Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:59 am BST

PDB ID	:	1GXC
Title	:	FHA domain from human Chk2 kinase in complex with a synthetic phosphopeptide
Authors	:	Li, J.; Williams, B.L.; Haire, L.F.; Goldberg, M.; Wilker, E.; Durocher, D.; Yaffe, M.B.; Jackson, S.P.; Smerdon, S.J.
Deposited on	:	2002-04-02
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

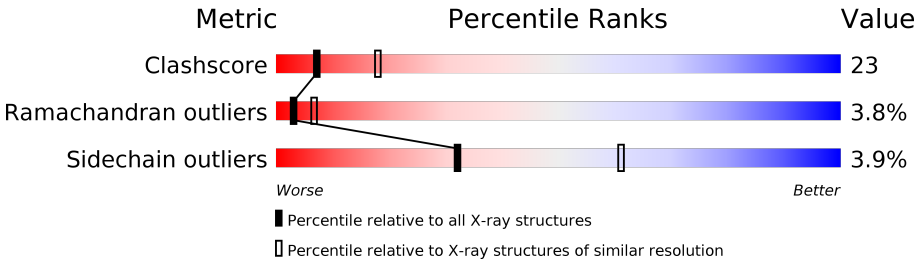
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	149	54% 21% • 22%
1	D	149	49% 27% •• 22%
1	G	149	34% 36% 6% • 22%
1	J	149	48% 26% • 22%
2	B	10	40% 30% 10% 20%
2	E	10	40% 30% 10% 20%
2	H	10	40% 30% 10% 20%
2	K	10	40% 40% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4247 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 SERINE/THREONINE-PROTEIN KINASE CHK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			964	617	170	174	3			
1	D	116	Total	C	N	O	S	0	0	0
			964	617	170	174	3			
1	G	116	Total	C	N	O	S	0	0	0
			964	617	170	174	3			
1	J	116	Total	C	N	O	S	0	0	0
			964	617	170	174	3			

- Molecule 2 is a protein called SYNTHETIC PHOSPHOPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			80	50	13	16	1			
2	E	8	Total	C	N	O	P	0	0	0
			80	50	13	16	1			
2	H	8	Total	C	N	O	P	0	0	0
			74	47	10	16	1			
2	K	8	Total	C	N	O	P	0	0	0
			74	47	10	16	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	3	Total	O	0	0
			3	3		
3	D	25	Total	O	0	0
			25	25		
3	E	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	8	Total O 8 8	0	0
3	J	20	Total O 20 20	0	0
3	K	3	Total O 3 3	0	0

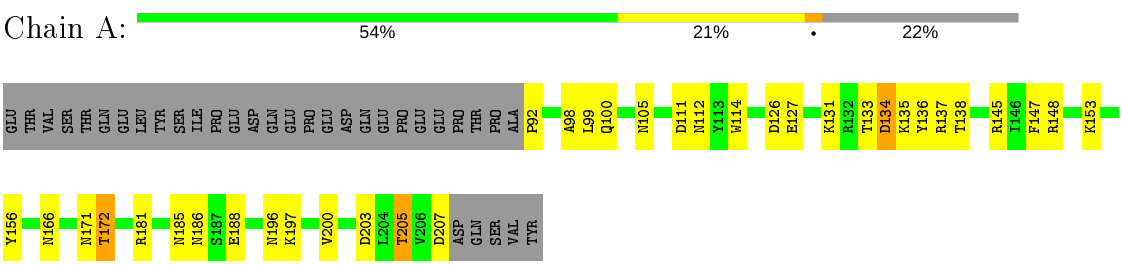
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

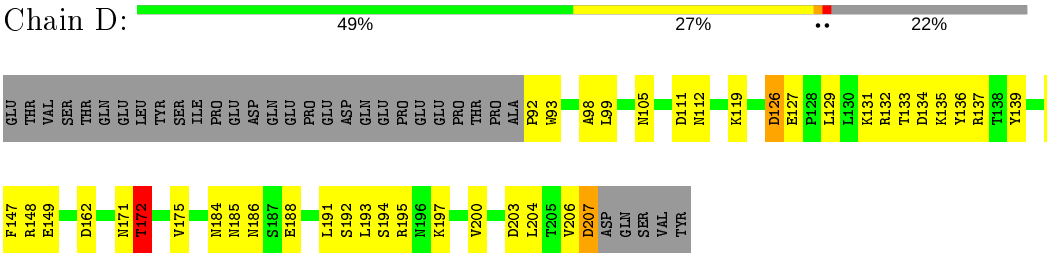
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE CHK2

