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	L2G	A	1506	-	-	0/21/46/46	0/3/7/7
2	L2G	B	1506	-	-	0/21/46/46	0/3/7/7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1506	L2G	C4-N2	-5.50	1.31	1.36
2	A	1506	L2G	C26-C24	-3.67	1.33	1.41
2	B	1506	L2G	C4-N2	-3.41	1.33	1.36
2	B	1506	L2G	C26-C24	-3.13	1.34	1.41
2	B	1506	L2G	C20-N8	2.35	1.41	1.36
2	A	1506	L2G	C32-C30	2.06	1.41	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1506	L2G	N3-C11-N4	-9.69	120.61	128.71
2	B	1506	L2G	N3-C11-N4	-9.65	120.64	128.71
2	B	1506	L2G	C10-N2-N1	-9.23	114.38	121.15
2	A	1506	L2G	C21-C26-C24	8.76	113.91	106.27
2	B	1506	L2G	C21-C26-C24	8.75	113.90	106.27
2	A	1506	L2G	C10-N2-N1	-8.62	114.83	121.15
2	B	1506	L2G	O1-C8-C12	4.55	120.10	114.83
2	A	1506	L2G	O1-C8-C12	4.12	119.60	114.83
2	B	1506	L2G	N3-C4-N2	3.52	132.75	127.68
2	A	1506	L2G	C3-C1-N1	3.51	125.53	120.72
2	A	1506	L2G	N3-C4-N2	3.41	132.59	127.68
2	B	1506	L2G	C3-C1-N1	3.38	125.36	120.72
2	B	1506	L2G	C26-C24-N8	-3.22	105.78	109.17
2	A	1506	L2G	C20-C21-C26	-3.09	103.64	106.17
2	A	1506	L2G	C26-C24-N8	-3.08	105.93	109.17
2	B	1506	L2G	C2-C4-N3	-2.84	120.09	125.71
2	A	1506	L2G	C2-C4-N3	-2.80	120.17	125.71
2	B	1506	L2G	C20-C21-C26	-2.71	103.94	106.17
2	B	1506	L2G	O1-C8-C6	-2.55	119.79	124.23
2	A	1506	L2G	C20-N8-C24	2.49	108.80	106.34
2	B	1506	L2G	C23-C28-N9	-2.49	104.56	110.58
2	A	1506	L2G	O1-C8-C6	-2.48	119.91	124.23
2	A	1506	L2G	C11-N3-C4	2.22	120.33	114.01
2	B	1506	L2G	C11-N3-C4	2.16	120.17	114.01
2	B	1506	L2G	C22-C27-N9	-2.13	105.42	110.58
2	B	1506	L2G	C12-N6-C18	-2.10	120.88	126.83
2	A	1506	L2G	C23-C28-N9	-2.07	105.57	110.58
2	B	1506	L2G	C30-C26-C21	-2.02	126.08	133.02

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	434/454 (95%)	0.50	8 (1%) 65 74	35, 51, 66, 75	0
1	B	434/454 (95%)	0.48	25 (5%) 22 26	35, 52, 66, 75	0
All	All	868/908 (95%)	0.49	33 (3%) 37 45	35, 52, 66, 75	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	443	PRO	4.3
1	B	182	LEU	3.6
1	B	409	ASN	3.4
1	B	449	LEU	3.3
1	A	183	ASP	3.1
1	A	182	LEU	3.0
1	B	407	ALA	3.0
1	B	408	ILE	2.9
1	A	187	PHE	2.8
1	B	357	ILE	2.8
1	B	447	ARG	2.7
1	B	451	ARG	2.5
1	A	105	GLY	2.5
1	B	271	MET	2.5
1	B	183	ASP	2.5
1	B	442	ASN	2.5
1	B	105	GLY	2.5
1	B	149	ILE	2.5
1	B	445	VAL	2.3
1	B	302	VAL	2.3
1	A	159	TYR	2.3
1	A	88	GLU	2.2
1	B	279	GLU	2.2
1	B	413	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	400	ILE	2.2
1	A	231	LYS	2.1
1	B	278	VAL	2.1
1	B	412	SER	2.1
1	B	439	GLY	2.1
1	B	84	MET	2.0
1	B	71	ILE	2.0
1	A	94	TRP	2.0
1	B	411	GLY	2.0

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	501	16/17	0.19	-0.84	49,52,54,54	0
1	PTR	B	501	16/17	0.19	-0.88	49,51,53,54	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
3	CA	B	1507	1/1	0.29	2.91	48,48,48,48	0
2	L2G	A	1506	46/46	0.24	0.51	40,46,63,67	0
2	L2G	B	1506	46/46	0.23	0.41	40,47,62,66	0
3	CA	A	1507	1/1	0.21	-0.82	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.