



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:14 AM UTC

PDB ID : 1HKC / pdb_00001hkc
Title : RECOMBINANT HUMAN HEXOKINASE TYPE I COMPLEXED WITH
GLUCOSE AND PHOSPHATE
Authors : Aleshin, A.E.; Honzatko, R.B.
Deposited on : 1998-07-01
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

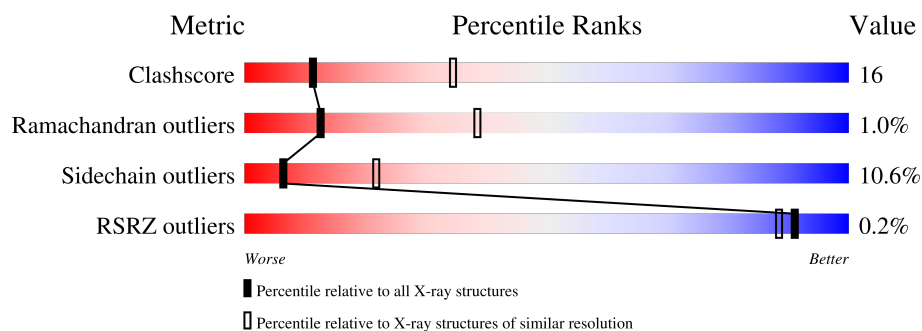
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of 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 $\leq 5\%$. 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	917	

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	PO4	A	920	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7206 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.

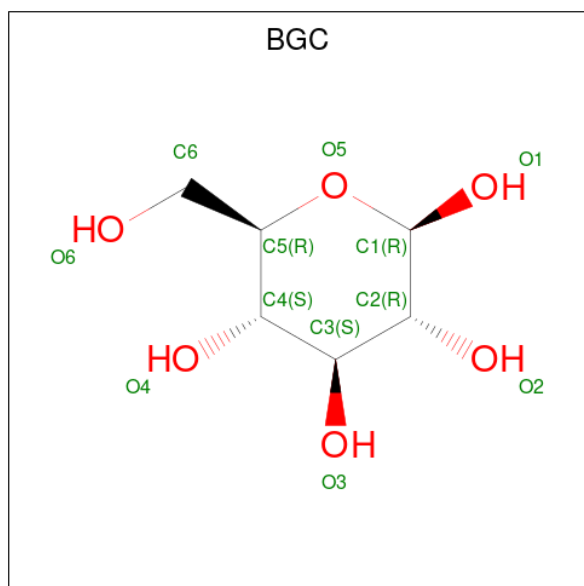
- Molecule 1 is a protein called D-GLUCOSE 6-PHOSPHOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	899	7032	4407	1241	1331	53	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	776	LEU	MET	SEE REMARK 999	UNP P19367

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

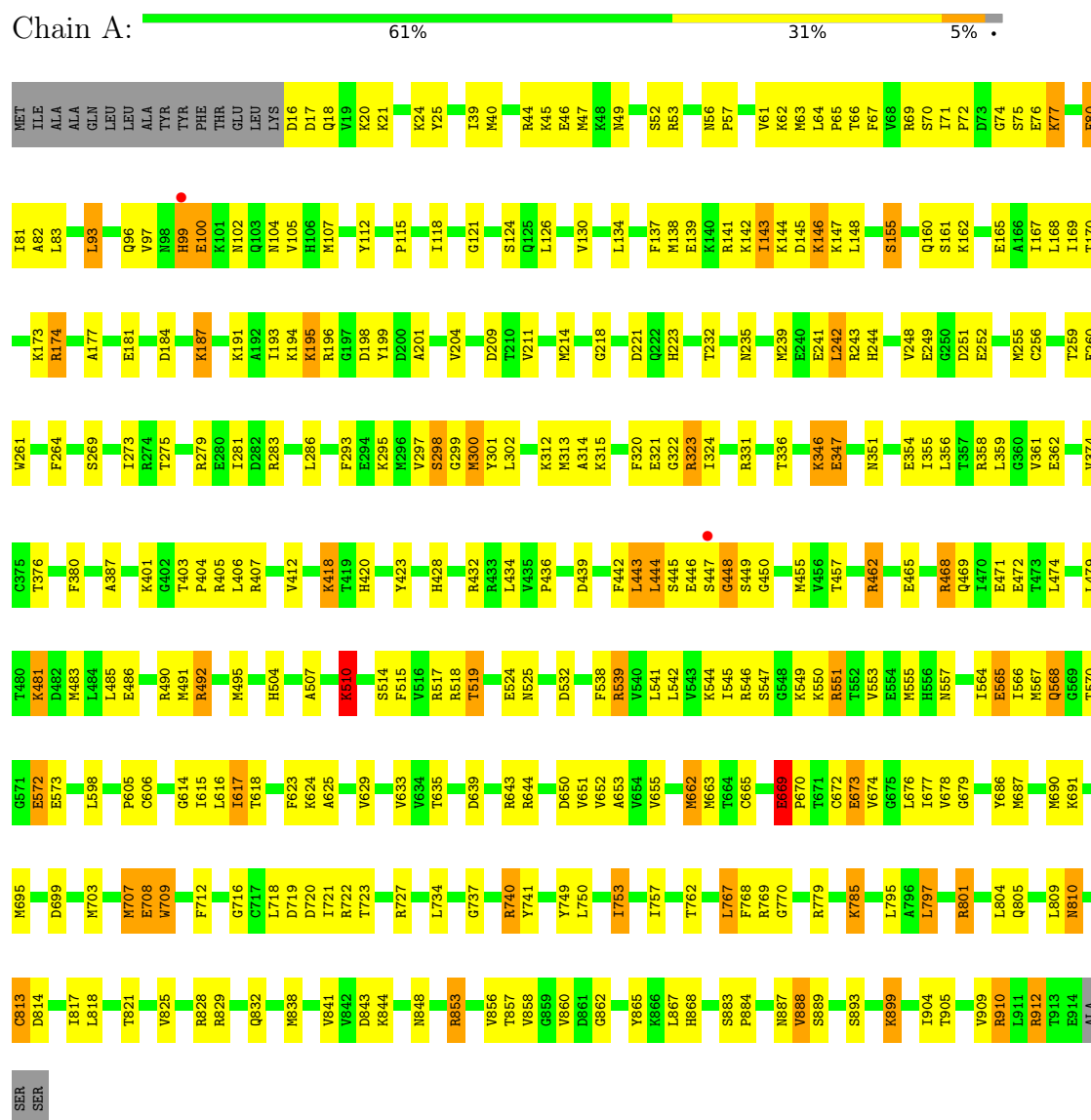
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: D-GLUCOSE 6-PHOSPHOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.09 Å 175.09 Å 99.47 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (8.00-2.80) 94.0 (8.