Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:52 PM GMT

PDB ID	:	1HKB
Title	:	CRYSTAL STRUCTURE OF RECOMBINANT HUMAN BRAIN HEXOKINASE TYPE I COMPLEXED WITH GLUCOSE AND GLUCOSE-6-PHOSPHATE
Authors	:	Aleshin, A.E.; Zeng, C.; Burenkov, G.P.; Bartunik, H.D.; Fromm, H.J.; Honzatko, R.B.
Deposited on	:	1997-12-01
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
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:

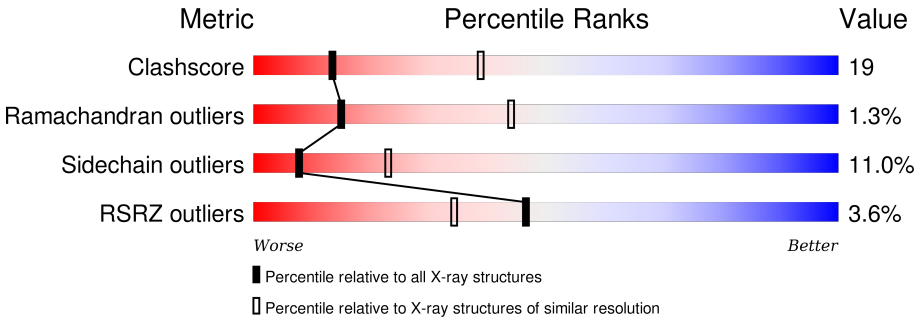
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	917	3% 59% 33% 5%
1	B	917	4% 61% 32% 5%

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
2	BGC	A	918	-	-	-	X
2	BGC	A	920	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G6P	A	919	X	-	-	-
3	G6P	A	921	X	-	-	-
3	G6P	B	919	X	-	-	-
3	G6P	B	921	X	-	-	-
4	CA	B	923	-	-	-	X

2 Entry composition

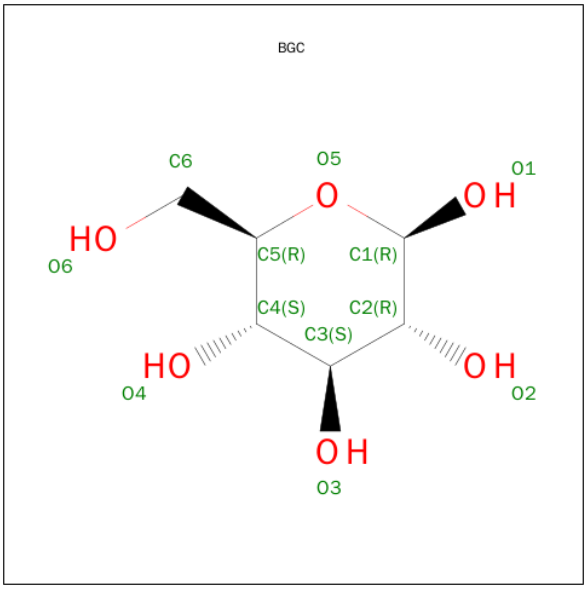
There are 5 unique types of molecules in this entry. The entry contains 14322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

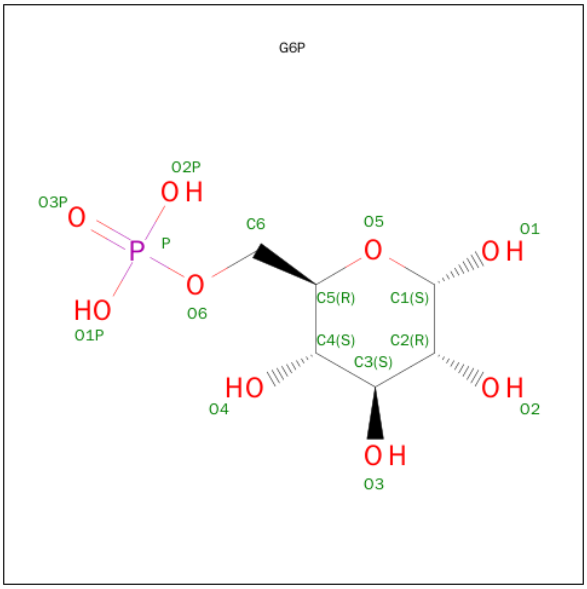
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	0	0	0
			7032	4407	1240	1332	53			
1	B	899	Total	C	N	O	S	0	0	0
			7032	4407	1240	1332	53			

- Molecule 2 is SUGAR (GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 16 6 9 1	0	0
3	A	1	Total C O P 16 6 9 1	0	0
3	B	1	Total C O P 16 6 9 1	0	0
3	B	1	Total C O P 16 6 9 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0

- Molecule 5 is water.

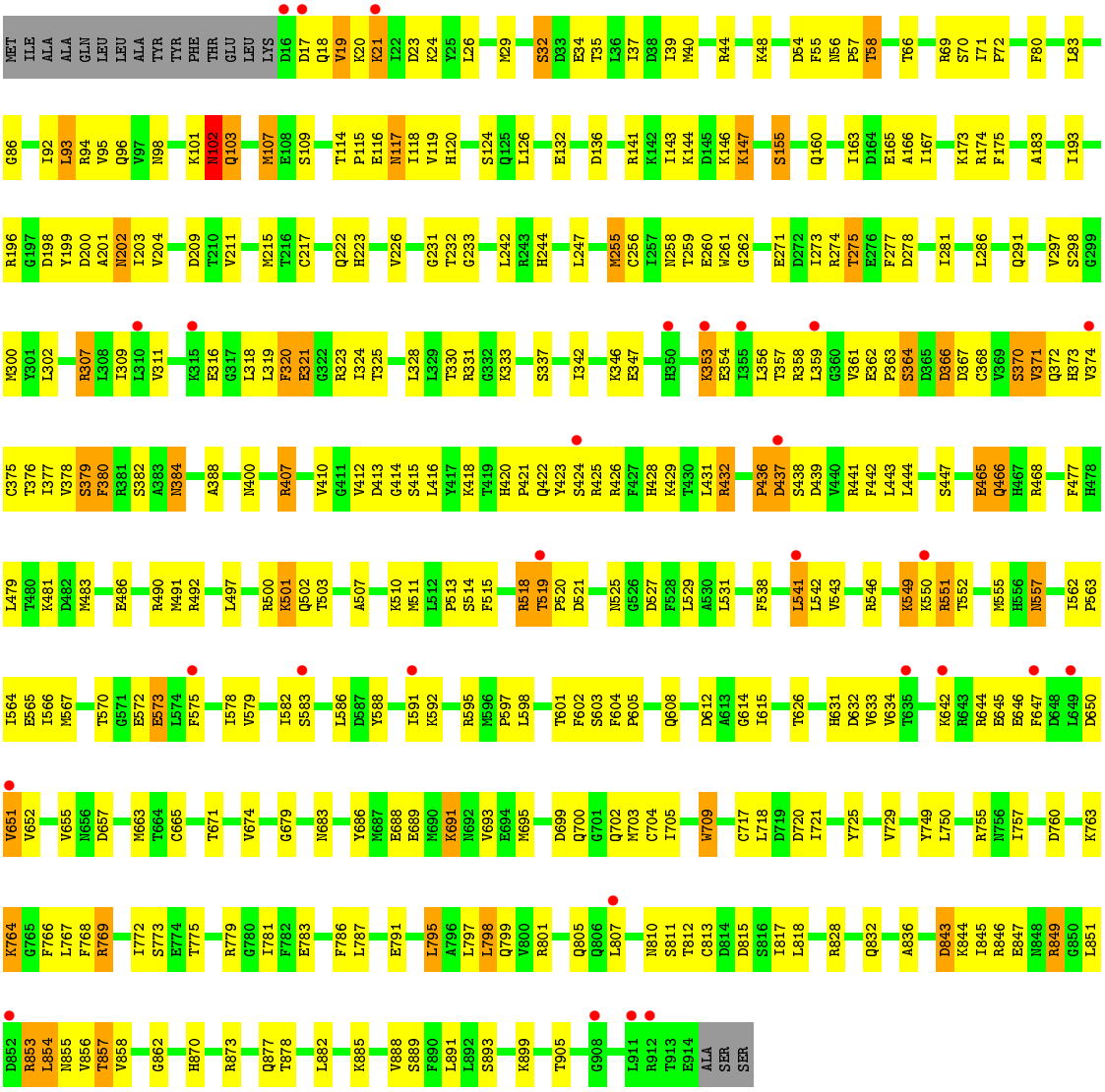
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	B	86	Total O 86 86	0	0

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.

