



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:03 AM GMT

PDB ID : 4FPA
Title : Crystal Structure of recombinant human Hexokinase type I mutant D413N
Glucose 6-Phosphate
Authors : Shen, L.; Honzatko, R.B.
Deposited on : 2012-06-21
Resolution : 2.48 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

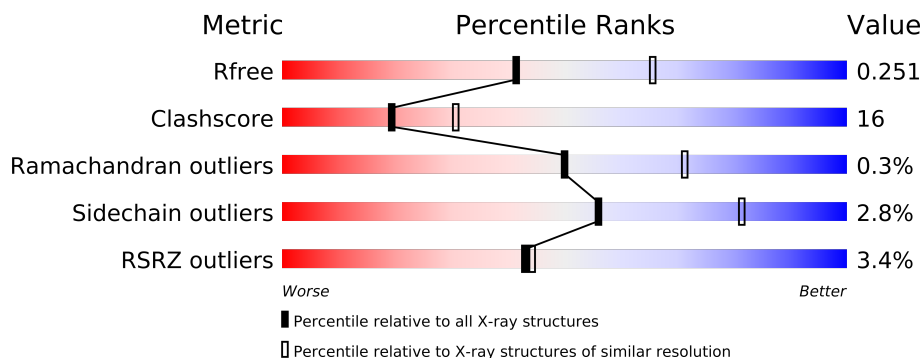
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.48 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3277 (2.50-2.46)
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (2.50-2.46)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	917	
1	B	917	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	BGC	B	1001	-	X
5	CIT	B	1007	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14391 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

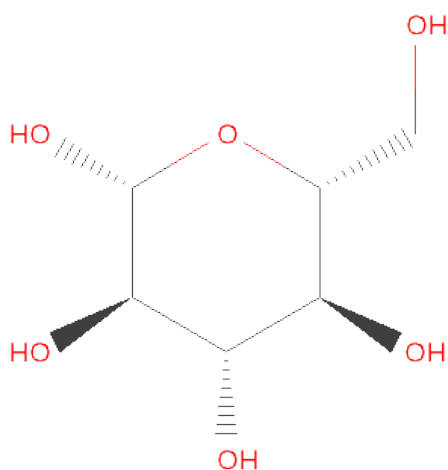
- Molecule 1 is a protein called Hexokinase-1.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	ASN	ASP	ENGINEERED MUTATION	UNP P19367
B	413	ASN	ASP	ENGINEERED MUTATION	UNP P19367

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C₆H₁₂O₆).



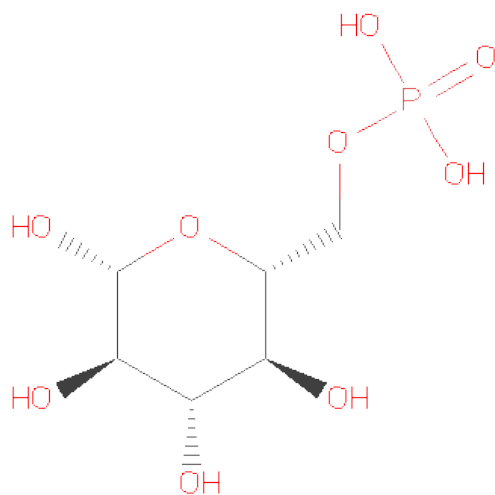
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 (BETA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: BG6) (formula: C₆H₁₃O₉P).

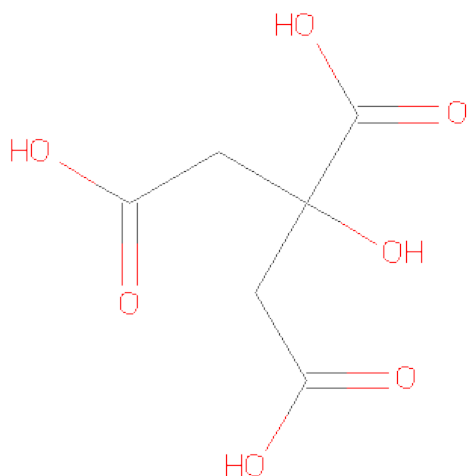


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O	0	0
			77	77		
6	B	108	Total	O	0	0
			108	108		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.61Å 121.14Å 119.89Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	44.15 – 2.48 44.15 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.15-2.48) 98.5 (44.15-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.238 , 0.256 0.237 , 0.251	Depositor DCC
R_{free} test set	4127 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.4	EDS
Estimated twinning fraction	0.007 for -h,-l,-k 0.000 for -h,l,k 0.019 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 82652 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14391	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, BGC, BG6, CIT

