



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:14 am GMT

PDB ID : 2C0I  
Title : SRC FAMILY KINASE HCK WITH BOUND INHIBITOR A-420983  
Authors : Borhani, D.W.; Burchat, A.; Calderwood, D.J.; Hirst, G.C.; Li, B.; Loew, A.  
Deposited on : 2005-09-03  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

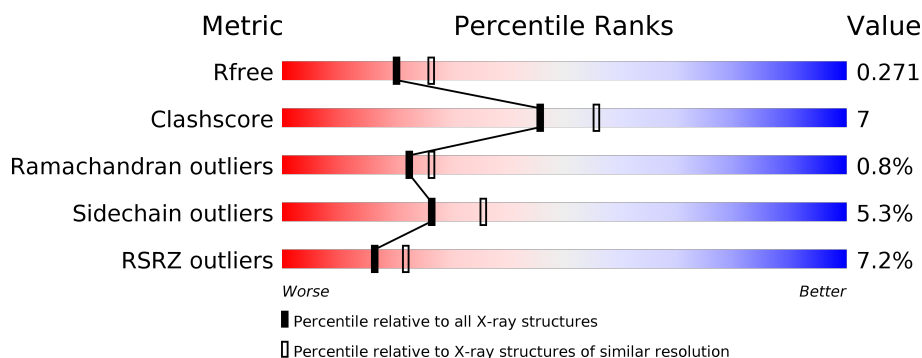
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	454	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7383 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.

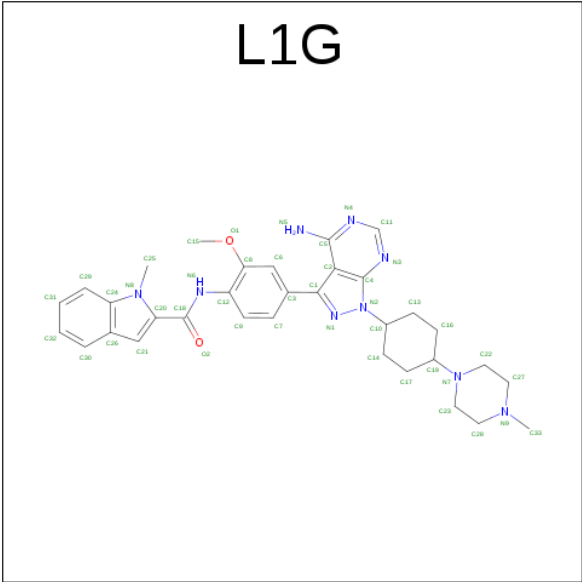
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE HCK.

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-{4-AMINO-1-[4-(4-METHYLPIPERAZIN-1-YL)-TRANS-CYCLOHEXYL]-1H-PYRAZOLO[3,4-D]PYRIMIDIN-3-YL}-2-METHOXYPHENYL)-1-METHYL-1H-INDOLE-2-CARBOXAMIDE (three-letter code: L1G) (formula: C<sub>33</sub>H<sub>39</sub>N<sub>9</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	33	9	2		
2	B	1	Total	C	N	O	0	0
			44	33	9	2		

- 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		

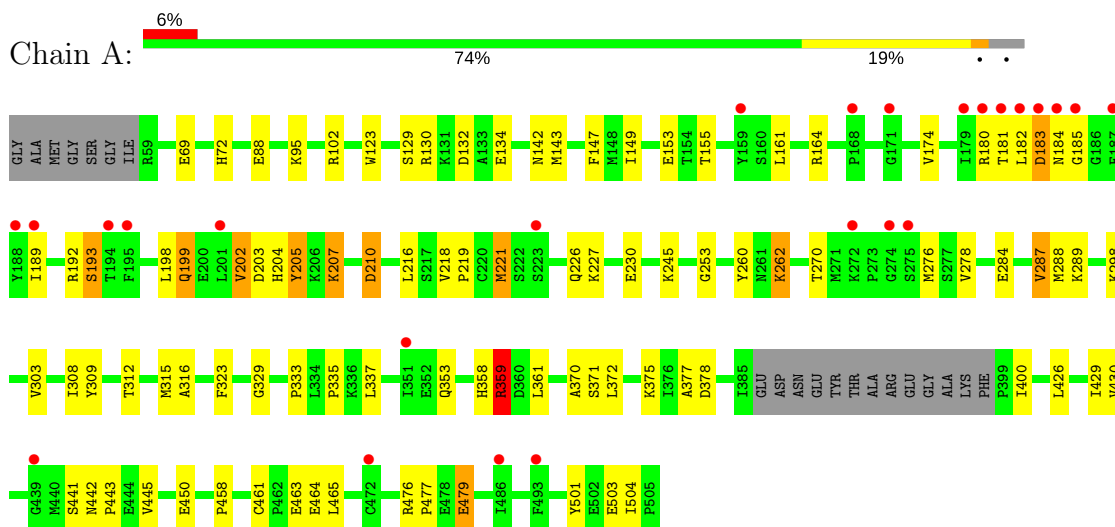
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total	O	0	0
			174	174		
4	B	99	Total	O	0	0
			99	99		