Chain A:



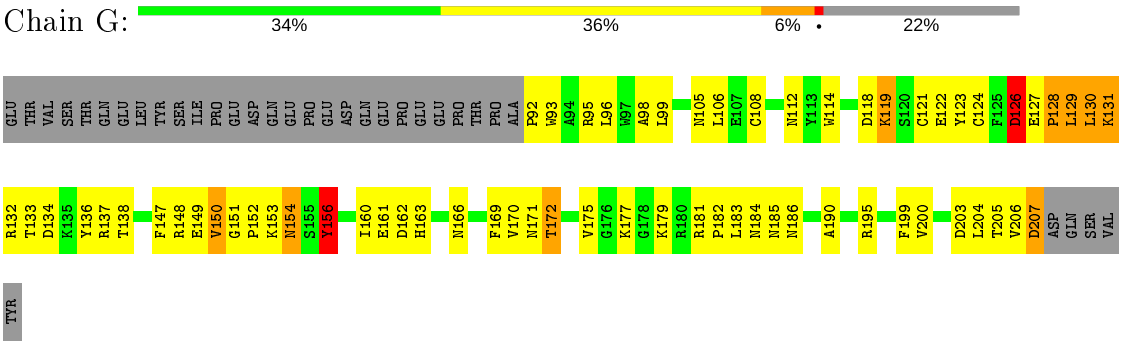
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE CHK2

Chain D:



- Molecule 1: SERINE/THREONINE-PROTEIN KINASE CHK2

Chain G:

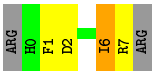


- Molecule 1: SERINE/THREONINE-PROTEIN KINASE CHK2

Chain J:

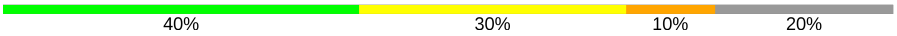
• Molecule 2: SYNTHETIC PHOSPHOPEPTIDE

Chain B:



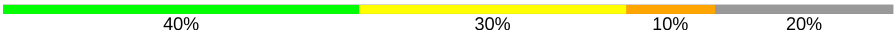
• Molecule 2: SYNTHETIC PHOSPHOPEPTIDE

Chain E:



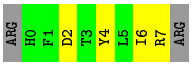
• Molecule 2: SYNTHETIC PHOSPHOPEPTIDE

Chain H:



• Molecule 2: SYNTHETIC PHOSPHOPEPTIDE

Chain K:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.82Å 82.88Å 129.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.6 (15.00-2.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.231 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4247	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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	0.50	0/990	0.78	2/1334 (0.1%)
1	D	0.61	0/990	0.83	1/1334 (0.1%)
1	G	0.40	0/990	0.78	4/1334 (0.3%)
1	J	0.47	0/990	0.84	4/1334 (0.3%)
2	B	0.53	0/70	0.89	1/90 (1.1%)
2	E	0.62	0/70	0.88	1/90 (1.1%)
2	H	0.45	0/64	0.89	1/83 (1.2%)
2	K	0.54	0/64	0.86	1/83 (1.2%)
All	All	0.50	0/4228	0.81	15/5682 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	134	ASP	CB-CG-OD2	7.73	125.26	118.30
1	A	134	ASP	CB-CG-OD2	6.94	124.55	118.30
1	J	101	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	126	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	126	ASP	CB-CG-OD2	5.69	123.42	118.30
1	G	162	ASP	CB-CG-OD2	5.61	123.35	118.30
2	H	2	ASP	CB-CG-OD2	5.61	123.35	118.30
1	G	126	ASP	CB-CG-OD2	5.56	123.31	118.30
1	G	118	ASP	CB-CG-OD2	5.42	123.17	118.30
1	J	162	ASP	CB-CG-OD2	5.39	123.15	118.30
1	G	207	ASP	CB-CG-OD2	5.32	123.09	118.30
1	J	207	ASP	CB-CG-OD2	5.28	123.05	118.30
2	K	2	ASP	CB-CG-OD2	5.23	123.01	118.30
2	B	2	ASP	CB-CG-OD2	5.20	122.98	118.30
2	E	2	ASP	CB-CG-OD2	5.16	122.94	118.30