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 2.81 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.174 , 0.241 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.089 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7206	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BGC, K

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	0.42	0/7138	0.92	16/9606 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	ILE	N-CA-C	-7.51	103.47	110.53
1	A	655	VAL	N-CA-C	7.46	120.34	108.85
1	A	707	MET	N-CA-C	6.63	118.51	111.28
1	A	510	LYS	N-CA-C	6.50	120.07	111.75
1	A	298	SER	N-CA-C	6.46	118.89	110.43
1	A	62	LYS	N-CA-C	6.32	118.98	111.71
1	A	374	VAL	N-CA-C	-6.19	104.71	110.53
1	A	387	ALA	N-CA-C	-5.96	104.70	111.14
1	A	669	GLU	CA-C-N	5.87	125.55	119.56
1	A	669	GLU	C-N-CA	5.87	125.55	119.56
1	A	868	HIS	CA-C-N	5.83	125.53	119.05
1	A	868	HIS	C-N-CA	5.83	125.53	119.05
1	A	653	ALA	N-CA-C	5.71	117.20	108.52
1	A	708	GLU	N-CA-C	-5.54	104.26	111.74
1	A	572	GLU	N-CA-C	-5.37	105.87	112.90
1	A	297	VAL	N-CA-C	5.02	119.77	109.34

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	7032	0	7092	229	0
2	A	12	0	12	1	0
3	A	10	0	0	2	0
4	A	2	0	0	0	0
5	A	150	0	0	2	0
All	All	7206	0	7104	229	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 16.