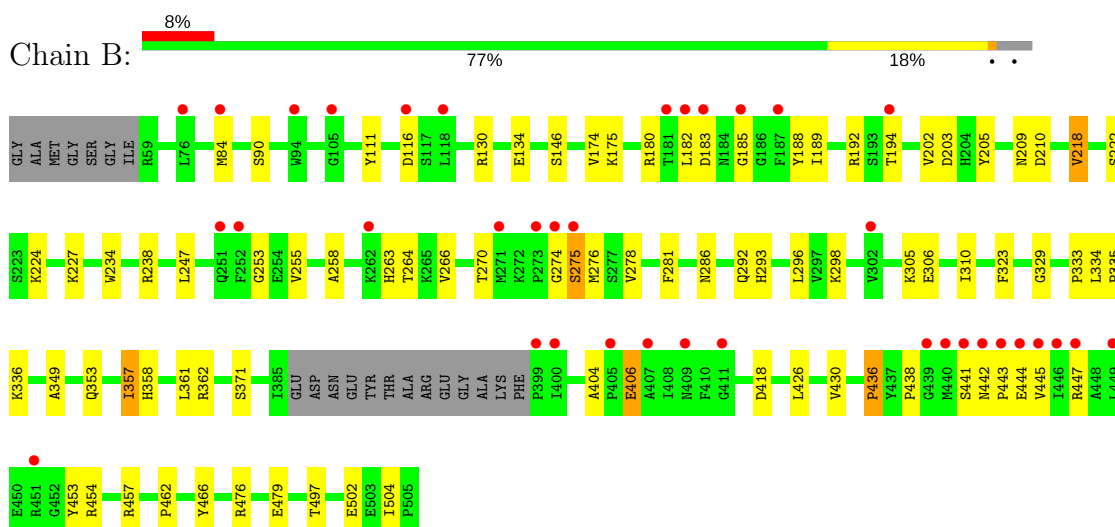
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



#### • Molecule 1: TYROSINE-PROTEIN KINASE HCK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.08Å 73.12Å 179.49Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	19.96 – 2.30 48.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.9 (19.96-2.30) 89.8 (48.81-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.222 , 0.274 0.222 , 0.271	Depositor DCC
$R_{free}$ test set	2515 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, L1G, 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	0.87	14/3573 (0.4%)	0.74	4/4823 (0.1%)
1	B	0.61	4/3581 (0.1%)	0.65	3/4834 (0.1%)
All	All	0.75	18/7154 (0.3%)	0.70	7/9657 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	LYS	CD-CE	18.24	1.96	1.51
1	B	444	GLU	CD-OE1	12.89	1.39	1.25
1	B	444	GLU	CD-OE2	10.23	1.36	1.25
1	A	193	SER	CB-OG	10.04	1.55	1.42
1	A	207	LYS	CE-NZ	9.88	1.73	1.49
1	A	205	TYR	CG-CD1	9.64	1.51	1.39
1	A	205	TYR	CE2-CZ	9.01	1.50	1.38
1	A	203	ASP	CG-OD1	8.80	1.45	1.25
1	A	203	ASP	CG-OD2	8.75	1.45	1.25
1	B	447	ARG	CZ-NH1	8.30	1.43	1.33
1	A	210	ASP	CG-OD1	8.28	1.44	1.25
1	A	192	ARG	NE-CZ	8.00	1.43	1.33
1	B	447	ARG	NE-CZ	7.64	1.43	1.33
1	A	210	ASP	CG-OD2	6.36	1.40	1.25
1	A	183	ASP	CG-OD1	5.89	1.38	1.25
1	A	204	HIS	CB-CG	5.73	1.60	1.50
1	A	207	LYS	CG-CD	5.38	1.70	1.52
1	A	192	ARG	CZ-NH1	5.24	1.39	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ARG	NE-CZ-NH2	-9.99	115.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	CB-CG-OD1	-7.67	111.40	118.30
1	A	192	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	207	LYS	CG-CD-CE	-5.96	94.00	111.90
1	B	444	GLU	OE1-CD-OE2	5.90	130.38	123.30
1	A	205	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	B	447	ARG	NH1-CZ-NH2	5.17	125.09	119.40