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	964	0	929	33	1
1	D	964	0	929	49	0
1	G	964	0	929	60	0
1	J	964	0	929	38	0
2	B	80	0	72	4	0
2	E	80	0	72	3	1
2	H	74	0	61	2	0
2	K	74	0	61	3	0
3	A	20	0	0	10	0
3	B	3	0	0	0	0
3	D	25	0	0	13	0
3	E	4	0	0	0	0
3	G	8	0	0	4	0
3	J	20	0	0	16	0
3	K	3	0	0	1	0
All	All	4247	0	3982	184	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 23.

All (184) 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:D:171:ASN:O	1:D:172:THR:HB	1.42	1.10
1:A:136:TYR:HB3	3:A:2007:HOH:O	1.62	1.00
1:J:112:ASN:ND2	1:J:145:ARG:HH11	1.63	0.96
1:A:181:ARG:HD3	3:A:2016:HOH:O	1.67	0.93
1:D:111:ASP:CB	3:D:2013:HOH:O	2.15	0.92
1:J:179:LYS:HA	3:J:2014:HOH:O	1.70	0.90
1:J:95:ARG:NH1	3:J:2002:HOH:O	2.05	0.89
1:D:92:PRO:N	3:D:2002:HOH:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:TYR:HB3	3:G:2002:HOH:O	1.73	0.88
1:J:112:ASN:HD21	1:J:145:ARG:HH11	1.22	0.86
1:J:206:VAL:HA	3:J:2019:HOH:O	1.74	0.86
1:J:133:THR:O	1:J:134:ASP:HB2	1.75	0.84
1:A:111:ASP:CB	3:A:2013:HOH:O	2.24	0.84
1:A:171:ASN:O	1:A:172:THR:HB	1.76	0.84
1:D:99:LEU:HD11	1:D:200:VAL:HG23	1.59	0.83
1:D:92:PRO:CD	3:D:2002:HOH:O	2.28	0.81
1:D:93:TRP:CE2	1:D:148:ARG:HD2	2.16	0.80
1:D:185:ASN:O	1:D:186:ASN:HB2	1.81	0.78
1:G:130:LEU:O	1:G:133:THR:HG23	1.84	0.78
1:J:112:ASN:ND2	1:J:145:ARG:NH1	2.33	0.77
1:D:98:ALA:H	1:D:105:ASN:ND2	1.82	0.76
1:G:112:ASN:HD22	1:G:147:PHE:HB3	1.52	0.75
1:D:92:PRO:N	3:D:2003:HOH:O	2.19	0.74
1:J:171:ASN:O	1:J:172:THR:HB	1.87	0.74
1:J:99:LEU:HD11	1:J:200:VAL:HG23	1.68	0.74
2:E:6:ILE:O	2:E:6:ILE:HG13	1.88	0.73
1:D:92:PRO:CD	3:D:2003:HOH:O	2.34	0.73
1:D:92:PRO:HD2	3:D:2003:HOH:O	1.87	0.73
1:A:98:ALA:H	1:A:105:ASN:ND2	1.87	0.73
1:G:98:ALA:H	1:G:105:ASN:ND2	1.88	0.72
2:B:6:ILE:O	2:B:7:ARG:HG3	1.92	0.69
1:G:119:LYS:HE2	1:G:119:LYS:HA	1.74	0.69
1:G:148:ARG:HB3	1:G:156:TYR:CE2	2.28	0.69
1:A:137:ARG:NH2	1:D:207:ASP:HB2	2.07	0.69
1:D:112:ASN:HD21	1:D:145:ARG:HD2	1.58	0.68
1:J:181:ARG:HD3	3:J:2015:HOH:O	1.94	0.68
1:D:133:THR:O	1:D:134:ASP:HB2	1.92	0.68
1:J:176:GLY:HA3	3:J:2013:HOH:O	1.95	0.66
1:G:129:LEU:HD23	1:G:130:LEU:N	2.11	0.65