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	0.26	0/7138	0.45	0/9606
1	B	0.25	0/7138	0.44	0/9606
All	All	0.26	0/14276	0.44	0/19212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7032	0	7092	224	0
1	B	7032	0	7092	246	0
2	A	24	0	24	2	0
2	B	24	0	24	0	0
3	A	32	0	22	2	0
3	B	32	0	22	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	13	0	5	1	0
5	B	13	0	5	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	77	0	0	4	0
6	B	108	0	0	6	0
All	All	14391	0	14286	465	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (465) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:132:GLU:HG3	1:A:196:ARG:NH2	1.62	1.15
1:B:797:LEU:HD11	1:B:817:ILE:HD11	1.26	1.13
1:B:518:ARG:HH12	1:B:521:ASP:HB3	1.14	1.09
1:B:518:ARG:NH1	1:B:521:ASP:HB3	1.67	1.06
1:B:480:THR:N	1:B:483:MET:HE3	1.70	1.06
1:B:66:THR:HG21	1:B:256:CYS:HB3	1.39	1.04
1:B:18:GLN:OE1	1:B:369:VAL:CG1	2.05	1.04
1:B:426:ARG:HH21	5:B:1007:CIT:H41	1.20	1.04
1:B:518:ARG:HH12	1:B:521:ASP:CB	1.73	1.02
1:B:480:THR:H	1:B:483:MET:CE	1.74	1.01
1:B:480:THR:H	1:B:483:MET:HE3	0.85	1.01
1:A:795:LEU:HD11	1:A:799:GLN:HG2	1.44	0.99
1:B:795:LEU:HD11	1:B:799:GLN:HG2	1.53	0.90
1:A:431:LEU:HD23	1:A:442:PHE:HZ	1.38	0.89
1:B:518:ARG:CZ	1:B:521:ASP:HB3	2.03	0.88
1:A:913:THR:O	1:A:913:THR:HG23	1.73	0.87
1:A:66:THR:HG22	1:A:256:CYS:O	1.76	0.86
1:B:356:LEU:HD11	1:B:371:VAL:HG21	1.55	0.85
1:B:18:GLN:OE1	1:B:369:VAL:HG12	1.76	0.85
1:B:595:ARG:NH1	1:B:650:ASP:HB2	1.93	0.83
1:B:735:ASN:HB2	1:B:738:LYS:HE3	1.59	0.82
1:A:505:ASN:HB2	6:A:1158:HOH:O	1.79	0.82
1:A:132:GLU:HG3	1:A:196:ARG:HH22	1.42	0.82
1:B:518:ARG:NH2	1:B:521:ASP:HB3	1.95	0.82
1:B:534:GLY:HA3	1:B:603:SER:HB2	1.62	0.81
1:A:361:VAL:O	1:A:363:PRO:HD3	1.83	0.79
1:A:323:ARG:NH2	1:A:362:GLU:HB2	1.98	0.79
1:B:687:MET:HE2	1:B:704:CYS:CB	2.12	0.79
1:B:539:ARG:CZ	1:B:559:ILE:HD11	2.13	0.78
1:B:687:MET:CE	1:B:704:CYS:HB2	2.13	0.77
1:B:564:ILE:HG23	1:B:565:GLU:N	2.00	0.77
1:A:767:LEU:HG	1:A:818:LEU:HD23	1.66	0.77
1:B:853:ARG:HB3	1:B:853:ARG:NH1	2.00	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:763:LYS:HG3	1:A:772:ILE:HD11	1.67	0.76
1:B:768:PHE:HA	1:B:769:ARG:HH21	1.49	0.76
1:A:786:PHE:CD2	1:A:807:LEU:HD11	2.20	0.76
1:B:575:PHE:O	1:B:579:VAL:HG23	1.86	0.76
1:A:234:THR:HG22	1:A:294:GLU:HG3	1.66	0.76
1:A:97:VAL:HG22	1:A:105:VAL:HA	1.67	0.75
1:B:18:GLN:NE2	1:B:366:ASP:O	2.18	0.75
1:B:778:THR:O	1:B:781:ILE:HG12	1.87	0.75