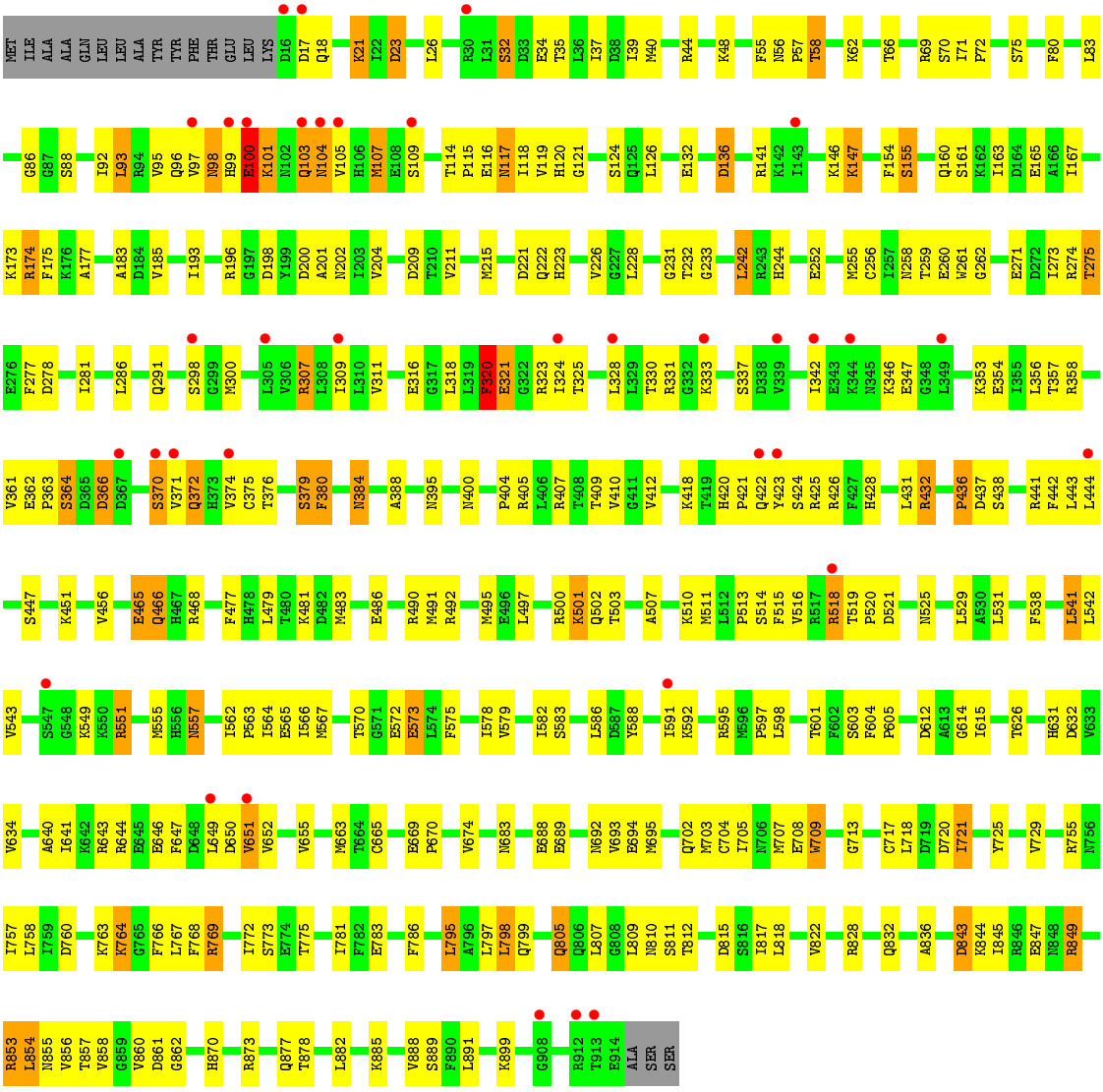
- Molecule 1: D-GLUCOSE 6-PHOSPHOTRANSFERASE

Chain A:



- Molecule 1: D-GLUCOSE 6-PHOSPHOTRANSFERASE

Chain B:


MET ILE ALA ALA GLN LEU LEU ALA TYR TYR PHE THR GLU LEU LYS D16 D17 Q18 K21 I22 D23 L26 R30 I31 S32 D33 E34 T35 L36 I37 D38 I39 M40 R44 K48 F55 N56 P57 T58 K62 T66 R69 S70 I71 F72 S75 F80 L83
G86 G87 S88 I92 L93 R94 V95 Q96 V97 N98 H99 E100 K101 N102 Q103 M104 V105 H106 M107 E108 S109 T114 P115 E116 N117 I118 V119 H120 G121 S124 Q125 L126 E132 D136 R141 K142 I143 K146 K147 F154 S155 Q160 S161 K162 I163 D164 E165 A166 I167
K173 R174 F175 K176 A177 A183 D184 V185 I193 R196 G197 D198 Y199 D200 A201 N202 I203 V204 D209 T210 V211 M215 D221 Q222 H223 V226 G227 L228 G231 T232 G233 L242 R243 H244 E252 M255 C256 I257 N258 T259 E260 W261 G262 E271 D272 I273 R274 T275
E276 F277 D278 I281 L286 Q291 S298 G299 M300 L305 V306 R307 L308 I309 L310 V311 E316 G317 L318 L319 F320 E321 G322 R323 I324 T325 L328 L329 T330 R331 G332 K333 S337 D338 V339 I342 E343 K344 N345 K346 E347 G348 L349 K353 E354 I355 L356 T357 R358
V361 E362 P363 S364 D365 D366 D367 S370 V371 Q372 H373 V374 C375 T376 S379 F380 N384 A388 N395 N400 P404 R405 L406 R407 T408 T409 V410 G411 V412 K418 T419 H420 P421 Q422 Y423 S424 R425 R426 F427 H428 L431 R432 P436 D437 S438 R441 F442 L443 L444
S447 K451 V456 E465 Q466 H467 R468 F477 H478 L479 T480 K481 D482 M483 E486 R490 M491 R492 M495 E496 L497 R500 K501 Q502 T503 A507 K510 M511 L512 P513 S514 F515 V516 R517 R518 T519 P520 D521 N525 L529 A530 L531 F538 L541 L542
V543 S547 G548 K549 K550 R551 N555 H556 N557 I562 P563 I564 E565 I566 M567 T570 G571 E572 E573 L574 F575 I578 V579 I582 S583 L586 D587 Y588 I591 K592 R595 M596 P597 L598 T601 F602 S603 F604 P605 D612 A613 G614 I615 T626 H631 D632 V633
V634 A640 I641 K642 R643 R644 E645 E646 F647 D648 L649 D650 V651 V652 V655 M663 T664 C665 E669 P670 V674 N683 E688 E689 N692 V693 E694 M695 Q702 M703 C704 I705 N706 M707 E708 W709 G713 C717 L718 D719 D720 I721 Y725 V729 R755 N756
I757 L758 I759 D760 K763 K764 G765 F766 L767 F768 R769 I772 S773 E774 T775 I781 F782 E783 F786 L795 A796 L797 L798 Q799 Q805 Q806 L807 G808 L809 N810 S811 T912 D815 S816 I817 L818 V822 R828 Q832 A836 D843 K844 I845 R846 E847 N848 R849
R853 L854 N855 V856 T857 V858 G859 V860 D861 G862 H870 R873 Q877 T878 L882 K885 V888 S889 F890 L891 K899 G903 R912 T913 E914 ALA SER SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.00Å 122.00Å 123.00Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 39.27 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.4 (8.00-2.80) 96.0 (39.27-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.200 , 0.270 0.277 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 69.7	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.007 for -h,-l,-k 0.019 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 58588 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14322	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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, BGC, G6P

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	0.38	0/7138	0.60	0/9606
1	B	0.39	0/7138	0.61	2/9606 (0.0%)
All	All	0.39	0/14276	0.61	2/19212 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	GLN	N-CA-C	-6.91	92.33	111.00
1	B	516	VAL	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7032	0	7090	282	0
1	B	7032	0	7090	259	0
2	A	24	0	24	3	0
2	B	24	0	24	2	0
3	A	32	0	22	6	0
3	B	32	0	22	5	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	56	0	0	2	0
5	B	86	0	0	2	0
All	All	14322	0	14272	531	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 19.

