Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:45 PM GMT

PDB ID	:	1QH4
Title	:	CRYSTAL STRUCTURE OF CHICKEN BRAIN-TYPE CREATINE KINASE AT 1.41 ANGSTROM RESOLUTION
Authors	:	Eder, M.; Schlattner, U.; Becker, A.; Wallimann, T.; Kabsch, W.; Fritz-Wolf, K.
Deposited on	:	1999-05-11
Resolution	:	1.41 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:

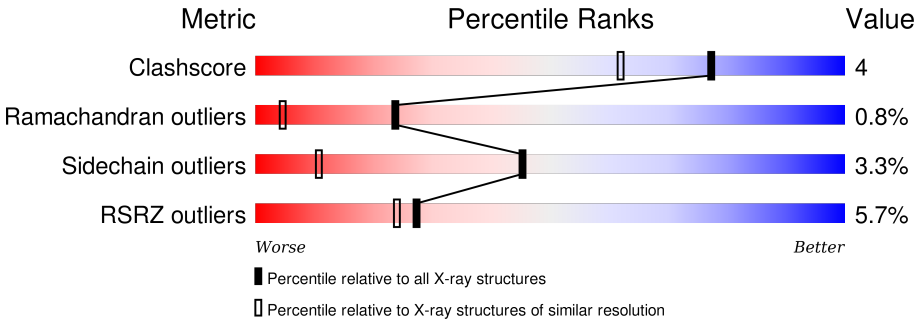
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.41 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))
Clashscore	102246	1743 (1.44-1.40)
Ramachandran outliers	100387	1698 (1.44-1.40)
Sidechain outliers	100360	1697 (1.44-1.40)
RSRZ outliers	91569	1632 (1.44-1.40)

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	380	8% 84% 15%
1	B	380	4% 89% 8%
1	C	380	4% 87% 12%
1	D	380	6% 82% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13559 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.

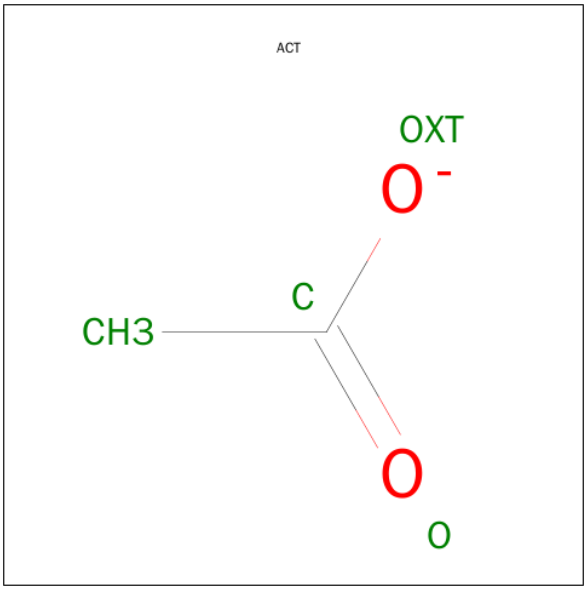
- Molecule 1 is a protein called CREATINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3005	1890	529	570	16			
1	B	380	Total	C	N	O	S	0	7	0
			3030	1907	535	571	17			
1	C	380	Total	C	N	O	S	0	6	0
			3021	1901	530	572	18			
1	D	380	Total	C	N	O	S	0	2	0
			3011	1895	529	570	17			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

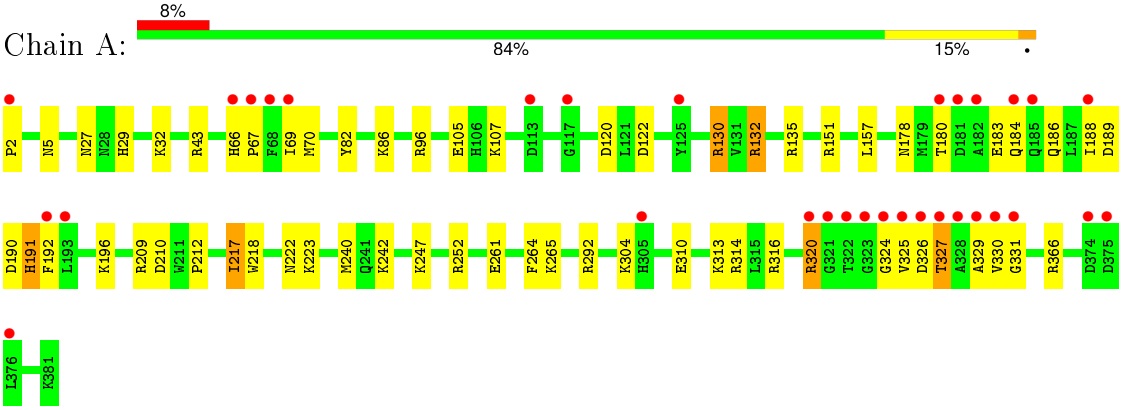
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	360	Total O 360 360	0	0
4	B	416	Total O 416 416	0	0
4	C	447	Total O 447 447	0	0
4	D	244	Total O 244 244	0	0