1:G:134:ASP:N	3:G:2002:HOH:O	2.28	0.65
1:J:98:ALA:H	1:J:105:ASN:ND2	1.96	0.64
1:A:148:ARG:HD3	1:A:156:TYR:CD2	2.32	0.64
1:A:188:GLU:OE2	1:A:197:LYS:HE2	1.98	0.63
1:G:171:ASN:O	1:G:172:THR:HB	1.96	0.63
1:D:149:GLU:HG2	3:J:2008:HOH:O	1.98	0.62
1:J:180:ARG:N	3:J:2014:HOH:O	2.32	0.62
1:A:207:ASP:C	3:A:2020:HOH:O	2.37	0.62
1:G:124:CYS:HB3	1:G:126:ASP:OD2	2.00	0.62
1:D:184:ASN:HB2	3:D:2020:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:HE22	1:A:196:ASN:ND2	1.98	0.62
1:D:171:ASN:O	1:D:172:THR:CB	2.30	0.61
1:G:127:GLU:HG2	1:G:128:PRO:HD2	1.81	0.61
1:J:150:VAL:HA	1:J:155:SER:O	1.99	0.61
1:A:100:GLN:HE22	1:A:196:ASN:HD21	1.46	0.61
1:G:99:LEU:HD11	1:G:200:VAL:CG2	2.30	0.61
1:D:204:LEU:HA	1:D:207:ASP:CB	2.30	0.61
1:A:127:GLU:HG2	3:A:2005:HOH:O	2.01	0.61
1:G:150:VAL:HA	1:G:156:TYR:HA	1.83	0.61
1:D:191:LEU:O	1:D:192:SER:HB2	2.01	0.60
1:G:99:LEU:HD11	1:G:200:VAL:HG23	1.82	0.60
1:J:148:ARG:HH11	1:J:148:ARG:HG2	1.67	0.59
1:G:98:ALA:H	1:G:105:ASN:HD22	1.51	0.59
1:J:181:ARG:CD	3:J:2015:HOH:O	2.51	0.59
1:G:99:LEU:HD21	1:G:200:VAL:HG23	1.85	0.59
1:G:122:GLU:N	1:G:122:GLU:OE1	2.36	0.59
1:G:170:VAL:HG12	1:G:171:ASN:HD22	1.69	0.58
1:D:134:ASP:O	1:D:137:ARG:HB2	2.03	0.58
1:D:204:LEU:HA	1:D:207:ASP:HB3	1.85	0.58
1:J:99:LEU:HD11	1:J:200:VAL:CG2	2.34	0.58
1:A:99:LEU:HD11	1:A:200:VAL:CG2	2.35	0.57
1:G:119:LYS:C	1:G:121:CYS:H	2.07	0.57
1:D:119:LYS:HD2	3:D:2007:HOH:O	2.04	0.57
1:G:170:VAL:HG12	1:G:171:ASN:ND2	2.20	0.56
1:A:99:LEU:HD11	1:A:200:VAL:HG23	1.87	0.56
1:A:131:LYS:HG2	1:A:136:TYR:CZ	2.41	0.55
1:G:93:TRP:CE2	1:G:148:ARG:HD2	2.41	0.55
1:G:133:THR:O	1:G:134:ASP:HB2	2.07	0.55
1:G:92:PRO:HA	1:G:108:CYS:O	2.06	0.55
1:G:130:LEU:O	1:G:131:LYS:C	2.45	0.55
2:E:6:ILE:O	2:E:7:ARG:HG3	2.08	0.54
1:G:169:PHE:HB2	1:G:190:ALA:HB3	1.89	0.54
1:D:206:VAL:O	1:D:207:ASP:C	2.46	0.54
1:G:160:ILE:HB	1:G:183:LEU:HD22	1.90	0.54
1:D:184:ASN:CB	3:D:2020:HOH:O	2.56	0.53
2:B:1:PHE:HD2	1:D:207:ASP:HA	1.73	0.53
1:J:206:VAL:CA	3:J:2019:HOH:O	2.43	0.53
1:D:112:ASN:HD22	1:D:147:PHE:HB3	1.73	0.53
1:J:157:ILE:HG22	1:J:159:TYR:CE1	2.44	0.53