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	58	0
1	B	3514	0	3466	49	0
2	A	44	0	39	1	0
2	B	44	0	39	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	174	0	0	4	1
4	B	99	0	0	4	0
All	All	7383	0	7005	103	1

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 7.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:NZ	1:A:207:LYS:CE	1.73	1.51
1:A:207:LYS:CE	1:A:207:LYS:CD	1.96	1.41
1:A:463:GLU:OE2	1:B:180:ARG:NH1	1.94	1.00
1:B:263[B]:HIS:HE1	4:B:2004:HOH:O	1.58	0.87
1:B:436:PRO:O	1:B:438:PRO:HD3	1.85	0.77
1:A:207:LYS:CE	1:A:207:LYS:CG	2.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HG	1:B:183:ASP:H	1.54	0.71
1:B:263[B]:HIS:HD2	1:B:264:THR:OG1	1.74	0.70
1:A:476:ARG:HB2	1:A:479:GLU:HG3	1.78	0.66
1:B:130:ARG:NH1	4:B:2014:HOH:O	2.29	0.63
1:A:147:PHE:CD1	1:A:216:LEU:HB3	2.33	0.63
1:B:175:LYS:HD2	1:B:502:GLU:OE2	1.99	0.62
1:A:129:SER:HB2	1:A:153:GLU:OE1	2.00	0.62
1:A:358:HIS:O	1:A:359:ARG:HB2	2.00	0.61
1:B:333:PRO:HB2	1:B:335:PRO:HD2	1.81	0.61
1:B:234:TRP:HE1	1:B:286:ASN:HD21	1.48	0.60
1:B:180:ARG:HG3	1:B:188:TYR:CE2	2.38	0.59
1:B:358:HIS:O	1:B:418:ASP:OD1	2.22	0.58
1:B:189:ILE:HG22	1:B:504:ILE:HG21	1.85	0.57
1:B:453:TYR:O	1:B:454:ARG:HD2	2.04	0.57
1:A:189:ILE:HG22	1:A:504:ILE:HG21	1.87	0.56
1:B:476:ARG:HB2	1:B:479:GLU:HG3	1.87	0.56
1:B:357:ILE:HG22	1:B:418:ASP:OD2	2.05	0.56
1:A:253:GLY:HA3	1:A:270:THR:O	2.04	0.56
1:A:312:THR:OG1	2:A:1506:L1G:H153	2.05	0.56
1:A:463:GLU:OE2	1:B:180:ARG:CZ	2.52	0.55
1:A:134:GLU:HA	1:A:174:VAL:HG21	1.87	0.55
1:A:218:VAL:CG2	1:A:219:PRO:HD2	2.36	0.55
1:A:183:ASP:C	1:A:185:GLY:H	2.10	0.54
1:A:132:ASP:OD2	4:A:2038:HOH:O	2.18	0.54
1:B:183:ASP:C	1:B:185:GLY:H	2.10	0.54
1:B:441:SER:O	1:B:445:VAL:HG23	2.08	0.54
1:B:182:LEU:HG	1:B:183:ASP:N	2.22	0.54
1:A:426:LEU:O	1:A:430:VAL:HG23	2.08	0.54
1:B:234:TRP:HE1	1:B:286:ASN:ND2	2.06	0.54
1:B:253:GLY:HA3	1:B:270:THR:O	2.07	0.54
1:B:134:GLU:HA	1:B:174:VAL:HG21	1.92	0.52
1:A:226:GLN:NE2	4:A:2056:HOH:O	2.41	0.51
1:B:183:ASP:O	1:B:185:GLY:N	2.36	0.51
1:A:198:LEU:O	1:A:202:VAL:HG12	2.10	0.51
1:A:218:VAL:HG22	1:A:219:PRO:HD2	1.93	0.51
1:B:189:ILE:CG2	1:B:504:ILE:HG21	2.41	0.50
1:B:274:GLY:O	1:B:275:SER:HB2	2.10	0.50
1:B:281:PHE:CE2	1:B:310:ILE:HD11	2.46	0.50
1:A:278:VAL:HG13	1:A:308:ILE:HD11	1.93	0.50
1:A:130:ARG:HD3	1:A:501:PTR:CE2	2.42	0.50
1:A:426:LEU:HD11	1:A:465:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:TYR:HE1	1:B:210:ASP:HB2	1.77	0.49