All (229) 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:184:ASP:HB3	1:A:187:LYS:HG3	1.45	0.94
1:A:204:VAL:HG21	1:A:457:THR:HG23	1.54	0.88
1:A:241:GLU:HB2	1:A:244:HIS:HD2	1.36	0.87
1:A:555:MET:HE1	1:A:899:LYS:HG3	1.56	0.87
1:A:814:ASP:HA	1:A:817:ILE:HD12	1.58	0.85
1:A:115:PRO:HD2	1:A:118:ILE:HD12	1.59	0.84
1:A:196:ARG:HG3	1:A:198:ASP:H	1.44	0.82
1:A:767:LEU:HG	1:A:818:LEU:HD23	1.63	0.80
1:A:346:LYS:HG3	1:A:347:GLU:HG3	1.65	0.78
1:A:232:THR:O	1:A:298:SER:HB2	1.84	0.76
1:A:676:LEU:HB3	1:A:860:VAL:HG12	1.68	0.74
1:A:169:ILE:HG22	1:A:170:THR:HG23	1.71	0.72
1:A:241:GLU:HB2	1:A:244:HIS:CD2	2.23	0.71
1:A:462:ARG:HB3	1:A:462:ARG:HH11	1.55	0.71
1:A:797:LEU:HD21	1:A:817:ILE:HG13	1.73	0.71
1:A:40:MET:HE1	1:A:434:LEU:HB3	1.74	0.70
1:A:617:ILE:HG13	1:A:618:THR:HG22	1.74	0.69
1:A:235:ASN:HB2	2:A:918:BGC:H5	1.75	0.69
1:A:97:VAL:HG21	1:A:455:MET:HE3	1.73	0.69
1:A:468:ARG:HD2	1:A:472:GLU:OE2	1.93	0.68
1:A:139:GLU:HG3	1:A:144:LYS:HE3	1.74	0.68
1:A:193:ILE:HD13	1:A:201:ALA:HB3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HD3	1:A:199:TYR:CE1	2.29	0.67
1:A:248:VAL:HG21	1:A:255:MET:HE1	1.76	0.67
1:A:492:ARG:HH11	1:A:492:ARG:HG3	1.58	0.67
1:A:25:TYR:CD2	1:A:313:MET:HE3	2.31	0.66
1:A:204:VAL:CG2	1:A:457:THR:HG23	2.27	0.65
1:A:481:LYS:O	1:A:485:LEU:HG	1.94	0.65
1:A:541:LEU:HG	1:A:557:ASN:HB3	1.79	0.65
1:A:909:VAL:O	1:A:912:ARG:HG3	1.97	0.65
1:A:479:LEU:HD23	1:A:829:ARG:HG3	1.79	0.64
1:A:315:LYS:HG3	1:A:324:ILE:HD11	1.79	0.64
1:A:248:VAL:HG21	1:A:255:MET:CE	2.28	0.63
1:A:428:HIS:HB3	1:A:432:ARG:NH1	2.14	0.63
1:A:428:HIS:HB3	1:A:432:ARG:HH12	1.63	0.62
1:A:214:MET:HE1	1:A:239:MET:HE2	1.80	0.62
1:A:652:VAL:HB	1:A:905:THR:HG23	1.80	0.61
1:A:145:ASP:OD2	1:A:146:LYS:HG3	2.00	0.61
1:A:821:THR:O	1:A:825:VAL:HG23	2.01	0.61
1:A:828:ARG:O	1:A:832:GLN:HG3	2.01	0.61
1:A:518:ARG:HG2	1:A:519:THR:O	2.01	0.61
1:A:214:MET:CE	1:A:239:MET:HE2	2.31	0.61
1:A:674:VAL:HB	1:A:858:VAL:HG22	1.81	0.60
1:A:445:SER:HB2	1:A:448:GLY:HA2	1.82	0.60
1:A:418:LYS:HD2	1:A:444:LEU:HD11	1.84	0.60
1:A:67:PHE:HE2	1:A:160:GLN:O	1.84	0.60