1:B:18:GLN:OE1	1:B:369:VAL:CB	2.35	0.74
1:B:66:THR:CG2	1:B:256:CYS:HB3	2.17	0.74
1:B:642:LYS:O	1:B:645:GLU:HG2	1.88	0.74
1:B:18:GLN:OE1	1:B:369:VAL:HB	1.87	0.74
1:A:786:PHE:CZ	1:A:790:ILE:HG13	2.23	0.73
1:B:767:LEU:HG	1:B:818:LEU:HD23	1.70	0.73
1:B:518:ARG:HH22	1:B:521:ASP:HB3	1.52	0.73
1:B:797:LEU:HD11	1:B:817:ILE:CD1	2.13	0.73
1:B:29:MET:HE1	1:B:381:ARG:CZ	2.18	0.73
1:B:35:THR:O	1:B:38:ASP:HB3	1.88	0.73
1:A:160:GLN:HG2	1:A:165:GLU:O	1.89	0.72
1:B:518:ARG:HH22	1:B:521:ASP:CB	2.01	0.72
1:B:431:LEU:HD22	1:B:442:PHE:HZ	1.53	0.72
1:B:687:MET:HE1	1:B:704:CYS:HB2	1.71	0.71
1:A:502:GLN:OE1	1:A:502:GLN:N	2.17	0.71
1:B:853:ARG:HH11	1:B:853:ARG:HB3	1.54	0.71
1:A:209:ASP:CG	1:A:229:ILE:HD12	2.11	0.71
1:B:688:GLU:OE1	1:B:689:GLU:OE1	2.07	0.71
1:B:420:HIS:HD2	1:B:423:TYR:H	1.39	0.70
1:A:570:THR:HA	1:A:626:THR:OG1	1.92	0.70
1:B:323:ARG:CZ	1:B:362:GLU:HB2	2.22	0.70
1:B:323:ARG:NH1	1:B:362:GLU:HB2	2.07	0.70
1:A:144:LYS:NZ	1:A:198:ASP:OD1	2.25	0.69
1:A:57:PRO:HG2	1:B:799:GLN:HE21	1.58	0.69
1:A:39:ILE:HD13	1:A:42:ARG:HH21	1.57	0.69
1:A:354:GLU:O	1:A:358:ARG:HG3	1.92	0.69
1:A:323:ARG:CZ	1:A:362:GLU:HB2	2.23	0.68
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.25	0.68
1:A:159:GLN:HB3	1:A:167:ILE:HB	1.75	0.68
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.07	0.68
1:A:799:GLN:NE2	1:B:58:THR:HB	2.08	0.68
1:A:398:ARG:HB3	1:A:398:ARG:HH11	1.59	0.68
1:B:267:ASP:OD1	1:B:269:SER:HB2	1.94	0.68
1:A:152:PHE:HB3	1:A:206:VAL:HG22	1.74	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:687:MET:CE	1:B:704:CYS:CB	2.72	0.67
1:A:56:ASN:N	1:A:57:PRO:HD2	2.09	0.67
1:B:122:SER:OG	1:B:125:GLN:HG3	1.94	0.67
1:B:160:GLN:HG2	1:B:165:GLU:O	1.93	0.67
1:B:351:ASN:O	1:B:355:ILE:HG12	1.95	0.67
1:B:810:ASN:HD22	1:B:810:ASN:H	1.43	0.66
1:B:772:ILE:HG22	1:B:777:LYS:HD2	1.78	0.66
1:A:241:GLU:O	1:A:245:ILE:HD12	1.95	0.66
1:A:132:GLU:CG	1:A:196:ARG:NH2	2.52	0.66
1:A:230:ILE:HD11	1:A:386:VAL:HG11	1.77	0.66
1:A:317:GLY:HA2	1:A:321:GLU:O	1.94	0.66
1:B:98:ASN:HB3	1:B:103:GLN:HB2	1.78	0.66
1:A:778:THR:HB	1:A:781:ILE:HD13	1.75	0.66
1:B:564:ILE:HG23	1:B:565:GLU:H	1.60	0.66
1:B:142:LYS:HE2	1:B:142:LYS:HA	1.78	0.66
1:B:760:ASP:O	1:B:764:LYS:HG2	1.96	0.66
1:B:425:ARG:HH22	5:B:1007:CIT:H42	1.61	0.66
1:A:245:ILE:HG12	1:A:257:ILE:HD11	1.77	0.66
1:A:280:GLU:HG3	1:A:283:ARG:NH2	2.11	0.65
1:A:913:THR:O	1:A:913:THR:CG2	2.45	0.65
1:A:309:ILE:O	1:A:313:MET:HG3	1.96	0.65