1:A:123:TRP:HZ2	1:A:199:GLN:HG2	1.78	0.49
1:B:426:LEU:O	1:B:430:VAL:HG23	2.13	0.49
1:B:274:GLY:O	1:B:275:SER:CB	2.61	0.48
1:B:238:ARG:NH2	1:B:305:LYS:O	2.46	0.48
1:B:404:ALA:HB1	1:B:406:GLU:OE2	2.14	0.48
1:A:303:VAL:HB	1:A:309:TYR:HB2	1.96	0.48
1:B:457:ARG:HG3	1:B:466:TYR:CG	2.49	0.47
1:A:149:ILE:HD13	1:A:161:LEU:HD13	1.97	0.47
1:A:155:THR:HG21	1:A:180:ARG:HH12	1.79	0.47
1:A:442:ASN:HB2	1:A:443:PRO:HD3	1.97	0.47
1:A:463:GLU:OE2	1:B:180:ARG:NH2	2.47	0.47
1:A:504:ILE:HG23	1:A:504:ILE:O	2.14	0.47
1:A:143:MET:HE3	1:A:218:VAL:HG12	1.97	0.47
1:A:315:MET:CE	1:A:375:LYS:HD2	2.44	0.47
1:B:247:LEU:HD12	1:B:255:VAL:HG12	1.97	0.46
1:B:263[B]:HIS:CE1	4:B:2004:HOH:O	2.47	0.46
1:A:284:GLU:O	1:A:288:MET:HG2	2.15	0.46
1:A:337:LEU:HB3	1:A:429:ILE:HG22	1.97	0.46
1:A:147:PHE:HB3	1:A:216:LEU:HD22	1.98	0.45
1:B:281:PHE:CZ	1:B:310:ILE:HD11	2.51	0.45
1:B:362:ARG:HD2	4:B:2057:HOH:O	2.15	0.45
1:A:123:TRP:HA	1:A:219:PRO:HB3	1.99	0.45
1:A:262:LYS:NZ	4:A:2074:HOH:O	2.48	0.45
1:B:504:ILE:O	1:B:504:ILE:HG23	2.16	0.45
1:A:142:ASN:OD1	1:A:221:MET:HG2	2.16	0.45
1:A:102:ARG:HD3	4:A:2023:HOH:O	2.16	0.44
1:A:458:PRO:HG2	1:A:461:CYS:HB2	1.98	0.44
1:B:111:TYR:HE2	1:B:224:LYS:HE3	1.82	0.44
1:B:442:ASN:HB2	1:B:443:PRO:HD3	1.98	0.44
1:B:84:MET:HE2	1:B:84:MET:HB3	1.76	0.44
1:A:333:PRO:HB2	1:A:335:PRO:HD2	2.00	0.44
1:A:371:SER:O	1:A:372:LEU:HB2	2.19	0.43
1:A:180:ARG:HD3	1:A:180:ARG:HA	1.81	0.43
1:A:155:THR:O	1:A:155:THR:HG22	2.19	0.42
1:A:230:GLU:OE1	1:A:260:TYR:OH	2.32	0.42
1:A:504:ILE:O	1:A:504:ILE:CG2	2.67	0.42
1:A:441:SER:O	1:A:445:VAL:HG23	2.19	0.42
1:A:72:HIS:CE1	1:A:230:GLU:HB2	2.53	0.42
1:A:464:GLU:HG2	1:B:497:THR:O	2.19	0.42
1:B:146:SER:HA	1:B:218:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:HG2	1:A:207:LYS:CE	2.48	0.42
1:A:284:GLU:O	1:A:287:VAL:HG12	2.19	0.42
1:B:334:LEU:HD21	1:B:462:PRO:CG	2.50	0.42
1:A:88:GLU:HB2	1:A:95:LYS:HB3	2.02	0.41
1:A:323:PHE:O	1:A:329:GLY:HA3	2.20	0.41
1:A:476:ARG:HA	1:A:477:PRO:HD3	1.92	0.41
1:B:258:ALA:HB3	1:B:266:VAL:HG23	2.02	0.41
1:A:316:ALA:HB3	1:A:370:ALA:HB2	2.03	0.41
1:B:323:PHE:O	1:B:329:GLY:HA3	2.21	0.41
1:A:218:VAL:HG23	1:A:219:PRO:HD2	2.03	0.41
1:B:292:GLN:HB2	1:B:292:GLN:HE21	1.63	0.41
1:A:377:ALA:O	1:A:378:ASP:HB2	2.20	0.40
1:B:293:HIS:HB3	1:B:296:LEU:HG	2.03	0.40
1:B:349:ALA:O	1:B:353:GLN:HB2	2.22	0.40
1:A:183:ASP:O	1:A:185:GLY:N	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2024:HOH:O	4:A:2079:HOH:O[2_555]	2.00	0.20