1:A:753:ILE:O	1:A:757:ILE:HG13	2.01	0.60
1:A:196:ARG:HD3	1:A:199:TYR:HE1	1.66	0.60
1:A:96:GLN:O	1:A:105:VAL:HG13	2.03	0.59
1:A:354:GLU:O	1:A:358:ARG:HG3	2.03	0.59
1:A:762:THR:O	1:A:770:GLY:HA2	2.02	0.59
1:A:718:LEU:O	1:A:722:ARG:HG3	2.03	0.59
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.67	0.58
1:A:184:ASP:CB	1:A:187:LYS:HG3	2.28	0.57
1:A:570:THR:C	1:A:572:GLU:H	2.12	0.57
1:A:797:LEU:CD2	1:A:817:ILE:HG13	2.34	0.57
1:A:551:ARG:HH11	1:A:551:ARG:CG	2.17	0.57
1:A:474:LEU:HD13	1:A:825:VAL:HG21	1.87	0.57
1:A:598:LEU:C	1:A:598:LEU:HD23	2.30	0.57
1:A:486:GLU:O	1:A:490:ARG:HG3	2.04	0.56
1:A:112:TYR:OH	1:A:137:PHE:HB2	2.05	0.56
1:A:18:GLN:HA	1:A:18:GLN:OE1	2.04	0.55
1:A:20:LYS:HG3	1:A:24:LYS:HE2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLY:C	1:A:76:GLU:H	2.15	0.55
1:A:99:HIS:C	1:A:100:GLU:HG2	2.32	0.55
1:A:507:ALA:O	1:A:510:LYS:HE2	2.07	0.55
1:A:71:ILE:HG12	5:A:999:HOH:O	2.07	0.54
1:A:66:THR:OG1	1:A:256:CYS:HB3	2.07	0.54
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.43	0.54
1:A:492:ARG:HH11	1:A:492:ARG:CG	2.18	0.54
1:A:44:ARG:HA	1:A:47:MET:HE3	1.90	0.54
1:A:723:THR:O	1:A:727:ARG:HG3	2.08	0.54
1:A:525:ASN:OD1	1:A:546:ARG:HA	2.07	0.53
1:A:673:GLU:O	1:A:686:TYR:HA	2.09	0.53
1:A:320:PHE:CD1	1:A:361:VAL:HG11	2.44	0.53
1:A:72:PRO:HA	1:A:76:GLU:OE2	2.09	0.52
1:A:712:PHE:O	1:A:741:TYR:HB2	2.09	0.52
1:A:856:VAL:O	1:A:888:VAL:HA	2.09	0.52
1:A:615:ILE:HD12	1:A:615:ILE:N	2.25	0.52
1:A:168:LEU:HD11	1:A:170:THR:O	2.10	0.52
1:A:252:GLU:OE2	1:A:813:CYS:HB2	2.10	0.52
1:A:315:LYS:HG3	1:A:324:ILE:CD1	2.39	0.52
1:A:614:GLY:O	1:A:633:VAL:HG22	2.09	0.52
1:A:20:LYS:HE3	1:A:24:LYS:NZ	2.25	0.51
1:A:403:THR:CG2	1:A:404:PRO:HD2	2.40	0.51
1:A:405:ARG:NH2	1:A:439:ASP:HB3	2.25	0.51
1:A:221:ASP:OD1	1:A:223:HIS:HB2	2.11	0.51
1:A:356:LEU:O	1:A:359:LEU:HB2	2.10	0.51
1:A:279:ARG:O	1:A:283:ARG:HG3	2.10	0.51
1:A:740:ARG:HH11	1:A:740:ARG:HG2	1.76	0.51
1:A:155:SER:HB3	1:A:209:ASP:CG	2.35	0.51
1:A:737:GLY:HA2	1:A:740:ARG:HE	1.75	0.51
1:A:93:LEU:HD22	1:A:450:GLY:HA3	1.92	0.50
1:A:740:ARG:HG2	1:A:740:ARG:NH1	2.26	0.50