All (531) 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:691:LYS:HD2	1:A:691:LYS:H	1.01	1.13
1:A:307:ARG:HH21	1:A:331:ARG:HA	1.22	1.00
1:A:550:LYS:HE3	1:A:552:THR:HG21	1.47	0.97
1:B:307:ARG:HH21	1:B:331:ARG:HA	1.31	0.95
1:A:689:GLU:HB3	1:A:691:LYS:HD3	1.47	0.95
1:A:691:LYS:HD2	1:A:691:LYS:N	1.85	0.91
1:B:420:HIS:HD2	1:B:423:TYR:H	1.15	0.89
1:A:691:LYS:CD	1:A:691:LYS:H	1.87	0.88
1:A:420:HIS:HD2	1:A:423:TYR:H	1.17	0.88
1:B:115:PRO:HD2	1:B:118:ILE:HD13	1.54	0.87
1:A:115:PRO:HD2	1:A:118:ILE:HD13	1.55	0.87
1:A:541:LEU:HD23	1:A:557:ASN:HB3	1.56	0.87
1:A:132:GLU:HG3	1:A:196:ARG:HH12	1.39	0.86
1:A:465:GLU:HA	1:A:465:GLU:OE1	1.76	0.84
1:B:465:GLU:OE1	1:B:465:GLU:HA	1.77	0.84
1:B:541:LEU:HD23	1:B:557:ASN:HB3	1.61	0.83
1:B:132:GLU:HG3	1:B:196:ARG:HH12	1.41	0.83
1:A:307:ARG:NH2	1:A:331:ARG:HA	1.94	0.81
1:A:26:LEU:HD11	1:A:374:VAL:HG13	1.63	0.80
1:A:321:GLU:HB3	1:A:323:ARG:HE	1.48	0.79
1:A:34:GLU:HA	1:A:37:ILE:HD12	1.65	0.78
1:A:421:PRO:HB2	1:A:422:GLN:HE21	1.47	0.78
1:A:323:ARG:NH1	1:A:362:GLU:HB2	2.00	0.77
1:A:58:THR:HB	1:B:799:GLN:NE2	2.00	0.77
1:A:18:GLN:O	1:A:21:LYS:HB3	1.85	0.77
1:B:421:PRO:HB2	1:B:422:GLN:HE21	1.49	0.76
1:B:307:ARG:NH2	1:B:331:ARG:HA	2.01	0.75
1:A:17:ASP:O	1:A:21:LYS:N	2.20	0.75
1:A:420:HIS:CD2	1:A:423:TYR:H	2.04	0.75
1:B:34:GLU:HA	1:B:37:ILE:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:LEU:HD22	1:B:799:GLN:HG2	1.69	0.74
1:B:428:HIS:O	1:B:432:ARG:HG2	1.87	0.74
1:B:321:GLU:HB3	1:B:323:ARG:HE	1.53	0.74
1:B:323:ARG:NH1	1:B:362:GLU:HB2	2.02	0.74
1:A:769:ARG:NH2	1:A:812:THR:HG23	2.02	0.74
1:B:18:GLN:HE21	1:B:18:GLN:HA	1.52	0.73
1:A:549:LYS:HG3	1:A:550:LYS:H	1.54	0.73
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.02	0.72
1:A:550:LYS:CE	1:A:552:THR:HG21	2.18	0.72
1:B:843:ASP:O	1:B:847:GLU:HG3	1.89	0.72
1:A:320:PHE:HB3	1:A:361:VAL:CG1	2.19	0.72
1:B:769:ARG:NH2	1:B:815:ASP:OD2	2.22	0.72
1:A:843:ASP:O	1:A:847:GLU:HG3	1.88	0.72
1:B:18:GLN:O	1:B:21:LYS:HB2	1.89	0.72
1:A:769:ARG:NH2	1:A:815:ASP:OD2	2.24	0.71
1:A:39:ILE:HD11	1:A:273:ILE:HD13	1.71	0.71
1:A:428:HIS:O	1:A:432:ARG:HG2	1.90	0.71
1:B:769:ARG:NH2	1:B:812:THR:HG23	2.05	0.71
1:A:58:THR:HB	1:B:799:GLN:HE22	1.54	0.71
1:A:797:LEU:HD21	1:A:817:ILE:HD11	1.71	0.71
1:A:132:GLU:HG3	1:A:196:ARG:NH1	2.06	0.71
1:B:431:LEU:CD2	1:B:442:PHE:HZ	2.04	0.71
1:A:324:ILE:HG23	1:A:328:LEU:HD23	1.72	0.71
1:B:420:HIS:CD2	1:B:423:TYR:H	2.04	0.70
1:A:795:LEU:HD22	1:A:799:GLN:HG2	1.71	0.70
1:B:486:GLU:O	1:B:490:ARG:HG3	1.90	0.70
1:B:39:ILE:HD11	1:B:273:ILE:HD13	1.73	0.70
1:A:674:VAL:HB	1:A:858:VAL:HG22	1.72	0.70
1:B:98:ASN:HD22	1:B:98:ASN:H	1.38	0.70
1:B:421:PRO:HB2	1:B:422:GLN:NE2	2.07	0.70
1:B:357:THR:OG1	1:B:363:PRO:HG2	1.92	0.69
1:B:497:LEU:O	1:B:503:THR:HG23	1.92	0.69
1:B:320:PHE:HB3	1:B:361:VAL:CG1	2.23	0.69
1:A:422:GLN:O	1:A:426:ARG:HG3	1.93	0.69
1:A:357:THR:OG1	1:A:363:PRO:HG2	1.93	0.69
1:A:421:PRO:HB2	1:A:422:GLN:NE2	2.06	0.69
1:A:486:GLU:O	1:A:490:ARG:HG3	1.94	0.68
1:A:431:LEU:HD23	1:A:442:PHE:HZ	1.57	0.68
1:B:674:VAL:HB	1:B:858:VAL:HG22	1.75	0.68
1:B:132:GLU:HG3	1:B:196:ARG:NH1	2.09	0.68
1:A:356:LEU:HD21	1:A:371:VAL:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ARG:HH21	1:A:812:THR:HG23	1.58	0.67
1:B:356:LEU:HD21	1:B:371:VAL:HG21	1.77	0.67
1:B:115:PRO:C	1:B:117:ASN:H	1.98	0.67
1:A:497:LEU:O	1:A:503:THR:HG23	1.93	0.66
1:A:418:LYS:HG3	1:A:444:LEU:HD11	1.75	0.66
1:B:324:ILE:HG23	1:B:328:LEU:HD23	1.78	0.66
1:B:422:GLN:O	1:B:426:ARG:HG3	1.96	0.66
1:A:320:PHE:HB3	1:A:361:VAL:HG13	1.78	0.66
1:B:514:SER:OG	1:B:704:CYS:HB3	1.96	0.65
1:A:514:SER:OG	1:A:704:CYS:HB3	1.95	0.65
1:B:320:PHE:CD1	1:B:361:VAL:HG11	2.32	0.65
1:B:769:ARG:HH21	1:B:812:THR:HG23	1.61	0.65
1:A:98:ASN:OD1	1:A:101:LYS:HB2	1.97	0.65
1:A:466:GLN:HG2	1:A:766:PHE:CE1	2.32	0.64
1:B:418:LYS:HG3	1:B:444:LEU:HD11	1.79	0.64
1:A:115:PRO:C	1:A:117:ASN:H	1.98	0.64
1:A:56:ASN:N	1:A:57:PRO:HD2	2.12	0.64
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.32	0.64
1:B:193:ILE:HD13	1:B:201:ALA:CB	2.28	0.64
1:B:431:LEU:HD23	1:B:442:PHE:HZ	1.61	0.64
1:B:26:LEU:HD21	1:B:309:ILE:HG21	1.79	0.64
1:B:380:PHE:CE2	1:B:426:ARG:HD3	2.33	0.64
1:A:767:LEU:CD2	1:A:818:LEU:HD23	2.28	0.64
1:B:768:PHE:HA	1:B:769:ARG:CZ	2.28	0.64
1:B:320:PHE:HB3	1:B:361:VAL:HG13	1.79	0.63
1:A:26:LEU:CD1	1:A:374:VAL:HG13	2.28	0.63
1:A:380:PHE:CE2	1:A:426:ARG:HD3	2.33	0.63
1:A:147:LYS:CD	1:A:147:LYS:H	2.11	0.63
1:A:795:LEU:CD2	1:A:799:GLN:HG2	2.29	0.63
1:A:799:GLN:NE2	1:B:58:THR:HB	2.13	0.63
1:A:767:LEU:HD21	1:A:818:LEU:HD23	1.80	0.63
1:A:160:GLN:HG2	1:A:165:GLU:O	1.99	0.62
1:B:75:SER:HA	1:B:99:HIS:NE2	2.15	0.62
1:B:147:LYS:CD	1:B:147:LYS:H	2.12	0.62
1:B:797:LEU:HD21	1:B:817:ILE:HD11	1.81	0.62
1:B:795:LEU:CD2	1:B:799:GLN:HG2	2.29	0.62
1:A:354:GLU:O	1:A:358:ARG:HG3	2.00	0.61
1:B:32:SER:O	1:B:35:THR:HB	1.99	0.61
1:B:307:ARG:HG2	1:B:307:ARG:NH1	2.14	0.61
1:A:768:PHE:HA	1:A:769:ARG:CZ	2.30	0.61
1:B:431:LEU:HD23	1:B:442:PHE:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HH21	1:B:395:ASN:HB3	1.63	0.61
1:A:320:PHE:CD1	1:A:361:VAL:HG11	2.35	0.61
1:A:500:ARG:HB2	1:A:503:THR:CG2	2.31	0.61
1:A:40:MET:HG3	1:A:388:ALA:O	2.01	0.60
1:A:95:VAL:HG22	1:A:107:MET:HB3	1.83	0.60
1:A:193:ILE:HD13	1:A:201:ALA:CB	2.31	0.60
1:B:441:ARG:NH2	1:B:443:LEU:HD13	2.15	0.60
1:B:114:THR:HG22	1:B:119:VAL:HG23	1.83	0.60
1:B:466:GLN:HG2	1:B:766:PHE:CE1	2.37	0.60
1:B:321:GLU:HB2	1:B:323:ARG:HH21	1.67	0.59
1:A:209:ASP:HB2	3:A:919:G6P:H1	1.84	0.59
1:B:354:GLU:O	1:B:358:ARG:HG3	2.01	0.59
1:B:56:ASN:N	1:B:57:PRO:HD2	2.16	0.59
1:B:502:GLN:N	1:B:502:GLN:OE1	2.33	0.59
1:B:437:ASP:OD1	1:B:437:ASP:N	2.36	0.59
1:B:18:GLN:NE2	1:B:18:GLN:HA	2.16	0.59
1:A:725:TYR:O	1:A:729:VAL:HG23	2.02	0.59
1:B:361:VAL:O	1:B:363:PRO:HD3	2.03	0.59
1:B:597:PRO:HA	1:B:650:ASP:HB3	1.84	0.59
1:A:665:CYS:HB3	1:A:891:LEU:HD23	1.85	0.59