## 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%)	404 (94%)	21 (5%)	5 (1%)	15	16
1	B	431/454 (95%)	406 (94%)	23 (5%)	2 (0%)	32	39
All	All	861/908 (95%)	810 (94%)	44 (5%)	7 (1%)	22	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ASP
1	B	275	SER
1	B	436	PRO
1	A	205	TYR
1	A	359	ARG
1	A	182	LEU
1	A	184	ASN

### 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%)	357 (94%)	21 (6%)	25	33
1	B	379/393 (96%)	360 (95%)	19 (5%)	28	39
All	All	757/786 (96%)	717 (95%)	40 (5%)	26	35

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

Mol	Chain	Res	Type
1	A	69	GLU
1	A	164	ARG
1	A	181	THR
1	A	193	SER
1	A	199	GLN
1	A	202	VAL
1	A	221	MET
1	A	227	LYS
1	A	245	LYS
1	A	262	LYS
1	A	276	MET
1	A	287	VAL
1	A	289	LYS
1	A	298	LYS
1	A	353	GLN
1	A	359	ARG
1	A	361	LEU

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Mol	Chain	Res	Type
1	A	400	ILE
1	A	450	GLU
1	A	479	GLU
1	A	503	GLU
1	B	90	SER
1	B	116	ASP
1	B	192	ARG
1	B	194	THR
1	B	202	VAL
1	B	203	ASP
1	B	209	ASN
1	B	218	VAL
1	B	222	SER
1	B	227	LYS
1	B	276	MET
1	B	278	VAL
1	B	298	LYS
1	B	306	GLU
1	B	336	LYS
1	B	357	ILE
1	B	361	LEU
1	B	371	SER
1	B	406	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	226	GLN
1	B	209	ASN
1	B	286	ASN
1	B	292	GLN

### 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	15,16,17	1.98	2 (13%)	19,22,24	0.72	0
1	PTR	B	501	1,3	15,16,17	1.80	1 (6%)	19,22,24	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	PTR	OH-CZ	-6.80	1.24	1.40
1	B	501	PTR	OH-CZ	-6.61	1.25	1.40
1	A	501	PTR	CA-C	2.85	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	501	PTR	1	0

## 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	L1G	A	1506	-	46,50,50	0.85	0	54,73,73	1.93	7 (12%)
2	L1G	B	1506	-	46,50,50	0.80	0	54,73,73	1.88	7 (12%)