1:A:80:PHE:CD1	1:A:80:PHE:N	2.78	0.50
1:A:838:MET:HE3	1:A:841:VAL:HB	1.93	0.50
1:A:20:LYS:O	1:A:24:LYS:HG3	2.11	0.50
1:A:20:LYS:HE3	1:A:24:LYS:HE2	1.93	0.50
1:A:517:ARG:NH2	1:A:690:MET:HE2	2.27	0.50
1:A:567:MET:HE3	1:A:623:PHE:CE1	2.47	0.50
1:A:716:GLY:O	1:A:719:ASP:HB2	2.12	0.50
1:A:720:ASP:OD1	1:A:721:ILE:HG23	2.12	0.49
1:A:81:ILE:HG22	1:A:82:ALA:H	1.77	0.49
1:A:455:MET:HE2	1:A:455:MET:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LEU:HD22	1:A:721:ILE:HD11	1.94	0.49
1:A:804:LEU:HD22	1:A:809:LEU:HD12	1.95	0.49
1:A:838:MET:HE3	1:A:838:MET:HA	1.94	0.49
1:A:69:ARG:HH12	1:A:242:LEU:HD21	1.77	0.49
1:A:174:ARG:HH11	1:A:300:MET:HE3	1.78	0.49
1:A:471:GLU:HA	1:A:471:GLU:OE1	2.12	0.49
1:A:242:LEU:C	1:A:244:HIS:H	2.19	0.48
1:A:376:THR:O	1:A:380:PHE:HB2	2.13	0.48
1:A:514:SER:O	1:A:515:PHE:HB2	2.11	0.48
1:A:674:VAL:HG11	1:A:838:MET:CE	2.43	0.48
1:A:768:PHE:HA	1:A:769:ARG:CZ	2.43	0.48
1:A:134:LEU:HB3	1:A:199:TYR:OH	2.12	0.48
1:A:551:ARG:CG	1:A:551:ARG:NH1	2.76	0.48
1:A:121:GLY:O	1:A:177:ALA:HA	2.14	0.48
1:A:170:THR:HA	1:A:181:GLU:HG2	1.95	0.48
1:A:767:LEU:CG	1:A:818:LEU:HD23	2.38	0.48
1:A:853:ARG:NH1	1:A:887:ASN:HB2	2.29	0.48
1:A:420:HIS:HB3	1:A:423:TYR:HB2	1.95	0.48
1:A:77:LYS:HA	1:A:97:VAL:O	2.13	0.48
1:A:81:ILE:HG22	1:A:82:ALA:N	2.28	0.48
1:A:81:ILE:HD11	1:A:148:LEU:HD12	1.95	0.48
1:A:707:MET:O	1:A:708:GLU:HB2	2.13	0.48
1:A:492:ARG:CG	1:A:492:ARG:NH1	2.76	0.48
1:A:676:LEU:HD23	1:A:860:VAL:CG1	2.43	0.48
1:A:434:LEU:O	1:A:436:PRO:HD3	2.14	0.47
1:A:275:THR:O	1:A:279:ARG:HG3	2.14	0.47
1:A:663:MET:HG3	1:A:904:ILE:HG12	1.96	0.47
1:A:56:ASN:N	1:A:57:PRO:CD	2.77	0.47
1:A:361:VAL:HG12	1:A:362:GLU:N	2.30	0.47
1:A:67:PHE:CE2	1:A:161:SER:HA	2.50	0.47
1:A:323:ARG:HG2	1:A:323:ARG:NH1	2.29	0.47
1:A:570:THR:OG1	1:A:573:GLU:HG3	2.15	0.47
1:A:45:LYS:HE2	1:A:49:ASN:HD21	1.80	0.46
1:A:884:PRO:HD2	5:A:1026:HOH:O	2.16	0.46
1:A:862:GLY:HA2	3:A:920:PO4:O1	2.16	0.46
1:A:860:VAL:HG21	1:A:865:TYR:CZ	2.51	0.46
1:A:769:ARG:NH2	1:A:810:ASN:O	2.49	0.46
1:A:678:VAL:O	1:A:862:GLY:HA3	2.16	0.46
1:A:20:LYS:HE3	1:A:24:LYS:CE	2.46	0.46