1:A:114:THR:HG22	1:A:119:VAL:HG23	1.84	0.58
1:B:95:VAL:HG22	1:B:107:MET:HB3	1.85	0.58
1:A:502:GLN:OE1	1:A:502:GLN:N	2.33	0.58
1:A:54:ASP:HB3	1:B:798:LEU:HD22	1.84	0.58
1:B:118:ILE:HG23	1:B:126:LEU:HA	1.85	0.58
1:A:361:VAL:O	1:A:363:PRO:HD3	2.03	0.58
1:B:870:HIS:CD2	1:B:873:ARG:HH21	2.21	0.58
1:B:420:HIS:CD2	1:B:423:TYR:HB2	2.39	0.58
1:B:501:LYS:HA	1:B:695:MET:SD	2.43	0.58
1:A:321:GLU:HB2	1:A:323:ARG:HH21	1.67	0.58
1:B:688:GLU:O	1:B:702:GLN:HB3	2.03	0.58
1:A:320:PHE:HB3	1:A:361:VAL:HG11	1.85	0.58
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.17	0.58
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.69	0.58
1:A:32:SER:O	1:A:35:THR:HB	2.04	0.57
1:B:98:ASN:HD22	1:B:98:ASN:N	1.98	0.57
1:A:23:ASP:OD1	1:A:373:HIS:NE2	2.30	0.57
1:A:783:GLU:HB2	1:A:786:PHE:CD2	2.39	0.57
1:A:307:ARG:CG	1:A:307:ARG:HH11	2.16	0.57
1:B:307:ARG:CG	1:B:307:ARG:HH11	2.17	0.57
1:B:500:ARG:HB2	1:B:503:THR:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:LEU:HD12	1:A:855:ASN:N	2.19	0.57
1:B:767:LEU:CD2	1:B:818:LEU:HD23	2.34	0.57
1:A:325:THR:HG23	1:A:361:VAL:HG23	1.85	0.57
1:B:507:ALA:O	1:B:510:LYS:HD3	2.04	0.56
1:A:797:LEU:HD21	1:A:817:ILE:CD1	2.34	0.56
1:A:380:PHE:CD2	1:A:426:ARG:HD3	2.41	0.56
1:B:854:LEU:HD12	1:B:855:ASN:N	2.20	0.56
1:B:330:THR:HB	1:B:333:LYS:HG3	1.86	0.56
1:A:330:THR:HB	1:A:333:LYS:HG3	1.87	0.56
1:A:328:LEU:HG	1:A:328:LEU:O	2.03	0.56
1:A:118:ILE:HG23	1:A:126:LEU:HA	1.87	0.56
1:B:196:ARG:C	1:B:198:ASP:H	2.08	0.56
1:B:513:PRO:HA	1:B:705:ILE:HD13	1.87	0.56
1:A:689:GLU:HB3	1:A:691:LYS:CD	2.30	0.56
1:A:420:HIS:CD2	1:A:423:TYR:HB2	2.41	0.56
1:A:465:GLU:OE1	1:A:468:ARG:NE	2.38	0.56
1:A:570:THR:OG1	1:A:573:GLU:HG3	2.06	0.56
1:A:331:ARG:HD2	1:B:588:TYR:CZ	2.41	0.55
1:A:646:GLU:HB3	1:A:647:PHE:CD1	2.41	0.55
1:B:862:GLY:HA2	3:B:921:G6P:H61	1.88	0.55
1:A:513:PRO:HA	1:A:705:ILE:HD13	1.88	0.55
1:A:202:ASN:O	1:A:204:VAL:HG23	2.06	0.55
1:A:173:LYS:HE2	2:A:918:BGC:O5	2.06	0.55
1:A:147:LYS:H	1:A:147:LYS:HD3	1.72	0.55
1:A:437:ASP:N	1:A:437:ASP:OD1	2.40	0.55
1:B:718:LEU:C	1:B:720:ASP:H	2.08	0.55
1:B:725:TYR:O	1:B:729:VAL:HG23	2.07	0.55
1:B:646:GLU:HB3	1:B:647:PHE:CD1	2.42	0.54
1:A:26:LEU:HD21	1:A:309:ILE:HG21	1.90	0.54
1:A:500:ARG:HB2	1:A:503:THR:HG22	1.89	0.54
1:B:693:VAL:HG12	1:B:693:VAL:O	2.07	0.54
1:B:325:THR:HG23	1:B:361:VAL:HG23	1.88	0.54
1:B:18:GLN:HA	1:B:21:LYS:HG3	1.89	0.54
1:A:441:ARG:NH2	1:A:443:LEU:HD13	2.23	0.54
1:A:597:PRO:HA	1:A:650:ASP:HB3	1.90	0.54
1:A:26:LEU:HD12	1:A:377:ILE:HD12	1.90	0.54
1:B:598:LEU:HD23	1:B:598:LEU:C	2.28	0.54
1:B:328:LEU:HG	1:B:328:LEU:O	2.08	0.54
1:A:196:ARG:C	1:A:198:ASP:H	2.12	0.54
1:A:277:PHE:CE1	1:A:309:ILE:HA	2.43	0.54
1:A:226:VAL:HB	1:A:410:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLY:HA3	3:B:919:G6P:O2P	2.07	0.53
1:B:767:LEU:HD21	1:B:818:LEU:HD23	1.90	0.53
1:B:604:PHE:HB3	1:B:605:PRO:HD2	1.90	0.53
1:B:380:PHE:CD2	1:B:426:ARG:HD3	2.44	0.53
1:A:700:GLN:OE1	1:A:700:GLN:N	2.36	0.53
1:A:86:GLY:HA3	1:A:155:SER:OG	2.09	0.53
1:B:500:ARG:HB2	1:B:503:THR:HG22	1.90	0.53
1:B:441:ARG:HH21	1:B:443:LEU:HD13	1.73	0.53
1:A:274:ARG:HH11	1:A:274:ARG:HG2	1.74	0.53
1:A:588:TYR:CZ	1:B:331:ARG:HD2	2.45	0.52
1:B:209:ASP:HB2	3:B:919:G6P:H1	1.91	0.52
1:B:86:GLY:HA3	1:B:155:SER:OG	2.08	0.52
1:A:688:GLU:O	1:A:702:GLN:HB3	2.09	0.52
1:B:320:PHE:HB3	1:B:361:VAL:HG11	1.90	0.52
1:A:101:LYS:O	1:A:102:ASN:CB	2.56	0.52
1:B:718:LEU:C	1:B:720:ASP:N	2.63	0.52
1:B:783:GLU:HB2	1:B:786:PHE:CD2	2.44	0.52
1:B:832:GLN:NE2	5:B:1125:HOH:O	2.43	0.52
1:B:160:GLN:HG2	1:B:165:GLU:O	2.10	0.52
1:A:321:GLU:CB	1:A:323:ARG:HE	2.21	0.52
1:A:376:THR:O	1:A:380:PHE:HB2	2.10	0.52
1:B:26:LEU:HD11	1:B:374:VAL:HG13	1.92	0.52
1:A:755:ARG:HG2	1:A:755:ARG:HH11	1.75	0.52
1:A:501:LYS:HA	1:A:695:MET:SD	2.50	0.52
1:B:88:SER:HB3	3:B:919:G6P:O1P	2.10	0.52
1:B:689:GLU:HB2	1:B:692:ASN:HD22	1.75	0.52
1:A:691:LYS:HB3	1:A:699:ASP:HB2	1.91	0.52
1:A:380:PHE:HE1	1:A:384:ASN:HD21	1.56	0.52
1:B:644:ARG:HG3	1:B:644:ARG:HH11	1.75	0.52
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.73	0.51
1:A:507:ALA:O	1:A:510:LYS:HD3	2.10	0.51
1:B:307:ARG:O	1:B:311:VAL:HG23	2.09	0.51
1:A:19:VAL:HG12	1:A:20:LYS:N	2.26	0.51
1:B:797:LEU:HD21	1:B:817:ILE:CD1	2.40	0.51
1:B:259:THR:O	1:B:260:GLU:HB2	2.09	0.51
1:B:543:VAL:HG22	1:B:555:MET:HB3	1.91	0.51
1:A:768:PHE:HA	1:A:769:ARG:NH1	2.26	0.51
1:B:83:LEU:HD23	1:B:92:ILE:HG23	1.93	0.51
1:A:353:LYS:HA	1:A:368:CYS:SG	2.51	0.51
1:B:465:GLU:OE1	1:B:468:ARG:NE	2.42	0.51
1:A:20:LYS:O	1:A:24:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLN:O	1:B:105:VAL:N	2.44	0.51
1:B:93:LEU:N	1:B:93:LEU:HD12	2.26	0.51
1:B:274:ARG:HG2	1:B:274:ARG:HH11	1.75	0.50
1:A:878:THR:O	1:A:882:LEU:HG	2.11	0.50
1:B:409:THR:HG23	1:B:441:ARG:HG2	1.93	0.50
1:A:477:PHE:CZ	1:A:757:ILE:HD11	2.46	0.50
1:A:520:PRO:HD3	1:A:663:MET:CE	2.41	0.50
1:B:614:GLY:O	1:B:632:ASP:HA	2.11	0.50
1:A:490:ARG:NH1	1:A:717:CYS:O	2.43	0.50
1:A:115:PRO:C	1:A:117:ASN:N	2.64	0.50
1:A:320:PHE:CG	1:A:361:VAL:HG11	2.47	0.50
1:A:307:ARG:CG	1:A:307:ARG:NH1	2.75	0.50
1:B:209:ASP:CB	3:B:919:G6P:H1	2.42	0.50
1:A:441:ARG:HH21	1:A:443:LEU:HD13	1.76	0.50
1:A:652:VAL:HB	1:A:905:THR:HG23	1.93	0.50
1:A:575:PHE:O	1:A:579:VAL:HG23	2.12	0.50
1:A:17:ASP:HA	1:A:20:LYS:HB2	1.92	0.50
1:B:575:PHE:O	1:B:579:VAL:HG23	2.11	0.50
1:A:518:ARG:NH1	1:A:521:ASP:N	2.59	0.50
1:B:193:ILE:HD13	1:B:201:ALA:HB3	1.93	0.49
1:A:259:THR:O	1:A:260:GLU:HB2	2.12	0.49
1:A:546:ARG:O	1:A:551:ARG:HA	2.12	0.49
1:A:598:LEU:HD23	1:A:598:LEU:C	2.32	0.49
1:A:604:PHE:HB3	1:A:605:PRO:HD2	1.93	0.49
1:B:878:THR:O	1:B:882:LEU:HG	2.12	0.49
1:B:320:PHE:CG	1:B:361:VAL:HG11	2.46	0.49
1:A:718:LEU:C	1:A:720:ASP:H	2.14	0.49
1:B:775:THR:HG21	1:B:807:LEU:O	2.12	0.49
1:A:93:LEU:N	1:A:93:LEU:HD12	2.27	0.49
1:A:870:HIS:CD2	1:A:873:ARG:HH21	2.30	0.49
1:B:325:THR:HG21	1:B:361:VAL:N	2.28	0.49