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.

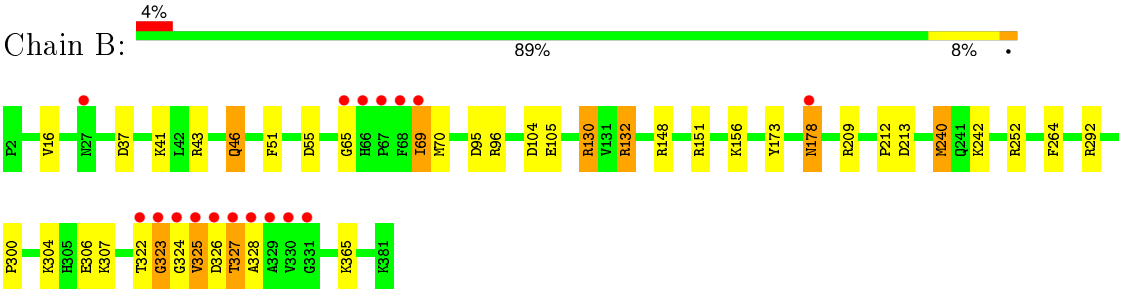
- Molecule 1: CREATINE KINASE

Chain A:



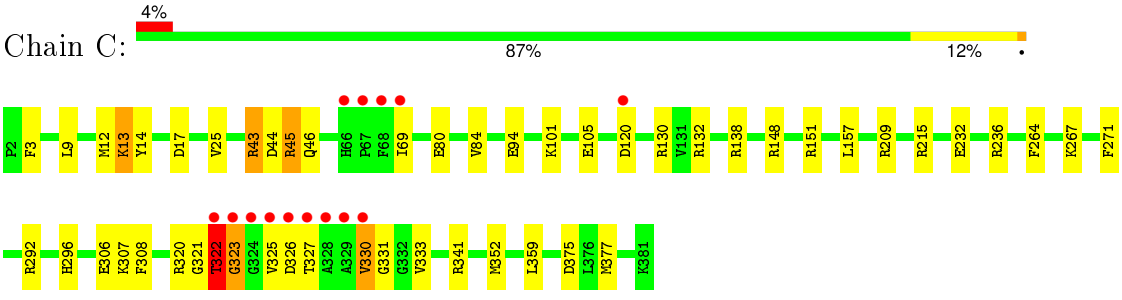
- Molecule 1: CREATINE KINASE

Chain B:



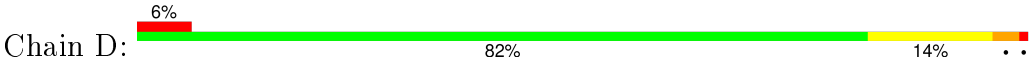
- Molecule 1: CREATINE KINASE

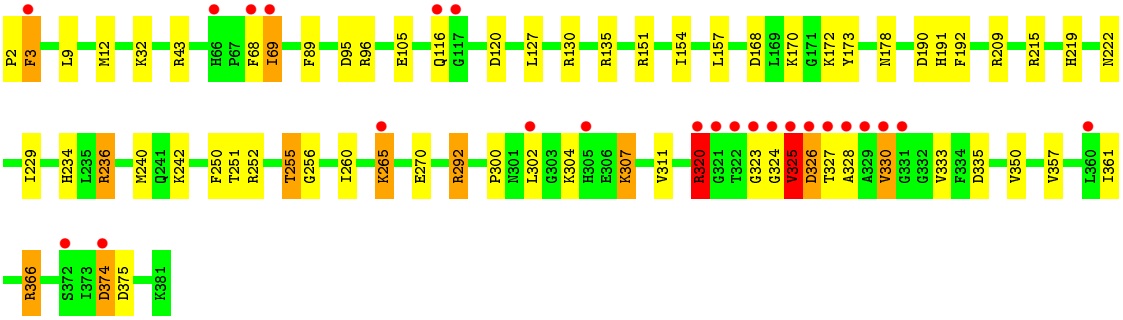
Chain C:



- Molecule 1: CREATINE KINASE

Chain D:




P2 F3 L9 M12 K32 R43 H66 P67 F68 I69 F89 D95 R96 E105 Q116 G117 D120 L127 R130 R135 R151 I154 L157 D168 I169 K170 G171 K172 Y173 N178 D190 H191 F192 R209 R215 H219 N222
I229 H234 L235 R236 M240 Q241 K242 F250 T251 R252 T255 G256 I260 K265 E270 R292 P300 N301 L302 G303 K304 H305 E306 K307 V311 R320 G321 T322 G323 G324 V325 D326 T327 A328 A329 V330 G331 G332 V333 F334 D335 V350 V357 L360 I361
R366 S372 I373 D374 D375 K381

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.43Å 175.99Å 95.40Å 90.00° 95.85° 90.00°	Depositor
Resolution (Å)	6.00 – 1.41 6.00 – 1.41	Depositor EDS
% Data completeness (in resolution range)	99.1 (6.00-1.41) 97.9 (6.00-1.41)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 1.41Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.137 , 0.188 0.144 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	13.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.70 , 103.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 297347 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13559	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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, ACT

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	0.53	0/3067	1.27	25/4136 (0.6%)
1	B	0.57	0/3127	1.26	22/4215 (0.5%)
1	C	0.59	0/3113	1.37	33/4197 (0.8%)
1	D	0.51	0/3083	1.26	23/4157 (0.6%)
All	All	0.55	0/12390	1.29	103/16705 (0.6%)

There are no bond length outliers.

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	130	ARG	CD-NE-CZ	29.40	164.76	123.60
1	C	292	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	B	43	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	C	43	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	A	252	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	A	209	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	B	292	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	C	43	ARG	CD-NE-CZ	10.03	137.64	123.60
1	B	43	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	C	236	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	C	132	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	132	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	B	209	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	D	43	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	C	151	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	A	292	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	330	VAL	C-N-CA	8.45	140.04	122.30
1	D	236	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	C	130	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	292	ARG	NE-CZ-NH2	-8.29	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	341	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	B	130	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	96	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	D	252	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	C	138	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	B	252[A]	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	B	252[B]	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	C	209	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	D	135	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	D	96	ARG	NE-CZ-NH1	-7.71	116.45	120.30
1	A	43	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	D	3	PHE	CB-CG-CD1	7.64	126.14	120.80
1	A	240	MET	CA-CB-CG	7.62	126.25	113.30
1	C	132	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	C	321	GLY	C-N-CA	7.49	140.43	121.70
1	C	46	GLN	CA-CB-CG	7.49	129.88	113.40
1	D	130	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	148	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	236	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	D	209	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	151	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	45	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	192	PHE	O-C-N	-6.84	111.75	122.70
1	C	375	ASP	CB-CG-OD1	-6.84	112.15	118.30
1	C	271	PHE	CB-CG-CD1	6.61	125.43	120.80
1	B	46	GLN	CA-CB-CG	6.55	127.82	113.40
1	A	209	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	C	236	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	264	PHE	CB-CG-CD1	6.46	125.32	120.80
1	B	156	LYS	CD-CE-NZ	6.39	126.39	111.70
1	B	105	GLU	OE1-CD-OE2	-6.38	115.65	123.30
1	D	320	ARG	CA-CB-CG	6.34	127.34	113.40
1	A	316	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	D	252	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	130	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	151	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	209	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	366	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	219	HIS	CA-CB-CG	6.03	123.85	113.60
1	A	82	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	D	89	PHE	CB-CG-CD1	5.97	124.98	120.80
1	D	135	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	TYR	CB-CG-CD2	5.91	124.55	121.00
1	B	213	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	96	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	B	213	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	264	PHE	CB-CG-CD1	5.81	124.87	120.80
1	A	210	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	B	104	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	122	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	17	ASP	CB-CG-OD1	5.71	123.43	118.30
1	C	308	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	C	157[A]	LEU	CA-CB-CG	5.70	128.41	115.30
1	C	157[B]	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	43	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	43	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	215	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	292	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	5	ASN	CA-C-O	5.51	131.68	120.10
1	C	13	LYS	CA-CB-CG	5.46	125.41	113.40
1	B	264	PHE	CB-CG-CD1	5.46	124.62	120.80
1	B	252[A]	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	252[B]	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	352	MET	CA-CB-CG	-5.33	104.23	113.30
1	A	157	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	105	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	D	192	PHE	CB-CG-CD1	5.25	124.47	120.80
1	C	14	TYR	CB-CG-CD1	5.22	124.13	121.00
1	A	320	ARG	CD-NE-CZ	5.18	130.85	123.60
1	B	173	TYR	CB-CG-CD2	5.17	124.10	121.00
1	C	271	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	A	192	PHE	CA-C-O	5.12	130.86	120.10
1	B	148	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	D	215	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	232	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	A	191	HIS	CA-CB-CG	5.08	122.24	113.60
1	D	157	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	366	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	95	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	320	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	135	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	D	151	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	196	LYS	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3005	0	2963	27	0
1	B	3030	0	3008	14	0
1	C	3021	0	2990	25	0
1	D	3011	0	2975	26	0
2	D	1	0	0	0	0
3	A	4	0	3	0	0
3	B	8	0	6	1	0
3	C	8	0	6	0	0
3	D	4	0	3	0	0
4	A	360	0	0	4	0
4	B	416	0	0	5	0
4	C	447	0	0	11	0
4	D	244	0	0	3	0
All	All	13559	0	11954	90	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 4.