1:A:53:ARG:HG3	1:A:53:ARG:HH11	1.80	0.45
1:A:259:THR:O	1:A:260:GLU:HB2	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ILE:O	1:A:546:ARG:HD3	2.16	0.45
1:A:39:ILE:CD1	1:A:273:ILE:HD13	2.47	0.45
1:A:314:ALA:O	1:A:322:GLY:HA2	2.15	0.45
1:A:491:MET:O	1:A:495:MET:HG3	2.16	0.45
1:A:542:LEU:HD21	1:A:544:LYS:HE3	1.98	0.45
1:A:515:PHE:HA	1:A:703:MET:SD	2.56	0.45
1:A:138:MET:O	1:A:142:LYS:N	2.50	0.45
1:A:209:ASP:OD1	1:A:209:ASP:N	2.48	0.45
1:A:299:GLY:O	1:A:336:THR:OG1	2.35	0.45
1:A:320:PHE:CG	1:A:361:VAL:HG11	2.52	0.45
1:A:465:GLU:O	1:A:469:GLN:HG3	2.16	0.45
1:A:407:ARG:HD3	1:A:407:ARG:C	2.42	0.44
1:A:639:ASP:HB3	1:A:643:ARG:HH21	1.82	0.44
1:A:65:PRO:HB3	1:A:255:MET:HE3	1.98	0.44
1:A:462:ARG:HH11	1:A:462:ARG:CB	2.26	0.44
1:A:504:HIS:CG	1:A:695:MET:HE2	2.52	0.44
1:A:564:ILE:HG23	1:A:565:GLU:N	2.32	0.44
1:A:805:GLN:HA	1:A:809:LEU:O	2.16	0.44
1:A:47:MET:CA	1:A:63:MET:HE2	2.48	0.44
1:A:785:LYS:HE3	1:A:867:LEU:HD13	1.98	0.44
1:A:261:TRP:CD1	1:A:261:TRP:C	2.95	0.44
1:A:445:SER:CB	1:A:448:GLY:HA2	2.47	0.44
1:A:665:CYS:HB2	1:A:893:SER:OG	2.18	0.44
1:A:65:PRO:CB	1:A:255:MET:HE3	2.47	0.44
1:A:570:THR:O	1:A:572:GLU:N	2.50	0.44
1:A:541:LEU:HG	1:A:557:ASN:CB	2.48	0.44
1:A:709:TRP:C	1:A:709:TRP:CD1	2.96	0.44
1:A:39:ILE:HD11	1:A:273:ILE:HD13	1.99	0.43
1:A:532:ASP:HB3	1:A:539:ARG:HG3	2.00	0.43
1:A:139:GLU:O	1:A:142:LYS:HG3	2.18	0.43
1:A:551:ARG:NH1	1:A:551:ARG:HG3	2.33	0.43
1:A:351:ASN:O	1:A:355:ILE:HD12	2.17	0.43
1:A:93:LEU:N	1:A:93:LEU:HD12	2.33	0.43
1:A:495:MET:HE2	1:A:844:LYS:HD3	2.00	0.43
1:A:412:VAL:CG2	1:A:442:PHE:HD1	2.32	0.43
1:A:662:MET:HE1	1:A:687:MET:SD	2.59	0.43
1:A:155:SER:HB2	1:A:173:LYS:NZ	2.33	0.43
1:A:838:MET:CE	1:A:841:VAL:HB	2.49	0.43
1:A:16:ASP:O	1:A:17:ASP:C	2.61	0.43
1:A:517:ARG:HH21	1:A:690:MET:HE2	1.82	0.42
1:A:134:LEU:O	1:A:138:MET:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:C	1:A:142:LYS:H	2.26	0.42
1:A:218:GLY:HA2	1:A:221:ASP:O	2.18	0.42
1:A:126:LEU:O	1:A:130:VAL:HG23	2.20	0.42
1:A:93:LEU:HD21	1:A:447:SER:OG	2.19	0.42
1:A:650:ASP:O	1:A:652:VAL:HG23	2.19	0.42
1:A:97:VAL:HG21	1:A:455:MET:CE	2.46	0.42