1:A:232:THR:O	1:A:300:MET:HB2	2.13	0.49
1:B:375:CYS:O	1:B:379:SER:HB3	2.13	0.49
1:B:196:ARG:C	1:B:198:ASP:N	2.65	0.49
1:B:376:THR:O	1:B:380:PHE:HB2	2.13	0.49
1:B:578:ILE:O	1:B:582:ILE:HG13	2.13	0.49
1:A:119:VAL:HG13	1:A:175:PHE:HA	1.94	0.49
1:B:836:ALA:HA	1:B:882:LEU:HD12	1.95	0.49
1:A:66:THR:HG21	1:A:211:VAL:HG21	1.95	0.49
1:B:40:MET:HG3	1:B:388:ALA:O	2.13	0.49
1:B:147:LYS:H	1:B:147:LYS:CE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ASN:HB2	2:A:920:BGC:H5	1.94	0.49
1:B:425:ARG:HG2	1:B:425:ARG:HH11	1.77	0.49
1:A:479:LEU:HA	1:A:483:MET:SD	2.53	0.48
1:B:634:VAL:HG13	1:B:651:VAL:HG11	1.94	0.48
1:B:232:THR:O	1:B:300:MET:HB2	2.13	0.48
1:B:115:PRO:C	1:B:117:ASN:N	2.65	0.48
1:A:325:THR:HG21	1:A:361:VAL:N	2.28	0.48
1:B:689:GLU:HB2	1:B:692:ASN:ND2	2.29	0.48
1:A:193:ILE:HD13	1:A:201:ALA:HB3	1.95	0.48
1:A:797:LEU:HD11	1:A:817:ILE:HG13	1.95	0.48
1:A:258:ASN:C	1:A:258:ASN:OD1	2.52	0.48
1:B:71:ILE:HA	1:B:215:MET:HE1	1.96	0.48
1:B:147:LYS:HD3	1:B:147:LYS:H	1.76	0.48
1:B:755:ARG:HH11	1:B:755:ARG:HG2	1.78	0.48
1:B:307:ARG:CG	1:B:307:ARG:NH1	2.75	0.48
1:A:66:THR:OG1	1:A:256:CYS:HB3	2.14	0.48
1:A:275:THR:HG23	1:A:278:ASP:OD2	2.14	0.48
1:B:202:ASN:O	1:B:204:VAL:HG23	2.14	0.48
1:A:578:ILE:O	1:A:582:ILE:HG13	2.14	0.47
1:A:307:ARG:O	1:A:311:VAL:HG23	2.14	0.47
1:A:549:LYS:CG	1:A:550:LYS:H	2.24	0.47
1:B:277:PHE:CE1	1:B:309:ILE:HA	2.49	0.47
1:B:570:THR:OG1	1:B:573:GLU:HG3	2.14	0.47
1:A:779:ARG:NH1	5:A:1145:HOH:O	2.47	0.47
1:A:425:ARG:HG2	1:A:425:ARG:HH11	1.79	0.47
1:A:115:PRO:O	1:A:117:ASN:N	2.46	0.47
1:A:83:LEU:HD23	1:A:92:ILE:HG23	1.96	0.47
1:B:860:VAL:HG12	1:B:861:ASP:N	2.29	0.47
1:B:98:ASN:N	1:B:98:ASN:ND2	2.61	0.47
1:B:105:VAL:HG11	1:B:451:LYS:HG3	1.96	0.47
1:B:62:LYS:NZ	5:B:1012:HOH:O	2.47	0.47
1:B:640:ALA:CA	1:B:643:ARG:HH21	2.27	0.47
1:B:119:VAL:HG13	1:B:175:PHE:HA	1.97	0.47
1:A:854:LEU:HD11	1:A:856:VAL:HB	1.97	0.47
1:A:755:ARG:NH1	1:A:755:ARG:HG2	2.28	0.47
1:A:364:SER:C	1:A:366:ASP:H	2.17	0.47
1:A:412:VAL:HG12	1:A:413:ASP:N	2.30	0.47
1:B:115:PRO:O	1:B:117:ASN:N	2.48	0.47
1:A:718:LEU:C	1:A:720:ASP:N	2.68	0.47
1:A:760:ASP:O	1:A:764:LYS:HG2	2.14	0.47
1:A:557:ASN:C	1:A:557:ASN:HD22	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:PHE:HE2	1:A:608:GLN:C	2.18	0.47
1:B:97:VAL:HA	1:B:104:ASN:O	2.15	0.47
1:A:120:HIS:NE2	1:A:174:ARG:O	2.46	0.47
1:A:167:ILE:HA	1:A:183:ALA:O	2.15	0.47
1:B:320:PHE:HE1	1:B:356:LEU:HD22	1.80	0.47
1:A:18:GLN:OE1	1:A:18:GLN:HA	2.15	0.47
1:B:121:GLY:O	1:B:177:ALA:HA	2.15	0.47
1:B:380:PHE:HE1	1:B:384:ASN:HD21	1.63	0.47
1:B:514:SER:O	1:B:515:PHE:HB2	2.15	0.47
1:B:479:LEU:HA	1:B:483:MET:SD	2.55	0.47
1:B:492:ARG:NE	1:B:844:LYS:HD2	2.29	0.47
1:A:763:LYS:HG2	1:A:772:ILE:HD11	1.95	0.46
1:B:703:MET:HG3	1:B:704:CYS:N	2.31	0.46
1:B:665:CYS:HB3	1:B:891:LEU:HD23	1.97	0.46
1:B:103:GLN:O	1:B:104:ASN:C	2.54	0.46
1:B:221:ASP:OD1	1:B:223:HIS:HB2	2.15	0.46
1:A:775:THR:HG21	1:A:807:LEU:O	2.15	0.46
1:B:167:ILE:HA	1:B:183:ALA:O	2.15	0.46
1:B:477:PHE:CZ	1:B:757:ILE:HD11	2.50	0.46
1:A:644:ARG:HG3	1:A:644:ARG:HH11	1.80	0.46
1:A:55:PHE:C	1:A:57:PRO:HD2	2.35	0.46
1:B:196:ARG:O	1:B:198:ASP:N	2.49	0.46
1:A:813:CYS:O	1:A:817:ILE:HD12	2.15	0.46
1:B:531:LEU:HD21	1:B:582:ILE:HD11	1.98	0.46
1:A:657:ASP:HB2	3:A:921:G6P:H1	1.98	0.46
1:A:514:SER:O	1:A:515:PHE:HB2	2.16	0.46
1:A:147:LYS:CE	1:A:147:LYS:H	2.28	0.46
1:A:20:LYS:O	1:A:24:LYS:HE3	2.16	0.46
1:B:364:SER:C	1:B:366:ASP:H	2.19	0.46
1:B:570:THR:HA	1:B:626:THR:OG1	2.15	0.46
1:A:614:GLY:O	1:A:632:ASP:HA	2.16	0.46
1:A:320:PHE:HE1	1:A:356:LEU:HD22	1.81	0.46
1:B:193:ILE:HD13	1:B:201:ALA:HB2	1.98	0.46
1:B:55:PHE:C	1:B:57:PRO:HD2	2.36	0.46
1:B:854:LEU:HD11	1:B:856:VAL:HB	1.97	0.46
1:B:26:LEU:CD1	1:B:374:VAL:HG13	2.46	0.45
1:B:161:SER:OG	1:B:165:GLU:OE1	2.22	0.45
1:A:543:VAL:HG22	1:A:555:MET:HB3	1.98	0.45
1:A:196:ARG:C	1:A:198:ASP:N	2.68	0.45
1:A:370:SER:O	1:A:374:VAL:HG23	2.16	0.45
1:A:564:ILE:HA	1:A:567:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASN:N	1:A:57:PRO:CD	2.79	0.45
1:B:612:ASP:O	1:B:634:VAL:HG21	2.16	0.45
1:B:173:LYS:HE2	2:B:918:BGC:O5	2.16	0.45
1:B:491:MET:O	1:B:495:MET:HG3	2.16	0.45
1:A:323:ARG:HH12	1:A:362:GLU:HB2	1.78	0.45
1:A:371:VAL:HG12	1:A:372:GLN:N	2.31	0.45
1:A:563:PRO:HG2	1:A:566:ILE:HG13	1.98	0.45
1:B:853:ARG:HA	1:B:885:LYS:O	2.17	0.45
1:B:768:PHE:HA	1:B:769:ARG:NH1	2.32	0.45
1:A:570:THR:HA	1:A:626:THR:OG1	2.16	0.45
1:A:510:LYS:O	1:A:511:MET:C	2.54	0.45
1:A:93:LEU:HD23	1:A:109:SER:HB3	1.98	0.45
1:B:755:ARG:NH1	1:B:755:ARG:HG2	2.32	0.45
1:B:252:GLU:OE1	1:B:812:THR:HB	2.17	0.45
1:B:490:ARG:NH1	1:B:717:CYS:O	2.49	0.45
1:B:26:LEU:HD21	1:B:309:ILE:CG2	2.46	0.45
1:A:846:ARG:HB2	1:A:854:LEU:HD23	1.98	0.45
1:B:120:HIS:NE2	1:B:174:ARG:O	2.49	0.45
1:A:247:LEU:HG	5:A:1034:HOH:O	2.17	0.45
1:A:71:ILE:HA	1:A:215:MET:HE1	1.98	0.45
1:B:242:LEU:HD23	1:B:252:GLU:O	2.17	0.45
1:A:233:GLY:HA2	1:A:298:SER:CB	2.47	0.45
1:A:492:ARG:NE	1:A:844:LYS:HD2	2.32	0.45
1:B:538:PHE:CD2	1:B:562:ILE:HD11	2.51	0.45
1:A:612:ASP:O	1:A:634:VAL:HG21	2.17	0.44
1:A:703:MET:HG3	1:A:704:CYS:N	2.32	0.44
1:B:758:LEU:HD22	1:B:767:LEU:HD11	1.99	0.44
1:A:828:ARG:O	1:A:832:GLN:HG3	2.17	0.44
1:B:763:LYS:HG2	1:B:772:ILE:HD11	1.99	0.44
1:B:275:THR:HG23	1:B:278:ASP:OD2	2.17	0.44
1:B:262:GLY:O	1:B:291:GLN:HA	2.17	0.44
1:B:17:ASP:O	1:B:18:GLN:C	2.55	0.44
1:B:856:VAL:O	1:B:888:VAL:HA	2.17	0.44
1:B:72:PRO:HD3	1:B:215:MET:CE	2.47	0.44
1:A:244:HIS:HE1	1:A:400:ASN:ND2	2.15	0.44
1:B:797:LEU:HD11	1:B:817:ILE:HG13	2.00	0.44
1:B:564:ILE:HA	1:B:567:MET:HB2	1.99	0.44
1:B:371:VAL:HG12	1:B:372:GLN:N	2.32	0.44
1:A:518:ARG:HH12	1:A:521:ASP:N	2.16	0.44
1:A:527:ASP:OD1	1:A:546:ARG:NH1	2.44	0.44
1:A:364:SER:O	1:A:367:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:PRO:C	1:A:438:SER:H	2.21	0.44
1:A:244:HIS:CE1	1:A:400:ASN:HD21	2.35	0.44
1:A:364:SER:C	1:A:366:ASP:N	2.71	0.44