All (90) 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:16:VAL:H	3:B:1501:ACT:H2	1.32	0.92
1:A:184:GLN:O	1:A:188:ILE:HG13	1.85	0.76
1:D:255:THR:HG22	4:D:1723:HOH:O	1.83	0.76
1:A:186:GLN:HA	1:A:189:ASP:OD2	1.87	0.75
1:C:359[B]:LEU:HG	4:C:1775:HOH:O	1.87	0.74
1:C:25:VAL:HG22	4:C:1927:HOH:O	1.87	0.74
1:D:265:LYS:O	1:D:265:LYS:HD2	1.88	0.72
1:B:306:GLU:HG2	4:B:1762:HOH:O	1.92	0.69
1:C:296:HIS:ND1	1:C:323:GLY:HA2	2.10	0.67
1:D:325:VAL:HB	1:D:326:ASP:OD1	1.96	0.65
1:D:292:ARG:HE	1:D:320:ARG:NH2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:PHE:HB2	4:D:1704:HOH:O	1.99	0.63
1:D:9:LEU:HD23	1:D:12[B]:MET:HE3	1.80	0.63
1:A:86:LYS:HE2	4:A:1641:HOH:O	1.97	0.62
1:A:66:HIS:CD2	1:A:67:PRO:HD2	2.35	0.61
1:D:250:PHE:CD1	1:D:350:VAL:HG21	2.36	0.60
1:A:324:GLY:O	1:A:329:ALA:HA	2.01	0.59
1:D:127:LEU:HD13	1:D:324:GLY:O	2.05	0.55
1:A:66:HIS:CG	1:A:67:PRO:HD2	2.41	0.55
1:C:43:ARG:HD3	4:C:1858:HOH:O	2.07	0.55
1:B:95:ASP:HB2	4:B:1672:HOH:O	2.07	0.54
1:D:190:ASP:O	1:D:191:HIS:HB2	2.08	0.54
1:A:190:ASP:O	1:A:191:HIS:HB2	2.09	0.53
1:C:359[B]:LEU:HD11	4:C:1628:HOH:O	2.07	0.52
1:C:359[B]:LEU:HD21	4:C:1628:HOH:O	2.09	0.52
1:C:327:THR:HG22	1:C:327:THR:O	2.10	0.52
1:C:69:ILE:O	1:C:69:ILE:HD12	2.10	0.51
1:C:9:LEU:O	1:C:12[A]:MET:HG2	2.10	0.51
4:A:1624:HOH:O	1:B:46:GLN:HG3	2.11	0.51
1:A:186:GLN:O	1:A:186:GLN:HG3	2.09	0.50
1:B:300:PRO:O	1:B:304:LYS:HG3	2.11	0.50
1:C:322:THR:O	1:C:323:GLY:O	2.29	0.49
1:C:296:HIS:CE1	1:C:323:GLY:HA2	2.46	0.49
1:D:300:PRO:O	1:D:304:LYS:HG2	2.13	0.49
1:A:326:ASP:O	1:A:326:ASP:OD1	2.30	0.49
1:D:307:LYS:O	1:D:311:VAL:HG23	2.13	0.48
1:D:69:ILE:HG23	1:D:69:ILE:O	2.14	0.47
1:D:366:ARG:HH12	1:D:375:ASP:CG	2.16	0.47
1:B:65:GLY:HA2	4:B:1915:HOH:O	2.13	0.47
1:C:94:GLU:OE2	1:C:101:LYS:HD3	2.14	0.47
1:A:261:GLU:OE2	1:A:265:LYS:HE2	2.15	0.47
1:A:180:THR:OG1	1:A:183:GLU:HG3	2.15	0.47
1:D:251:THR:O	1:D:255:THR:HG23	2.15	0.46
1:A:217:ILE:HG12	1:A:218:TRP:N	2.30	0.46
1:B:327:THR:O	1:B:328:ALA:HB2	2.16	0.46
1:D:173:TYR:CE1	1:D:229:ILE:HD12	2.51	0.46
1:B:365:LYS:NZ	4:B:1691:HOH:O	2.49	0.45
1:A:105:GLU:OE1	1:A:107:LYS:NZ	2.50	0.45