1:J:93:TRP:C	1:J:204:LEU:HB2	2.30	0.52
1:A:92:PRO:CD	3:A:2001:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HB2	3:A:2014:HOH:O	2.09	0.52
1:J:112:ASN:HD21	1:J:145:ARG:HD2	1.74	0.52
1:D:193:LEU:O	1:D:195:ARG:N	2.43	0.52
1:D:99:LEU:HD11	1:D:200:VAL:CG2	2.34	0.52
1:G:148:ARG:HB3	1:G:156:TYR:CZ	2.45	0.51
1:G:95:ARG:NH1	3:J:2007:HOH:O	2.40	0.51
1:A:98:ALA:H	1:A:105:ASN:HD22	1.54	0.51
1:J:137:ARG:HH11	1:J:137:ARG:HB3	1.75	0.51
1:D:126:ASP:O	1:D:127:GLU:C	2.49	0.51
1:G:129:LEU:HD23	1:G:129:LEU:C	2.32	0.50
2:E:6:ILE:O	2:E:6:ILE:CG1	2.54	0.50
1:A:137:ARG:HH21	1:D:207:ASP:HB2	1.75	0.50
1:G:149:GLU:O	1:G:150:VAL:O	2.29	0.50
1:D:133:THR:N	3:D:2010:HOH:O	2.45	0.50
1:G:151:GLY:O	1:G:154:ASN:N	2.45	0.49
1:D:129:LEU:HD23	1:D:129:LEU:C	2.33	0.49
2:H:4:TYR:CE2	2:H:6:ILE:HG22	2.48	0.49
1:D:132:ARG:CA	3:D:2010:HOH:O	2.60	0.49
1:J:132:ARG:C	3:J:2007:HOH:O	2.51	0.49
1:D:204:LEU:HA	1:D:207:ASP:HB2	1.95	0.49
1:J:94:ALA:HB3	1:J:108:CYS:HB2	1.95	0.49
1:J:161:GLU:HG3	1:J:179:LYS:O	2.12	0.49
1:G:134:ASP:O	1:G:137:ARG:HB2	2.13	0.49
1:D:204:LEU:O	1:D:207:ASP:HB3	2.13	0.48
1:J:148:ARG:NH1	1:J:148:ARG:HG2	2.28	0.48
1:G:96:LEU:HB2	1:G:106:LEU:HB3	1.96	0.48
1:A:134:ASP:O	1:A:137:ARG:HB2	2.13	0.48
1:G:175:VAL:HG12	1:G:179:LYS:O	2.14	0.48
1:A:207:ASP:OXT	3:A:2020:HOH:O	2.18	0.48
2:B:1:PHE:CD2	1:D:207:ASP:HA	2.49	0.48
1:G:195:ARG:HG3	1:G:195:ARG:HH11	1.79	0.47
1:D:98:ALA:H	1:D:105:ASN:HD21	1.58	0.47
1:G:95:ARG:HD2	1:J:134:ASP:OD1	2.15	0.47
1:J:179:LYS:CA	3:J:2014:HOH:O	2.44	0.47
1:A:156:TYR:N	3:A:2015:HOH:O	2.45	0.47
1:G:128:PRO:O	1:G:130:LEU:N	2.47	0.47
1:D:132:ARG:C	3:D:2010:HOH:O	2.53	0.47
1:G:95:ARG:HG2	3:G:2001:HOH:O	2.13	0.47
1:J:171:ASN:O	1:J:172:THR:CB	2.59	0.47
1:G:138:THR:HB	1:G:166:ASN:ND2	2.30	0.47
1:J:92:PRO:CD	3:J:2001:HOH:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ASN:HB2	1:D:203:ASP:HB2	1.97	0.46
1:G:133:THR:O	1:G:134:ASP:CB	2.63	0.46
1:D:204:LEU:CA	1:D:207:ASP:HB3	2.45	0.46
1:A:138:THR:HB	1:A:166:ASN:ND2	2.31	0.46
1:A:185:ASN:HB2	1:A:203:ASP:HB3	1.96	0.46
1:G:134:ASP:O	1:G:137:ARG:N	2.48	0.46