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	L1G	A	1506	-	-	0/15/42/42	0/7/7/7
2	L1G	B	1506	-	-	0/15/42/42	0/7/7/7

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1506	L1G	N3-C11-N4	-9.41	120.66	128.86
2	A	1506	L1G	N3-C11-N4	-9.17	120.87	128.86
2	A	1506	L1G	C26-C24-N8	-4.17	104.79	109.17
2	B	1506	L1G	C26-C24-N8	-3.55	105.43	109.17
2	A	1506	L1G	C20-C21-C26	-3.07	102.72	106.55
2	B	1506	L1G	C20-C21-C26	-3.06	102.73	106.55
2	A	1506	L1G	C2-C5-N4	-2.28	116.75	122.78
2	B	1506	L1G	O1-C8-C6	-2.09	120.66	124.17
2	B	1506	L1G	C11-N4-C5	2.08	122.41	118.77
2	A	1506	L1G	C1-N1-N2	2.15	106.89	105.19
2	A	1506	L1G	C11-N4-C5	2.95	123.94	118.77
2	B	1506	L1G	O1-C8-C12	3.19	118.97	114.81
2	B	1506	L1G	C21-C26-C24	5.65	111.20	106.27
2	A	1506	L1G	C21-C26-C24	5.82	111.35	106.27

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
2	A	1506	L1G	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	433/454 (95%)	0.74	25 (5%)	24 30	37, 50, 63, 74	0
1	B	433/454 (95%)	0.71	37 (8%)	11 16	38, 50, 63, 73	0
All	All	866/908 (95%)	0.73	62 (7%)	16 22	37, 50, 63, 74	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	GLY	7.0
1	A	187	PHE	6.7
1	A	182	LEU	5.2
1	B	439	GLY	4.9
1	A	185	GLY	4.8
1	B	399	PRO	4.6
1	B	445	VAL	4.3
1	B	275	SER	4.3
1	B	449	LEU	4.1
1	A	274	GLY	4.0
1	A	180	ARG	3.9
1	B	451	ARG	3.8
1	B	447	ARG	3.8
1	B	409	ASN	3.7
1	B	182	LEU	3.6
1	A	179	ILE	3.6
1	B	271	MET	3.6
1	B	400	ILE	3.5
1	B	446	ILE	3.5
1	A	184	ASN	3.2
1	B	183	ASP	3.1
1	B	443	PRO	3.0
1	A	188	TYR	3.0
1	B	444	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	189	ILE	2.9
1	A	181	THR	2.8
1	B	407	ALA	2.7
1	B	273	PRO	2.7
1	A	351	ILE	2.7
1	A	201	LEU	2.7
1	B	274	GLY	2.7
1	A	183	ASP	2.7
1	B	411	GLY	2.6
1	A	486	ILE	2.6
1	B	405	PRO	2.5
1	B	84	MET	2.5
1	A	195	PHE	2.5
1	A	272	LYS	2.5
1	B	118	LEU	2.4
1	A	168	PRO	2.4
1	B	187	PHE	2.4
1	B	442	ASN	2.4
1	A	493	PHE	2.3
1	A	159	TYR	2.2
1	B	302	VAL	2.2
1	B	194	THR	2.2
1	B	251	GLN	2.2
1	B	262	LYS	2.2
1	B	76	LEU	2.2
1	A	472	CYS	2.1
1	A	223	SER	2.1
1	B	105	GLY	2.1
1	B	181	THR	2.1
1	A	194	THR	2.1
1	A	171	GLY	2.1
1	B	94	TRP	2.0
1	A	439	GLY	2.0
1	B	441	SER	2.0
1	B	116	ASP	2.0
1	B	252	PHE	2.0
1	B	440	MET	2.0
1	A	275	SER	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PTR	A	501	16/17	0.97	0.16	-	45,48,49,49	0
1	PTR	B	501	16/17	0.97	0.16	-	45,47,49,49	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CA	B	1507	1/1	0.98	0.21	1.41	44,44,44,44	0
3	CA	A	1507	1/1	0.97	0.20	1.02	44,44,44,44	0
2	L1G	B	1506	44/44	0.95	0.17	-0.04	39,41,44,46	0
2	L1G	A	1506	44/44	0.96	0.16	-0.47	38,41,45,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.