1:A:787:LEU:O	1:A:791:GLU:HG3	2.18	0.44
1:B:228:LEU:HD23	1:B:412:VAL:HG13	2.00	0.44
1:A:302:LEU:HD22	1:A:378:VAL:HG12	2.00	0.44
1:A:552:THR:HB	1:B:117:ASN:OD1	2.17	0.43
1:B:105:VAL:HG11	1:B:451:LYS:CG	2.48	0.43
1:A:500:ARG:NH2	1:A:503:THR:HG21	2.32	0.43
1:B:543:VAL:HG22	1:B:555:MET:CB	2.48	0.43
1:B:718:LEU:HD22	1:B:721:ILE:HD11	2.00	0.43
1:A:518:ARG:HH12	1:A:521:ASP:H	1.66	0.43
1:B:211:VAL:HG22	1:B:256:CYS:SG	2.58	0.43
1:A:853:ARG:HA	1:A:885:LYS:O	2.17	0.43
1:A:311:VAL:HG22	1:A:328:LEU:HG	2.00	0.43
1:B:702:GLN:HE22	1:B:849:ARG:HH21	1.67	0.43
1:A:862:GLY:HA2	3:A:921:G6P:H61	2.00	0.43
1:A:798:LEU:HD21	1:B:55:PHE:CE1	2.52	0.43
1:B:718:LEU:O	1:B:720:ASP:N	2.52	0.43
1:A:836:ALA:HA	1:A:882:LEU:HD12	1.99	0.43
1:B:518:ARG:NH1	1:B:521:ASP:N	2.66	0.43
1:A:342:ILE:O	1:A:372:GLN:HG3	2.18	0.43
1:A:518:ARG:HG3	1:A:519:THR:O	2.19	0.43
1:A:211:VAL:HG22	1:A:256:CYS:SG	2.59	0.43
1:A:29:MET:CE	1:A:275:THR:HG21	2.49	0.43
1:B:66:THR:OG1	1:B:256:CYS:HB3	2.19	0.43
1:B:601:THR:HA	1:B:655:VAL:O	2.19	0.43
1:B:669:GLU:HA	1:B:670:PRO:HD2	1.84	0.43
1:B:551:ARG:NH1	1:B:551:ARG:HG3	2.33	0.43
1:A:432:ARG:HG2	1:A:432:ARG:H	1.52	0.43
1:B:44:ARG:NH2	1:B:395:ASN:HB3	2.32	0.43
1:A:573:GLU:HG3	1:A:573:GLU:H	1.57	0.43
1:A:407:ARG:HG2	1:A:439:ASP:HB2	2.00	0.43
1:A:316:GLU:HB2	1:A:318:LEU:HD12	1.99	0.43
1:B:321:GLU:CB	1:B:323:ARG:HE	2.26	0.43
1:A:320:PHE:CE1	1:A:356:LEU:HD22	2.54	0.43
1:B:146:LYS:HA	1:B:147:LYS:NZ	2.34	0.43
1:A:646:GLU:HB3	1:A:647:PHE:HD1	1.83	0.43
1:A:94:ARG:NH1	1:A:143:ILE:HG21	2.33	0.43
1:B:56:ASN:N	1:B:57:PRO:CD	2.81	0.43
1:B:845:ILE:O	1:B:849:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ARG:HH11	1:B:551:ARG:HG3	1.83	0.43
1:A:375:CYS:O	1:A:379:SER:HB3	2.18	0.43
1:A:209:ASP:CB	3:A:919:G6P:H1	2.49	0.42
1:B:23:ASP:OD1	1:B:23:ASP:N	2.52	0.42
1:B:370:SER:O	1:B:374:VAL:HG23	2.18	0.42
1:A:255:MET:HG3	1:A:256:CYS:N	2.34	0.42
1:A:601:THR:HA	1:A:655:VAL:O	2.19	0.42
1:A:602:PHE:CE2	1:A:633:VAL:HG11	2.54	0.42
1:B:860:VAL:HG12	1:B:861:ASP:H	1.85	0.42
1:B:529:LEU:HD11	1:B:586:LEU:HD21	2.01	0.42
1:B:436:PRO:C	1:B:438:SER:H	2.23	0.42
1:B:805:GLN:HA	1:B:809:LEU:O	2.19	0.42
1:B:93:LEU:HD23	1:B:109:SER:HB3	2.01	0.42
1:A:709:TRP:CD1	1:A:709:TRP:C	2.92	0.42
1:A:538:PHE:CD2	1:A:562:ILE:HD11	2.54	0.42
1:A:671:THR:OG1	1:A:857:THR:HG23	2.20	0.42
1:A:231:GLY:HA3	3:A:919:G6P:O1P	2.20	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.82	0.42
1:B:563:PRO:HG2	1:B:566:ILE:HG13	2.01	0.42
1:B:118:ILE:CG2	1:B:126:LEU:HA	2.48	0.42
1:A:217:CYS:HB3	1:A:443:LEU:HD23	2.00	0.42
1:A:54:ASP:HB3	1:B:798:LEU:CD2	2.50	0.42
1:B:364:SER:C	1:B:366:ASP:N	2.73	0.42
1:B:244:HIS:HE1	1:B:400:ASN:ND2	2.17	0.42
1:A:297:VAL:HG13	1:A:382:SER:OG	2.20	0.42
1:A:849:ARG:HB3	1:A:851:LEU:HG	2.01	0.42
1:B:136:ASP:C	1:B:136:ASP:OD1	2.58	0.42
1:B:342:ILE:O	1:B:372:GLN:HG3	2.19	0.42
1:B:828:ARG:O	1:B:832:GLN:HG3	2.20	0.42
1:B:233:GLY:HA2	1:B:298:SER:CB	2.50	0.42
1:A:693:VAL:O	1:A:693:VAL:HG12	2.20	0.42
1:B:258:ASN:OD1	1:B:258:ASN:C	2.59	0.41
1:B:226:VAL:HB	1:B:410:VAL:HG22	2.01	0.41
1:B:518:ARG:CG	1:B:518:ARG:HH11	2.33	0.41
1:A:586:LEU:HA	1:A:586:LEU:HD23	1.87	0.41
1:B:713:GLY:HA2	1:B:717:CYS:SG	2.60	0.41
1:B:320:PHE:CE1	1:B:356:LEU:HD22	2.55	0.41
1:A:400:ASN:HD22	1:A:400:ASN:HA	1.66	0.41
1:A:173:LYS:HE2	2:A:918:BGC:C1	2.50	0.41
1:A:856:VAL:O	1:A:888:VAL:HA	2.21	0.41
1:A:650:ASP:O	1:A:652:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:HD21	1:A:582:ILE:HD11	2.02	0.41
1:B:432:ARG:H	1:B:432:ARG:HG2	1.51	0.41
1:A:428:HIS:O	1:A:431:LEU:HB3	2.21	0.41
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.56	0.41
1:B:760:ASP:O	1:B:764:LYS:HG2	2.20	0.41
1:A:319:LEU:HD21	1:A:370:SER:HB2	2.01	0.41
1:A:634:VAL:HG13	1:A:651:VAL:HG11	2.02	0.41
1:A:529:LEU:HD11	1:A:586:LEU:HD21	2.03	0.41
1:A:48:LYS:HE3	1:A:48:LYS:HB2	1.90	0.41
1:B:316:GLU:HB2	1:B:318:LEU:HD12	2.01	0.41
1:A:146:LYS:HA	1:A:147:LYS:NZ	2.36	0.41
1:A:72:PRO:HD3	1:A:215:MET:CE	2.50	0.41
1:B:100:GLU:CG	1:B:101:LYS:H	2.34	0.41
1:B:48:LYS:HE3	1:B:48:LYS:HB2	1.88	0.41
1:A:320:PHE:CB	1:A:361:VAL:HG11	2.51	0.41
1:A:101:LYS:HD2	1:A:103:GLN:HE22	1.86	0.41
1:A:160:GLN:HG2	1:A:166:ALA:HA	2.02	0.41
1:A:798:LEU:HD21	1:B:55:PHE:CZ	2.56	0.41
1:B:650:ASP:O	1:B:652:VAL:HG23	2.20	0.41
1:B:215:MET:HG3	1:B:456:VAL:CG2	2.51	0.41
1:A:679:GLY:HA3	3:A:921:G6P:O1P	2.21	0.41
1:B:641:ILE:HD11	1:B:649:LEU:HD12	2.03	0.41
1:B:683:ASN:HA	1:B:709:TRP:CD1	2.56	0.41
1:A:749:TYR:O	1:A:750:LEU:C	2.59	0.41
1:A:413:ASP:OD1	1:A:414:GLY:N	2.54	0.41
1:A:302:LEU:HD12	1:A:416:LEU:HD11	2.03	0.41
1:B:154:PHE:CE2	1:B:185:VAL:HG11	2.55	0.41
1:B:274:ARG:NH1	1:B:274:ARG:HG2	2.35	0.40
1:A:232:THR:O	1:A:298:SER:OG	2.34	0.40
1:B:615:ILE:HA	1:B:631:HIS:O	2.21	0.40
1:A:615:ILE:HA	1:A:631:HIS:O	2.22	0.40
1:B:510:LYS:O	1:B:511:MET:C	2.59	0.40
1:A:671:THR:OG1	1:A:857:THR:CG2	2.69	0.40
1:B:707:MET:O	1:B:708:GLU:HB2	2.20	0.40
1:A:262:GLY:O	1:A:291:GLN:HA	2.21	0.40
1:A:598:LEU:HD23	1:A:598:LEU:O	2.21	0.40
1:A:144:LYS:HD3	1:A:199:TYR:HB3	2.03	0.40
1:A:705:ILE:HD13	1:A:705:ILE:HA	1.91	0.40
1:A:518:ARG:CG	1:A:518:ARG:HH11	2.34	0.40
1:A:491:MET:HE3	1:A:709:TRP:CE3	2.57	0.40
1:B:520:PRO:HD3	1:B:663:MET:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:TYR:HB2	1:A:845:ILE:HD11	2.02	0.40
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.87	0.40
1:A:801:ARG:NH1	1:A:813:CYS:SG	2.94	0.40
1:B:818:LEU:O	1:B:822:VAL:HG23	2.21	0.40
1:B:215:MET:HG3	1:B:456:VAL:HG23	2.02	0.40
1:A:29:MET:HE3	1:A:275:THR:HG21	2.03	0.40
1:B:551:ARG:H	1:B:551:ARG:HG2	1.61	0.40
1:B:683:ASN:HB2	2:B:920:BGC:H5	2.03	0.40
1:A:642:LYS:O	1:A:645:GLU:HG2	2.21	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%)	810 (90%)	76 (8%)	11 (1%)	16	47
1	B	897/917 (98%)	811 (90%)	73 (8%)	13 (1%)	14	42
All	All	1794/1834 (98%)	1621 (90%)	149 (8%)	24 (1%)	15	44