1:C:44:ASP:O	1:D:2:PRO:N	2.49	0.45
1:B:130:ARG:HG3	1:B:240[B]:MET:HB3	1.98	0.45
1:C:80:GLU:HG3	4:C:1730:HOH:O	2.17	0.45
1:A:29:HIS:CE1	1:A:70:MET:HE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:THR:OG1	1:B:323:GLY:N	2.50	0.45
1:A:310:GLU:OE2	1:A:313:LYS:NZ	2.50	0.45
1:C:331:GLY:HA2	4:C:1910:HOH:O	2.18	0.44
1:D:326:ASP:OD1	1:D:326:ASP:N	2.50	0.44
1:A:325:VAL:HG23	1:A:326:ASP:N	2.33	0.44
1:D:120:ASP:OD1	1:D:120:ASP:N	2.50	0.44
1:D:256:GLY:O	1:D:260:ILE:HG13	2.18	0.44
1:C:307:LYS:NZ	4:C:1831:HOH:O	2.49	0.44
1:C:325:VAL:O	1:C:326:ASP:HB3	2.18	0.44
1:D:374:ASP:OD1	1:D:374:ASP:N	2.50	0.43
1:A:2:PRO:HB2	1:B:46:GLN:OE1	2.18	0.43
1:A:310:GLU:O	1:A:314:ARG:HG2	2.19	0.43
1:A:325:VAL:CG2	1:A:327:THR:HG22	2.49	0.43
1:A:222:ASN:O	1:A:223:LYS:HB2	2.19	0.43
1:A:217:ILE:HB	4:A:1754:HOH:O	2.19	0.43
1:A:27:ASN:ND2	1:A:66:HIS:O	2.50	0.42
1:C:13:LYS:NZ	4:C:1952:HOH:O	2.50	0.42
1:D:324:GLY:N	1:D:333:VAL:HG11	2.34	0.42
1:A:261:GLU:O	1:A:265:LYS:HD3	2.20	0.42
1:A:32:LYS:CD	1:A:70:MET:HE2	2.50	0.42
1:A:130:ARG:HG3	4:A:1635:HOH:O	2.20	0.42
1:D:168:ASP:OD1	1:D:222:ASN:ND2	2.53	0.42
1:B:178:ASN:ND2	4:B:1823:HOH:O	2.52	0.42
1:A:132:ARG:O	1:A:132:ARG:HG3	2.18	0.42
1:D:323:GLY:O	1:D:330:VAL:HG13	2.20	0.41
1:C:45:ARG:NH1	1:C:84:VAL:O	2.53	0.41
1:C:306:GLU:HG2	4:C:1619:HOH:O	2.20	0.41
1:C:94:GLU:OE2	1:C:101:LYS:NZ	2.50	0.41
1:D:270:GLU:HB2	4:D:1683:HOH:O	2.21	0.41
1:D:292:ARG:HH22	1:D:335:ASP:CG	2.24	0.41
1:A:32:LYS:HD3	1:A:70:MET:HE2	2.03	0.41
1:D:154:ILE:HD13	1:D:234:HIS:CD2	2.56	0.41
1:C:267:LYS:NZ	4:C:1517:HOH:O	2.54	0.41
1:C:330:VAL:HG11	1:C:333:VAL:CG2	2.51	0.41
1:C:307:LYS:HD2	1:C:377:MET:CE	2.50	0.40
1:B:37:ASP:OD2	1:B:41:LYS:NZ	2.50	0.40
1:B:51:PHE:CE1	1:B:55:ASP:HB3	2.56	0.40
1:D:357:VAL:O	1:D:361:ILE:HG13	2.21	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	378/380 (100%)	363 (96%)	13 (3%)	2 (0%)	34	9
1	B	385/380 (101%)	370 (96%)	10 (3%)	5 (1%)	15	2
1	C	384/380 (101%)	372 (97%)	10 (3%)	2 (0%)	34	9
1	D	380/380 (100%)	365 (96%)	12 (3%)	3 (1%)	24	4
All	All	1527/1520 (100%)	1470 (96%)	45 (3%)	12 (1%)	24	4

