Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:52 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 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:

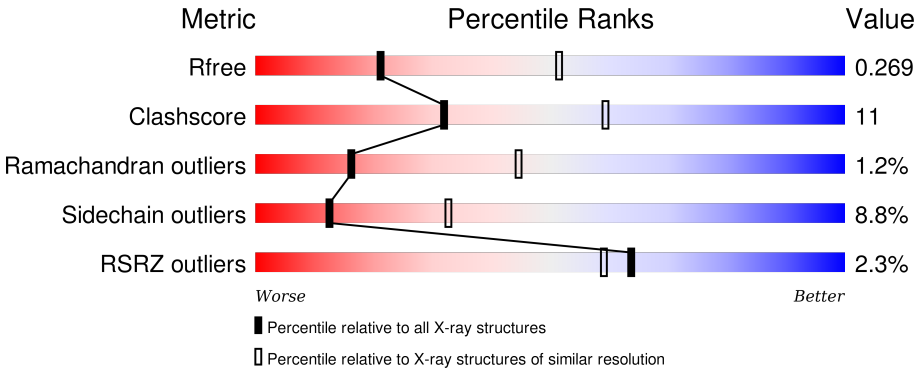
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

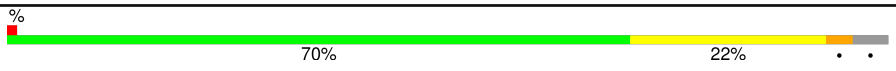
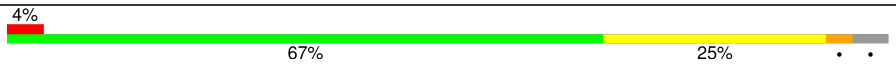
The reported resolution of this entry is 2.85 Å.

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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (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. 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	454	
1	B	454	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 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.

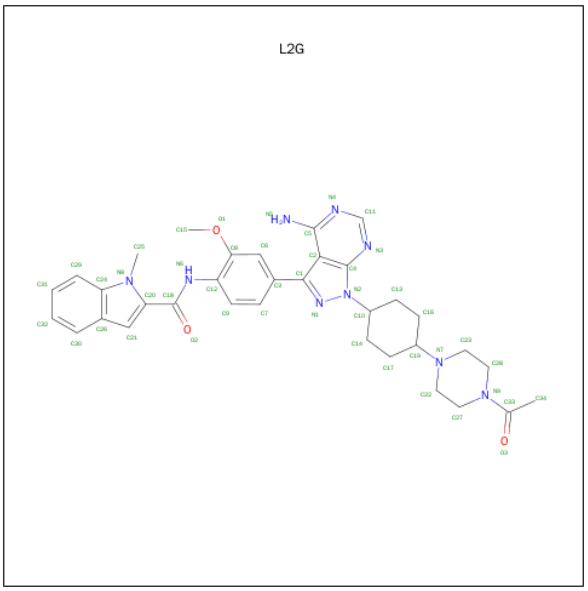
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE HCK.

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-ACETYLPIPERAZIN-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: $C_{34}H_{39}N_9O_3$).



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

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

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

- Molecule 4 is water.

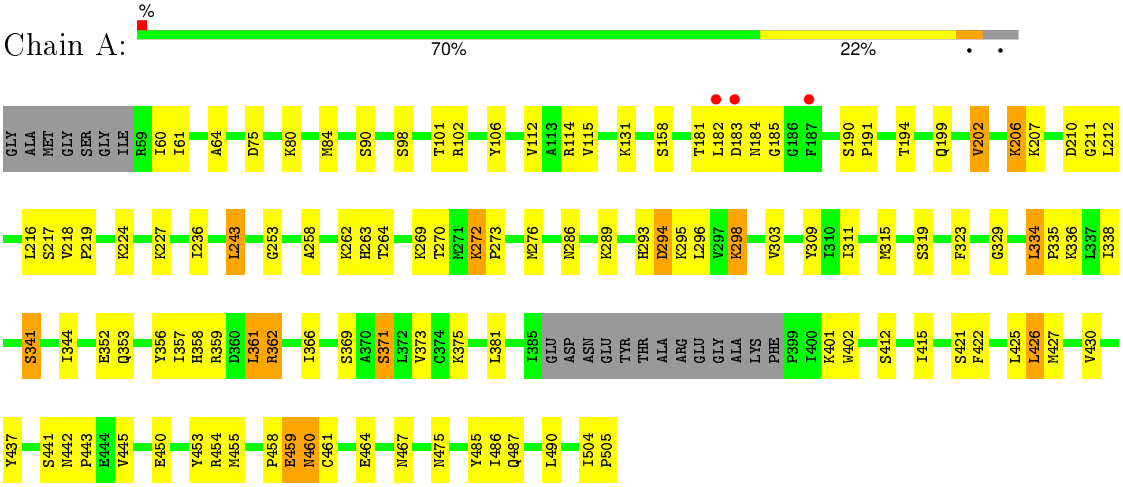
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	159	Total O 159 159	0	0
4	B	89	Total O 89 89	0	0