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	346	LYS
1	B	100	GLU
1	B	104	ASN
1	B	346	LYS
1	B	549	LYS
1	A	116	GLU
1	A	591	ILE
1	B	116	GLU

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Mol	Chain	Res	Type
1	B	591	ILE
1	A	222	GLN
1	B	222	GLN
1	A	437	ASP
1	B	320	PHE
1	B	372	GLN
1	B	694	GLU
1	A	415	SER
1	B	436	PRO
1	A	436	PRO
1	A	203	ILE
1	A	371	VAL
1	B	651	VAL
1	A	651	VAL
1	B	404	PRO

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	774/788 (98%)	687 (89%)	87 (11%)	7 22
1	B	774/788 (98%)	691 (89%)	83 (11%)	8 24
All	All	1548/1576 (98%)	1378 (89%)	170 (11%)	8 23

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	21	LYS
1	A	32	SER
1	A	44	ARG
1	A	58	THR
1	A	69	ARG
1	A	70	SER
1	A	80	PHE

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Mol	Chain	Res	Type
1	A	93	LEU
1	A	96	GLN
1	A	102	ASN
1	A	103	GLN
1	A	107	MET
1	A	117	ASN
1	A	124	SER
1	A	136	ASP
1	A	141	ARG
1	A	147	LYS
1	A	155	SER
1	A	163	ILE
1	A	200	ASP
1	A	202	ASN
1	A	223	HIS
1	A	242	LEU
1	A	255	MET
1	A	261	TRP
1	A	271	GLU
1	A	275	THR
1	A	281	ILE
1	A	286	LEU
1	A	307	ARG
1	A	320	PHE
1	A	321	GLU
1	A	337	SER
1	A	347	GLU
1	A	353	LYS
1	A	364	SER
1	A	366	ASP
1	A	370	SER
1	A	379	SER
1	A	380	PHE
1	A	384	ASN
1	A	407	ARG
1	A	424	SER
1	A	429	LYS
1	A	432	ARG
1	A	447	SER
1	A	465	GLU
1	A	466	GLN
1	A	481	LYS

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Mol	Chain	Res	Type
1	A	501	LYS
1	A	518	ARG
1	A	519	THR
1	A	525	ASN
1	A	541	LEU
1	A	542	LEU
1	A	549	LYS
1	A	551	ARG
1	A	557	ASN
1	A	565	GLU
1	A	572	GLU
1	A	573	GLU
1	A	583	SER
1	A	592	LYS
1	A	595	ARG
1	A	603	SER
1	A	691	LYS
1	A	709	TRP
1	A	721	ILE
1	A	764	LYS
1	A	769	ARG
1	A	773	SER
1	A	781	ILE
1	A	795	LEU
1	A	798	LEU
1	A	805	GLN
1	A	810	ASN
1	A	811	SER
1	A	843	ASP
1	A	849	ARG
1	A	853	ARG
1	A	854	LEU
1	A	857	THR
1	A	877	GLN
1	A	889	SER
1	A	893	SER
1	A	899	LYS
1	B	21	LYS
1	B	23	ASP
1	B	32	SER
1	B	58	THR
1	B	69	ARG