1:A:115:PRO:O	1:A:118:ILE:HB	2.19	0.42
1:A:481:LYS:O	1:A:481:LYS:HG2	2.18	0.42
1:A:74:GLY:C	1:A:76:GLU:N	2.74	0.42
1:A:264:PHE:O	1:A:293:PHE:HB2	2.20	0.42
1:A:801:ARG:O	1:A:805:GLN:HG3	2.20	0.42
1:A:64:LEU:HD21	1:A:169:ILE:HD11	2.02	0.41
1:A:97:VAL:HG11	1:A:455:MET:HE1	2.01	0.41
1:A:141:ARG:HB3	1:A:143:ILE:HG12	2.02	0.41
1:A:146:LYS:HG3	1:A:146:LYS:H	1.58	0.41
1:A:749:TYR:O	1:A:750:LEU:C	2.63	0.41
1:A:810:ASN:HD22	1:A:810:ASN:HA	1.74	0.41
1:A:53:ARG:HG3	1:A:53:ARG:NH1	2.35	0.41
1:A:115:PRO:HB2	1:A:118:ILE:HG13	2.02	0.41
1:A:174:ARG:NH1	1:A:300:MET:HE3	2.35	0.41
1:A:194:LYS:O	1:A:195:LYS:C	2.63	0.41
1:A:679:GLY:HA3	3:A:920:PO4:O1	2.21	0.41
1:A:909:VAL:HG23	1:A:910:ARG:N	2.35	0.41
1:A:66:THR:HG21	1:A:211:VAL:CG2	2.50	0.41
1:A:624:LYS:O	1:A:625:ALA:C	2.64	0.41
1:A:17:ASP:O	1:A:21:LYS:HG3	2.20	0.41
1:A:74:GLY:O	1:A:76:GLU:N	2.54	0.41
1:A:403:THR:HG23	1:A:404:PRO:HD2	2.03	0.41
1:A:564:ILE:O	1:A:568:GLN:HG3	2.21	0.41
1:A:46:GLU:HB3	1:A:61:VAL:CG2	2.51	0.41
1:A:242:LEU:HD13	1:A:242:LEU:HA	1.93	0.41
1:A:443:LEU:HD12	1:A:443:LEU:HA	1.95	0.41
1:A:672:CYS:HA	1:A:857:THR:O	2.21	0.41
1:A:20:LYS:HA	1:A:20:LYS:HD2	1.77	0.40
1:A:405:ARG:HH22	1:A:439:ASP:HB3	1.86	0.40
1:A:524:GLU:O	1:A:547:SER:HB3	2.20	0.40
1:A:532:ASP:O	1:A:538:PHE:HB2	2.21	0.40
1:A:160:GLN:HB3	1:A:165:GLU:O	2.21	0.40
1:A:676:LEU:HD23	1:A:860:VAL:HG11	2.03	0.40
1:A:616:LEU:HD23	1:A:629:VAL:HA	2.03	0.40
1:A:669:GLU:HA	1:A:670:PRO:HD2	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:HD13	1:A:734:LEU:HA	1.95	0.40
1:A:795:LEU:HD23	1:A:795:LEU:HA	1.78	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	897/917 (98%)	841 (94%)	47 (5%)	9 (1%)	12 38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	147	LYS
1	A	251	ASP
1	A	446	GLU
1	A	75	SER
1	A	243	ARG
1	A	605	PRO
1	A	651	VAL
1	A	448	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	774/788 (98%)	692 (89%)	82 (11%)	6	22

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	70	SER
1	A	77	LYS
1	A	80	PHE
1	A	83	LEU
1	A	93	LEU
1	A	99	HIS
1	A	100	GLU
1	A	102	ASN
1	A	107	MET
1	A	124	SER