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.

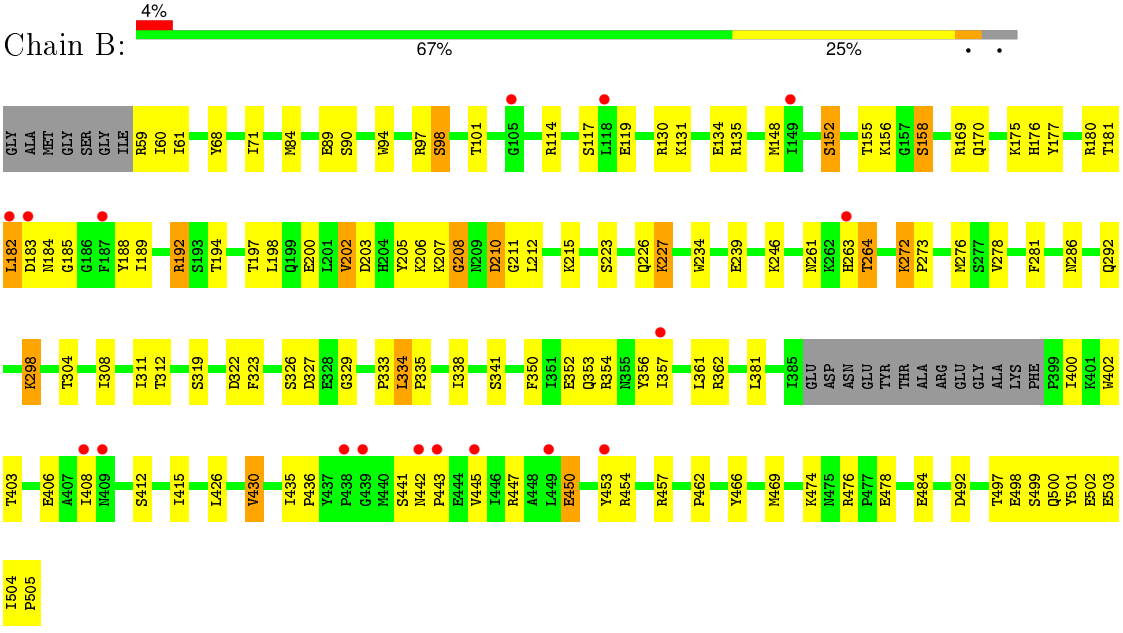
- Molecule 1: TYROSINE-PROTEIN KINASE HCK

Chain A:



- Molecule 1: TYROSINE-PROTEIN KINASE HCK

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.27 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.273 0.198 , 0.269	Depositor DCC
R_{free} test set	1440 reflections (5.26%)	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 , 72.1	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 28905 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[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: 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(^{o})	Ideal(^{o})
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 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	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

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 11.

All (150) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ASN:O	1:B:263[B]:HIS:ND1	2.45	0.49
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:202:VAL:O	1:A:206:LYS:HB2	2.22	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	430/454 (95%)	398 (93%)	27 (6%)	5 (1%)	16	44
1	B	431/454 (95%)	398 (92%)	28 (6%)	5 (1%)	16	44
All	All	861/908 (95%)	796 (92%)	55 (6%)	10 (1%)	16	44

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 (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	378/393 (96%)	349 (92%)	29 (8%)	16 39
1	B	379/393 (96%)	342 (90%)	37 (10%)	10 27
All	All	757/786 (96%)	691 (91%)	66 (9%)	12 33

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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
1	B	442	ASN