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	THR
1	A	331	GLY
1	B	325	VAL
1	C	323	GLY
1	C	322	THR
1	B	323	GLY
1	B	327	THR
1	D	327	THR
1	D	328	ALA
1	B	69	ILE
1	B	324	GLY
1	D	325	VAL

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	330/330 (100%)	320 (97%)	10 (3%)	48 13
1	B	337/330 (102%)	326 (97%)	11 (3%)	45 11
1	C	336/330 (102%)	333 (99%)	3 (1%)	84 62
1	D	332/330 (101%)	311 (94%)	21 (6%)	22 2
All	All	1335/1320 (101%)	1290 (97%)	45 (3%)	45 10

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ILE
1	A	120	ASP
1	A	132	ARG
1	A	178	ASN
1	A	212	PRO
1	A	217	ILE
1	A	242	LYS
1	A	247	LYS
1	A	304	LYS
1	A	320	ARG
1	B	69	ILE
1	B	70	MET
1	B	132	ARG
1	B	178	ASN
1	B	212	PRO
1	B	240[A]	MET
1	B	240[B]	MET
1	B	242	LYS
1	B	307	LYS
1	B	325	VAL
1	B	326	ASP
1	C	120	ASP
1	C	322	THR
1	C	330	VAL
1	D	3	PHE
1	D	32	LYS
1	D	68	PHE
1	D	69	ILE
1	D	105	GLU
1	D	116	GLN
1	D	170	LYS
1	D	172	LYS
1	D	178	ASN

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Mol	Chain	Res	Type
1	D	236	ARG
1	D	240	MET
1	D	242	LYS
1	D	255	THR
1	D	265	LYS
1	D	302	LEU
1	D	307	LYS
1	D	320	ARG
1	D	325	VAL
1	D	326	ASP
1	D	330	VAL
1	D	374	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	178	ASN
1	A	222	ASN
1	A	268	ASN
1	A	286	ASN
1	B	178	ASN
1	B	296	HIS
1	B	318	GLN
1	D	178	ASN
1	D	296	HIS

5.3.3 RNA

There are no RNA molecules 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 (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	ACT	A	1502	-	1,3,3	1.84	0	0,3,3	0.00	-
3	ACT	B	1501	-	1,3,3	1.69	0	0,3,3	0.00	-
3	ACT	B	1503	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
3	ACT	C	1504	-	1,3,3	1.27	0	0,3,3	0.00	-
3	ACT	C	1505	-	1,3,3	2.71	1 (100%)	0,3,3	0.00	-
3	ACT	D	1506	-	1,3,3	1.80	0	0,3,3	0.00	-

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	ACT	A	1502	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1501	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1503	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1504	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1505	-	-	0/0/0/0	0/0/0/0
3	ACT	D	1506	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1503	ACT	CH3-C	2.26	1.52	1.48
3	C	1505	ACT	CH3-C	2.71	1.52	1.48