1	A	143	ILE
1	A	146	LYS
1	A	155	SER
1	A	162	LYS
1	A	167	ILE
1	A	174	ARG
1	A	187	LYS
1	A	191	LYS
1	A	195	LYS
1	A	242	LEU
1	A	249	GLU
1	A	269	SER
1	A	281	ILE
1	A	286	LEU
1	A	300	MET
1	A	302	LEU
1	A	312	LYS
1	A	321	GLU
1	A	323	ARG
1	A	331	ARG
1	A	346	LYS
1	A	347	GLU
1	A	401	LYS
1	A	406	LEU
1	A	418	LYS
1	A	443	LEU
1	A	444	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	449	SER
1	A	462	ARG
1	A	468	ARG
1	A	481	LYS
1	A	483	MET
1	A	492	ARG
1	A	510	LYS
1	A	519	THR
1	A	539	ARG
1	A	549	LYS
1	A	550	LYS
1	A	551	ARG
1	A	553	VAL
1	A	565	GLU
1	A	566	ILE
1	A	568	GLN
1	A	606	CYS
1	A	617	ILE
1	A	635	THR
1	A	644	ARG
1	A	662	MET
1	A	669	GLU
1	A	673	GLU
1	A	677	ILE
1	A	691	LYS
1	A	699	ASP
1	A	709	TRP
1	A	740	ARG
1	A	767	LEU
1	A	779	ARG
1	A	785	LYS
1	A	797	LEU
1	A	801	ARG
1	A	810	ASN
1	A	813	CYS
1	A	843	ASP
1	A	848	ASN
1	A	853	ARG
1	A	883	SER
1	A	888	VAL
1	A	889	SER
1	A	899	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	910	ARG
1	A	912	ARG

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

Mol	Chain	Res	Type
1	A	49	ASN
1	A	102	ASN
1	A	103	GLN
1	A	104	ASN
1	A	160	GLN
1	A	202	ASN
1	A	244	HIS
1	A	466	GLN
1	A	537	ASN
1	A	810	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	BGC	A	918	-	12,12,12	0.46	0	17,17,17	0.59	0
3	PO4	A	920	-	4,4,4	1.50	0	6,6,6	0.50	0
3	PO4	A	919	-	4,4,4	1.87	2 (50%)	6,6,6	0.51	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	BGC	A	918	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	919	PO4	P-O3	-2.18	1.48	1.54
3	A	919	PO4	P-O4	-2.15	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	918	BGC	1	0
3	A	920	PO4	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	899/917 (98%)	-0.90	2 (0%) 91 88	6, 27, 75, 100	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	SER	3.8
1	A	99	HIS	3.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	A	922	1/1	0.62	0.10	46,46,46,46	0
3	PO4	A	920	5/5	0.81	0.21	79,83,85,94	0
4	K	A	921	1/1	0.91	0.06	40,40,40,40	0
2	BGC	A	918	12/12	0.95	0.09	26,37,46,55	0
3	PO4	A	919	5/5	0.98	0.06	26,30,35,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.