5.3.3 RNA

There are no RNA molecules 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	14,16,17	1.88	1 (7%)	18,22,24	0.91	0
1	PTR	B	501	1,3	14,16,17	1.89	1 (7%)	18,22,24	1.07	2 (11%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	PTR	OH-CZ	-6.77	1.24	1.40
1	B	501	PTR	OH-CZ	-6.58	1.24	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	501	PTR	P-OH-CZ	2.09	129.77	123.76
1	B	501	PTR	O2P-P-O1P	2.25	117.82	110.58

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	B	501	PTR	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	-	48,52,52	1.08	3 (6%)	61,76,76	2.18	9 (14%)
2	L2G	B	1506	-	48,52,52	0.92	2 (4%)	61,76,76	2.22	11 (18%)

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	-	-	0/19/46/46	0/7/7/7
2	L2G	B	1506	-	-	0/19/46/46	0/7/7/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1506	L2G	C26-C24	-3.62	1.33	1.41
2	B	1506	L2G	C26-C24	-3.09	1.34	1.41
2	A	1506	L2G	C32-C30	2.04	1.41	1.36
2	B	1506	L2G	C21-C20	2.16	1.40	1.38
2	A	1506	L2G	C21-C20	2.19	1.40	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1506	L2G	N3-C11-N4	-10.82	120.61	128.89
2	B	1506	L2G	N3-C11-N4	-10.78	120.64	128.89
2	B	1506	L2G	C26-C24-N8	-3.22	105.78	109.17
2	A	1506	L2G	C26-C24-N8	-3.08	105.93	109.17
2	B	1506	L2G	C23-C28-N9	-2.60	104.56	110.49
2	B	1506	L2G	O1-C8-C6	-2.59	119.79	124.21
2	A	1506	L2G	O1-C8-C6	-2.52	119.91	124.21
2	A	1506	L2G	C20-C21-C26	-2.34	103.64	106.55
2	B	1506	L2G	C22-C27-N9	-2.23	105.42	110.49
2	B	1506	L2G	C12-N6-C18	-2.22	120.88	127.06
2	A	1506	L2G	C23-C28-N9	-2.16	105.57	110.49
2	B	1506	L2G	C20-C21-C26	-2.09	103.94	106.55
2	B	1506	L2G	C30-C26-C21	-2.04	126.08	133.00
2	A	1506	L2G	C28-N9-C27	2.02	116.30	112.56
2	B	1506	L2G	C3-C1-N1	3.60	125.36	120.71
2	A	1506	L2G	O1-C8-C12	3.70	119.60	114.87
2	A	1506	L2G	C3-C1-N1	3.73	125.53	120.71
2	B	1506	L2G	O1-C8-C12	4.10	120.10	114.87
2	B	1506	L2G	C21-C26-C24	8.75	113.90	106.27
2	A	1506	L2G	C21-C26-C24	8.76	113.91	106.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1506	L2G	4	0
2	B	1506	L2G	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	433/454 (95%)	0.34	3 (0%) 89 88	35, 51, 66, 75	0
1	B	433/454 (95%)	0.39	17 (3%) 43 36	35, 52, 66, 75	0
All	All	866/908 (95%)	0.36	20 (2%) 64 59	35, 52, 66, 75	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	PHE	3.5
1	B	443	PRO	3.3
1	A	182	LEU	3.1
1	A	183	ASP	2.8
1	B	182	LEU	2.7
1	B	183	ASP	2.5
1	B	263[A]	HIS	2.5
1	B	408	ILE	2.4
1	B	105	GLY	2.4
1	B	439	GLY	2.4
1	B	445	VAL	2.3
1	B	453	TYR	2.2
1	B	357	ILE	2.2
1	B	449	LEU	2.2
1	B	149	ILE	2.1
1	B	438	PRO	2.1
1	B	409	ASN	2.1
1	B	187	PHE	2.1
1	B	118	LEU	2.0
1	B	442	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PTR	A	501	16/17	0.97	0.20	-	49,52,54,54	0
1	PTR	B	501	16/17	0.97	0.17	-	49,51,53,54	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CA	B	1507	1/1	0.96	0.25	2.56	48,48,48,48	0
2	L2G	A	1506	46/46	0.97	0.25	0.80	40,46,63,67	0
2	L2G	B	1506	46/46	0.96	0.23	0.14	40,47,62,66	0
3	CA	A	1507	1/1	0.98	0.21	-0.59	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.