1:G:186:ASN:OD1	2:K:4:TYR:HB2	2.16	0.46
1:G:206:VAL:O	1:G:207:ASP:C	2.55	0.46
1:G:181:ARG:HD3	3:G:2004:HOH:O	2.16	0.45
2:K:7:ARG:CB	3:K:2003:HOH:O	2.63	0.45
1:J:111:ASP:O	1:J:147:PHE:HB2	2.17	0.45
1:G:177:LYS:C	1:G:179:LYS:H	2.20	0.45
1:J:206:VAL:C	3:J:2019:HOH:O	2.53	0.45
1:D:142:LYS:HE3	3:D:2011:HOH:O	2.15	0.45
1:G:114:TRP:HB2	1:G:122:GLU:OE1	2.16	0.45
1:G:128:PRO:O	1:G:129:LEU:C	2.54	0.45
2:H:1:PHE:H	2:H:1:PHE:HD2	1.63	0.44
1:A:112:ASN:HD22	1:A:147:PHE:HB3	1.81	0.44
1:G:161:GLU:OE1	1:G:163:HIS:NE2	2.50	0.44
1:A:148:ARG:HD3	1:A:156:TYR:CE2	2.52	0.44
2:B:1:PHE:HB3	1:D:206:VAL:HG12	1.98	0.43
1:G:93:TRP:O	1:G:204:LEU:HB2	2.18	0.43
1:J:148:ARG:HA	1:J:158:ALA:HA	1.99	0.43
1:D:93:TRP:NE1	1:D:148:ARG:HD2	2.32	0.43
1:A:185:ASN:O	1:A:186:ASN:HB2	2.19	0.43
1:G:206:VAL:HG12	1:G:207:ASP:N	2.32	0.43
1:A:133:THR:O	1:A:135:LYS:N	2.47	0.43
1:J:133:THR:N	3:J:2007:HOH:O	2.52	0.43
1:A:203:ASP:OD1	1:A:205:THR:HB	2.19	0.42
1:A:114:TRP:CZ2	1:A:145:ARG:HD3	2.54	0.42
1:D:136:TYR:HA	1:D:139:TYR:CD1	2.54	0.42
1:G:130:LEU:O	1:G:132:ARG:N	2.52	0.42
1:G:200:VAL:HG21	2:K:4:TYR:CE2	2.54	0.42
1:A:112:ASN:ND2	1:A:145:ARG:HH11	2.17	0.42
1:A:112:ASN:HD21	1:A:145:ARG:HD2	1.85	0.41
1:G:171:ASN:O	1:G:172:THR:CB	2.63	0.41
1:D:188:GLU:OE1	1:D:197:LYS:HD3	2.20	0.41
1:J:179:LYS:C	3:J:2014:HOH:O	2.56	0.41
1:D:204:LEU:C	1:D:207:ASP:HB3	2.40	0.41
1:G:203:ASP:OD1	1:G:205:THR:HB	2.21	0.41
1:J:111:ASP:HA	1:J:148:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:LYS:C	1:G:121:CYS:N	2.74	0.41
1:G:153:LYS:O	1:G:154:ASN:C	2.59	0.41
1:J:203:ASP:OD1	1:J:205:THR:HB	2.20	0.41
1:A:181:ARG:CD	3:A:2016:HOH:O	2.45	0.41
1:G:181:ARG:HA	1:G:182:PRO:HD3	1.98	0.41
1:D:93:TRP:CH2	1:D:148:ARG:HG3	2.55	0.41
1:G:131:LYS:HA	1:G:136:TYR:CD2	2.56	0.41
1:G:123:TYR:CE2	1:G:199:PHE:HZ	2.39	0.41
1:G:99:LEU:HD11	1:G:200:VAL:HG22	2.02	0.41
1:J:117:ARG:HB2	1:J:141:LYS:HA	2.03	0.40
1:D:134:ASP:O	1:D:135:LYS:C	2.55	0.40
1:D:162:ASP:HB2	1:D:175:VAL:HB	2.03	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)
1:A:188:GLU:OE1	2:E:4:TYR:OH[4_567]	2.18	0.02