1:A:619:TRP:HB3	1:A:623:PHE:O	1.95	0.65
1:B:644:ARG:NE	1:B:646:GLU:OE1	2.29	0.65
1:B:431:LEU:CD2	1:B:442:PHE:HZ	2.10	0.65
1:A:40:MET:HG3	1:A:388:ALA:O	1.96	0.65
1:A:407:ARG:HG2	1:A:439:ASP:HB2	1.78	0.65
1:A:93:LEU:HD22	1:A:450:GLY:HA3	1.79	0.65
1:B:405:ARG:HD2	1:B:437:ASP:HB3	1.79	0.64
1:A:24:LYS:O	1:A:27:TYR:HB3	1.97	0.64
1:A:356:LEU:HD11	1:A:371:VAL:HG21	1.80	0.64
1:B:693:VAL:HG12	1:B:693:VAL:O	1.98	0.64
1:B:405:ARG:HB3	1:B:405:ARG:HH11	1.63	0.64
1:B:405:ARG:HB3	1:B:405:ARG:NH1	2.13	0.64
1:B:539:ARG:HB3	1:B:559:ILE:HD13	1.79	0.63
1:A:196:ARG:HG2	1:A:198:ASP:HB2	1.80	0.63
1:A:663:MET:HG3	1:A:904:ILE:HD11	1.81	0.63
1:B:423:TYR:HB3	6:B:1181:HOH:O	1.99	0.63
1:B:810:ASN:HD22	1:B:810:ASN:N	1.97	0.62
1:B:134:LEU:O	1:B:138:MET:HG3	1.99	0.62
1:B:583:SER:OG	1:B:592:LYS:NZ	2.32	0.62
1:A:320:PHE:O	1:A:321:GLU:HB2	1.99	0.62
1:B:813:CYS:O	1:B:817:ILE:HG12	1.98	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:426:ARG:HE	5:B:1007:CIT:H22	1.65	0.61
1:A:420:HIS:HD2	1:A:423:TYR:N	1.98	0.61
1:A:799:GLN:HE22	1:B:58:THR:HB	1.65	0.61
1:A:66:THR:CG2	1:A:256:CYS:HB3	2.30	0.61
1:B:854:LEU:HD12	1:B:855:ASN:N	2.15	0.61
1:A:795:LEU:HD11	1:A:799:GLN:CG	2.26	0.61
1:B:101:LYS:C	1:B:103:GLN:H	2.04	0.61
1:A:767:LEU:HD13	1:A:768:PHE:CE2	2.35	0.61
1:B:18:GLN:OE1	1:B:369:VAL:HG11	1.99	0.60
1:B:29:MET:HE1	1:B:381:ARG:NH2	2.15	0.60
1:B:687:MET:HE2	1:B:704:CYS:HA	1.83	0.60
1:B:768:PHE:CE1	1:B:811:SER:HB3	2.37	0.60
1:B:782:PHE:HD1	1:B:786:PHE:CE1	2.19	0.60
1:A:558:LYS:HD3	1:A:560:TYR:OH	2.01	0.60
1:B:687:MET:HE2	1:B:704:CYS:CA	2.31	0.60
1:B:98:ASN:ND2	1:B:101:LYS:HD2	2.17	0.59
1:B:426:ARG:HH21	5:B:1007:CIT:C4	2.06	0.59
1:B:768:PHE:HE1	1:B:811:SER:HB3	1.65	0.59
1:B:763:LYS:HG3	1:B:772:ILE:HD11	1.83	0.59
1:A:912:ARG:C	1:A:914:GLU:H	2.06	0.59
1:B:66:THR:HG23	1:B:68:VAL:H	1.68	0.59
1:A:910:ARG:O	1:A:914:GLU:HB2	2.02	0.59
1:B:471:GLU:HG3	6:B:1161:HOH:O	2.02	0.59
1:A:398:ARG:HB3	1:A:398:ARG:NH1	2.16	0.59
1:B:564:ILE:CG2	1:B:565:GLU:N	2.65	0.59
1:B:18:GLN:HE22	1:B:366:ASP:C	2.06	0.59
1:A:209:ASP:OD1	1:A:229:ILE:HD12	2.03	0.59
1:B:58:THR:HG22	1:B:58:THR:O	2.03	0.58
1:A:193:ILE:HD13	1:A:201:ALA:HB3	1.86	0.58
1:B:193:ILE:HD13	1:B:201:ALA:HB3	1.86	0.58
1:A:644:ARG:NE	1:A:646:GLU:OE1	2.28	0.58
1:A:361:VAL:C	1:A:363:PRO:HD3	2.24	0.57
1:B:564:ILE:CG2	1:B:565:GLU:H	2.17	0.57
1:A:546:ARG:O	1:A:551:ARG:HA	2.05	0.57
1:B:479:LEU:HA	1:B:483:MET:HE1	1.85	0.57