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Mol	Chain	Res	Type
1	B	70	SER
1	B	80	PHE
1	B	93	LEU
1	B	96	GLN
1	B	98	ASN
1	B	100	GLU
1	B	101	LYS
1	B	107	MET
1	B	117	ASN
1	B	124	SER
1	B	136	ASP
1	B	141	ARG
1	B	147	LYS
1	B	155	SER
1	B	163	ILE
1	B	174	ARG
1	B	200	ASP
1	B	242	LEU
1	B	255	MET
1	B	261	TRP
1	B	271	GLU
1	B	275	THR
1	B	281	ILE
1	B	286	LEU
1	B	307	ARG
1	B	320	PHE
1	B	321	GLU
1	B	337	SER
1	B	347	GLU
1	B	353	LYS
1	B	364	SER
1	B	366	ASP
1	B	370	SER
1	B	379	SER
1	B	380	PHE
1	B	384	ASN
1	B	405	ARG
1	B	407	ARG
1	B	424	SER
1	B	432	ARG
1	B	447	SER
1	B	465	GLU

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Mol	Chain	Res	Type
1	B	466	GLN
1	B	481	LYS
1	B	501	LYS
1	B	518	ARG
1	B	519	THR
1	B	525	ASN
1	B	541	LEU
1	B	542	LEU
1	B	551	ARG
1	B	557	ASN
1	B	565	GLU
1	B	572	GLU
1	B	573	GLU
1	B	583	SER
1	B	592	LYS
1	B	595	ARG
1	B	603	SER
1	B	709	TRP
1	B	721	ILE
1	B	764	LYS
1	B	769	ARG
1	B	773	SER
1	B	781	ILE
1	B	795	LEU
1	B	798	LEU
1	B	805	GLN
1	B	810	ASN
1	B	811	SER
1	B	843	ASP
1	B	849	ARG
1	B	853	ARG
1	B	854	LEU
1	B	857	THR
1	B	877	GLN
1	B	889	SER
1	B	899	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	117	ASN
1	A	159	GLN
1	A	202	ASN
1	A	222	GLN
1	A	384	ASN
1	A	400	ASN
1	A	466	GLN
1	A	525	ASN
1	A	556	HIS
1	A	557	ASN
1	A	692	ASN
1	A	805	GLN
1	A	806	GLN
1	A	848	ASN
1	A	870	HIS
1	B	96	GLN
1	B	98	ASN
1	B	103	GLN
1	B	104	ASN
1	B	159	GLN
1	B	202	ASN
1	B	222	GLN
1	B	384	ASN
1	B	400	ASN
1	B	466	GLN
1	B	525	ASN
1	B	556	HIS
1	B	557	ASN
1	B	692	ASN
1	B	702	GLN
1	B	771	GLN
1	B	805	GLN
1	B	806	GLN
1	B	848	ASN
1	B	870	HIS

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	0.49	0	17,17,17	0.94	1 (5%)
3	G6P	A	919	-	16,16,16	0.75	0	23,24,24	0.89	1 (4%)
2	BGC	A	920	-	12,12,12	0.46	0	17,17,17	0.89	1 (5%)
3	G6P	A	921	-	16,16,16	0.79	0	23,24,24	1.23	4 (17%)
2	BGC	B	918	-	12,12,12	0.36	0	17,17,17	0.75	0
3	G6P	B	919	-	16,16,16	0.84	1 (6%)	23,24,24	1.07	2 (8%)
2	BGC	B	920	-	12,12,12	0.35	0	17,17,17	0.57	0
3	G6P	B	921	-	16,16,16	0.82	0	23,24,24	0.96	1 (4%)

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
3	G6P	A	919	-	1/1/6/6	0/6/26/26	0/1/1/1
2	BGC	A	920	-	-	0/2/22/22	0/1/1/1
3	G6P	A	921	-	1/1/6/6	0/6/26/26	0/1/1/1
2	BGC	B	918	-	-	0/2/22/22	0/1/1/1
3	G6P	B	919	-	1/1/6/6	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	920	-	-	0/2/22/22	0/1/1/1
3	G6P	B	921	-	1/1/6/6	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	919	G6P	P-O1P	-2.19	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	920	BGC	C1-C2-C3	-2.66	106.47	110.43
3	A	921	G6P	C3-C4-C5	-2.17	106.41	110.20
3	B	919	G6P	O2P-P-O6	2.15	112.75	106.56
3	B	921	G6P	O1P-P-O6	2.21	112.94	106.56
3	A	921	G6P	O2P-P-O6	2.29	113.17	106.56
3	A	919	G6P	O2P-P-O6	2.30	113.19	106.56
3	B	919	G6P	O6-P-O3P	2.30	113.00	107.14
3	A	921	G6P	C6-C5-C4	2.33	117.30	112.03
3	A	921	G6P	O1P-P-O6	2.44	113.60	106.56
2	A	918	BGC	O5-C1-C2	2.71	114.11	109.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	919	G6P	C1
3	B	919	G6P	C1
3	B	921	G6P	C1
3	A	921	G6P	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	918	BGC	2	0
3	A	919	G6P	3	0
2	A	920	BGC	1	0
3	A	921	G6P	3	0
2	B	918	BGC	1	0
3	B	919	G6P	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	920	BGC	1	0
3	B	921	G6P	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	899/917 (98%)	0.25	28 (3%)	52	40	7, 41, 92, 100	0
1	B	899/917 (98%)	0.25	36 (4%)	42	30	8, 37, 87, 100	0
All	All	1798/1834 (98%)	0.25	64 (3%)	46	34	7, 39, 89, 100	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	908	GLY	5.2
1	B	103	GLN	4.8
1	A	649	LEU	4.0
1	A	550	LYS	3.7
1	B	374	VAL	3.7
1	B	370	SER	3.6
1	A	374	VAL	3.6
1	A	17	ASP	3.6
1	B	913	THR	3.4
1	B	99	HIS	3.3
1	A	21	LYS	3.3
1	B	16	ASP	3.1
1	A	647	PHE	2.9
1	A	908	GLY	2.8
1	B	109	SER	2.8
1	A	911	LEU	2.8
1	B	305	LEU	2.7
1	A	359	LEU	2.7
1	B	349	LEU	2.7
1	A	315	LYS	2.7
1	B	547	SER	2.6
1	B	298	SER	2.6
1	B	328	LEU	2.6
1	A	350	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	104	ASN	2.5
1	A	583	SER	2.5
1	A	355	ILE	2.5
1	B	342	ILE	2.5
1	A	852	ASP	2.5
1	B	651	VAL	2.5
1	A	642	LYS	2.5
1	B	422	GLN	2.4
1	B	423	TYR	2.4
1	B	649	LEU	2.4
1	A	310	LEU	2.4
1	B	324	ILE	2.4
1	B	105	VAL	2.3
1	A	16	ASP	2.3
1	B	143	ILE	2.3
1	B	17	ASP	2.3
1	B	339	VAL	2.3
1	A	912	ARG	2.2
1	B	333	LYS	2.2
1	B	344	LYS	2.2
1	A	424	SER	2.2
1	A	591	ILE	2.2
1	A	807	LEU	2.2
1	A	353	LYS	2.1
1	B	97	VAL	2.1
1	B	30	ARG	2.1
1	B	912	ARG	2.1
1	A	519	THR	2.1
1	B	591	ILE	2.1
1	A	437	ASP	2.1
1	B	100	GLU	2.1
1	A	635	THR	2.0
1	A	541	LEU	2.0
1	A	651	VAL	2.0
1	B	371	VAL	2.0
1	B	367	ASP	2.0
1	B	518	ARG	2.0
1	B	444	LEU	2.0
1	B	309	ILE	2.0
1	A	575	PHE	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
2	BGC	A	918	12/12	0.83	0.33	2.81	32,50,61,68	0
2	BGC	A	920	12/12	0.88	0.28	2.70	13,20,28,32	0
4	CA	B	923	1/1	0.86	0.32	2.14	91,91,91,91	0
2	BGC	B	918	12/12	0.88	0.29	1.39	6,16,23,26	0
4	CA	A	923	1/1	0.55	0.30	1.27	70,70,70,70	0
3	G6P	B	921	16/16	0.95	0.26	0.92	13,30,45,51	0
3	G6P	A	921	16/16	0.86	0.26	0.49	5,12,23,23	0
3	G6P	B	919	16/16	0.87	0.27	0.47	25,37,47,51	0
2	BGC	B	920	12/12	0.92	0.18	-0.14	10,22,33,37	0
3	G6P	A	919	16/16	0.90	0.20	-0.15	37,57,68,71	0
4	CA	B	922	1/1	0.69	0.11	-1.39	70,70,70,70	0
4	CA	A	922	1/1	0.95	0.08	-2.07	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.