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	114/149 (76%)	104 (91%)	10 (9%)	0	100 100
1	D	114/149 (76%)	103 (90%)	8 (7%)	3 (3%)	5 13
1	G	114/149 (76%)	90 (79%)	14 (12%)	10 (9%)	1 1
1	J	114/149 (76%)	100 (88%)	11 (10%)	3 (3%)	5 13
2	B	5/10 (50%)	4 (80%)	1 (20%)	0	100 100
2	E	5/10 (50%)	4 (80%)	0	1 (20%)	0 0
2	H	5/10 (50%)	4 (80%)	0	1 (20%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	K	5/10 (50%)	5 (100%)	0	0	100 100
All	All	476/636 (75%)	414 (87%)	44 (9%)	18 (4%)	3 7

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	194	SER
1	G	128	PRO
1	G	129	LEU
1	G	131	LYS
1	G	150	VAL
1	G	126	ASP
1	G	130	LEU
1	G	156	TYR
1	D	131	LYS
1	G	185	ASN
1	J	153	LYS
1	J	154	ASN
1	G	152	PRO
1	G	154	ASN
2	H	1	PHE
1	D	172	THR
1	J	205	THR
2	E	6	ILE

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	103/136 (76%)	101 (98%)	2 (2%)	57 82
1	D	103/136 (76%)	101 (98%)	2 (2%)	57 82
1	G	103/136 (76%)	99 (96%)	4 (4%)	32 61
1	J	103/136 (76%)	96 (93%)	7 (7%)	16 36
2	B	7/9 (78%)	6 (86%)	1 (14%)	3 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	7/9 (78%)	7 (100%)	0	100 100
2	H	6/9 (67%)	6 (100%)	0	100 100
2	K	6/9 (67%)	5 (83%)	1 (17%)	2 5
All	All	438/580 (76%)	421 (96%)	17 (4%)	32 61

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	THR
1	A	205	THR
2	B	6	ILE
1	D	172	THR
1	D	207	ASP
1	G	119	LYS
1	G	156	TYR
1	G	172	THR
1	G	184	ASN
1	J	118	ASP
1	J	129	LEU
1	J	137	ARG
1	J	156	TYR
1	J	172	THR
1	J	180	ARG
1	J	207	ASP
2	K	6	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	112	ASN
1	A	186	ASN
1	A	196	ASN
1	D	105	ASN
1	D	112	ASN
1	D	196	ASN
1	G	105	ASN
1	G	112	ASN
1	G	171	ASN
1	J	100	GLN

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Mol	Chain	Res	Type
1	J	105	ASN
1	J	112	ASN
1	J	196	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
2	TPO	H	3	2	8,10,11	1.63	1 (12%)	10,14,16	1.24	1 (10%)
2	TPO	K	3	2	8,10,11	1.66	1 (12%)	10,14,16	1.09	1 (10%)
2	TPO	B	3	2	8,10,11	1.81	1 (12%)	10,14,16	1.11	1 (10%)
2	TPO	E	3	2	8,10,11	1.53	1 (12%)	10,14,16	1.07	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
2	TPO	H	3	2	-	0/9/11/13	-
2	TPO	K	3	2	-	0/9/11/13	-
2	TPO	B	3	2	-	0/9/11/13	-
2	TPO	E	3	2	-	0/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	TPO	P-OG1	-4.68	1.50	1.59
2	K	3	TPO	P-OG1	-4.36	1.51	1.59
2	H	3	TPO	P-OG1	-4.13	1.51	1.59
2	E	3	TPO	P-OG1	-3.95	1.51	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	3	TPO	CG2-CB-CA	-3.03	107.19	113.16
2	B	3	TPO	CG2-CB-CA	-2.43	108.38	113.16
2	K	3	TPO	CG2-CB-CA	-2.39	108.44	113.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.