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
3	B	1501	ACT	1	0

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, 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	380/380 (100%)	0.28	32 (8%)	14	11	10, 25, 54, 103	0
1	B	380/380 (100%)	-0.20	17 (4%)	37	33	9, 19, 38, 101	0
1	C	380/380 (100%)	-0.25	14 (3%)	45	42	10, 18, 36, 98	0
1	D	380/380 (100%)	0.23	24 (6%)	23	20	9, 29, 58, 102	0
All	All	1520/1520 (100%)	0.01	87 (5%)	27	24	9, 21, 51, 103	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	ALA	23.5
1	B	325	VAL	19.6
1	C	325	VAL	18.2
1	A	330	VAL	17.9
1	A	328	ALA	15.2
1	D	330	VAL	14.5
1	C	327	THR	14.0
1	A	324	GLY	13.1
1	B	68	PHE	13.1
1	C	328	ALA	12.4
1	B	330	VAL	12.1
1	D	325	VAL	12.1
1	B	324	GLY	12.0
1	D	327	THR	11.8
1	A	329	ALA	11.6
1	C	68	PHE	11.3
1	D	328	ALA	11.0
1	A	325	VAL	10.6
1	C	330	VAL	10.3
1	D	324	GLY	10.2
1	A	327	THR	10.1

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Mol	Chain	Res	Type	RSRZ
1	B	327	THR	10.0
1	C	329	ALA	9.5
1	A	322	THR	9.2
1	D	329	ALA	8.9
1	C	326	ASP	8.8
1	B	329	ALA	8.6
1	C	69	ILE	8.5
1	A	331	GLY	8.0
1	D	322	THR	7.8
1	B	326	ASP	7.5
1	A	68	PHE	7.4
1	B	323	GLY	7.4
1	D	68	PHE	7.3
1	C	324	GLY	7.1
1	C	67	PRO	6.8
1	C	322	THR	6.8
1	A	321	GLY	6.6
1	D	323	GLY	6.3
1	A	326	ASP	6.2
1	C	323	GLY	6.0
1	D	326	ASP	6.0
1	A	323	GLY	5.9
1	B	67	PRO	5.6
1	A	66	HIS	5.5
1	A	67	PRO	5.3
1	A	69	ILE	5.0
1	D	69	ILE	4.5
1	D	321	GLY	4.4
1	D	331	GLY	4.0
1	C	66	HIS	4.0
1	B	66	HIS	3.8
1	A	180	THR	3.8
1	A	181	ASP	3.7
1	B	322	THR	3.7
1	D	66	HIS	3.7
1	A	182	ALA	3.6
1	D	320	ARG	3.4
1	A	374	ASP	3.4
1	A	125	TYR	3.0
1	A	320	ARG	2.9
1	B	27	ASN	2.9
1	A	376	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	ILE	2.8
1	D	374	ASP	2.6
1	D	117	GLY	2.6
1	A	2	PRO	2.5
1	D	3	PHE	2.5
1	A	185	GLN	2.5
1	A	193	LEU	2.5
1	A	375	ASP	2.4
1	C	120	ASP	2.4
1	D	265	LYS	2.4
1	B	178	ASN	2.3
1	B	331	GLY	2.3
1	D	372	SER	2.2
1	A	113	ASP	2.2
1	D	116	GLN	2.2
1	A	117	GLY	2.1
1	A	192	PHE	2.1
1	B	65	GLY	2.1
1	D	360	LEU	2.1
1	D	305	HIS	2.1
1	B	69	ILE	2.1
1	D	302	LEU	2.1
1	A	305	HIS	2.1
1	A	184	GLN	2.0

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

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

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	ACT	D	1506	4/4	0.95	0.10	1.81	26,31,31,33	0
3	ACT	C	1505	4/4	0.91	0.11	1.36	49,52,52,58	0
3	ACT	B	1503	4/4	0.96	0.09	0.65	33,39,40,45	0
3	ACT	A	1502	4/4	0.97	0.07	0.37	27,32,34,41	0
3	ACT	C	1504	4/4	0.97	0.07	0.35	19,27,32,35	0
2	CA	D	382	1/1	1.00	0.02	-2.14	12,12,12,12	0
3	ACT	B	1501	4/4	0.88	0.16	-	27,34,40,45	0

6.5 Other polymers (i)

There are no such residues in this entry.