1:B:619:TRP:CD1	1:B:624:LYS:HA	2.40	0.57
1:B:605:PRO:HB3	1:B:708:GLU:HG3	1.87	0.57
1:B:56:ASN:N	1:B:57:PRO:HD2	2.19	0.57
1:B:426:ARG:NH2	5:B:1007:CIT:H41	2.04	0.56
1:A:595:ARG:HD2	1:A:648:ASP:OD2	2.05	0.56
1:B:265:GLY:HA2	1:B:269:SER:HB3	1.87	0.56
1:A:389:THR:O	1:A:392:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:768:PHE:HE1	1:A:811:SER:HB3	1.71	0.56
1:B:644:ARG:HD3	1:B:646:GLU:OE1	2.05	0.56
1:A:235:ASN:HA	1:A:261:TRP:CD1	2.40	0.56
1:B:687:MET:HE2	1:B:704:CYS:HB2	1.82	0.56
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.04	0.56
1:A:66:THR:HG21	1:A:256:CYS:HB3	1.87	0.55
1:B:420:HIS:HD2	1:B:423:TYR:N	2.02	0.55
1:A:307:ARG:O	1:A:311:VAL:HG23	2.05	0.55
1:A:688:GLU:OE1	1:A:848:ASN:ND2	2.38	0.55
1:A:155:SER:HA	1:A:208:ASN:ND2	2.20	0.55
1:A:760:ASP:O	1:A:764:LYS:HG2	2.05	0.55
1:B:724:HIS:HA	1:B:727:ARG:NH1	2.21	0.55
1:B:230:ILE:HD11	1:B:386:VAL:HG11	1.87	0.55
1:B:565:GLU:CG	1:B:566:ILE:N	2.70	0.55
1:B:342:ILE:HG22	1:B:342:ILE:O	2.06	0.55
1:A:171:TRP:HB3	1:A:175:PHE:O	2.06	0.55
1:A:126:LEU:O	1:A:129:HIS:HB3	2.07	0.55
1:B:76:GLU:H	1:B:76:GLU:CD	2.10	0.55
1:B:565:GLU:HG2	1:B:566:ILE:H	1.70	0.55
1:B:101:LYS:O	1:B:103:GLN:N	2.40	0.54
1:A:558:LYS:HD3	1:A:560:TYR:CZ	2.42	0.54
1:A:420:HIS:HD2	1:A:423:TYR:H	1.53	0.54
1:A:320:PHE:C	1:A:322:GLY:H	2.10	0.54
1:B:59:ALA:HB1	6:B:1172:HOH:O	2.07	0.54
1:A:739:GLN:O	1:A:743:LYS:HG3	2.07	0.54
1:A:418:LYS:HG3	1:A:444:LEU:HD11	1.88	0.54
1:A:72:PRO:HD3	1:A:215:MET:CE	2.38	0.54
1:B:786:PHE:CE2	1:B:803:ILE:HG22	2.42	0.54
1:A:168:LEU:HD23	1:A:180:VAL:HG12	1.89	0.54
1:B:602:PHE:CE2	1:B:633:VAL:HG11	2.42	0.54
1:A:380:PHE:HD2	1:A:426:ARG:HD3	1.72	0.54
1:B:479:LEU:HA	1:B:483:MET:CE	2.38	0.53
1:A:608:GLN:OE1	1:A:654:VAL:HG13	2.08	0.53
1:A:244:HIS:HD2	1:A:396:ARG:NH2	2.06	0.53
1:B:418:LYS:HG2	1:B:444:LEU:HD21	1.90	0.53
1:A:422:GLN:OE1	1:A:425:ARG:NH2	2.37	0.53
1:A:575:PHE:O	1:A:579:VAL:HG23	2.08	0.53
1:B:212:GLY:HA3	1:B:449:SER:HB2	1.89	0.53
1:A:58:THR:OG1	1:B:799:GLN:NE2	2.42	0.53
1:B:565:GLU:CG	1:B:566:ILE:H	2.22	0.53
1:B:910:ARG:HG2	1:B:914:GLU:OE2	2.09	0.53
1:A:502:GLN:CD	1:A:502:GLN:H	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:LEU:HD23	1:A:199:TYR:HE1	1.71	0.53
1:A:738:LYS:HE2	6:A:1148:HOH:O	2.08	0.53
1:B:505:ASN:HB2	6:B:1185:HOH:O	2.09	0.53
1:B:29:MET:CE	1:B:381:ARG:CZ	2.86	0.53
1:B:735:ASN:HB2	1:B:738:LYS:CE	2.33	0.52
1:B:673:GLU:CD	1:B:849:ARG:HH22	2.13	0.52
1:A:351:ASN:O	1:A:355:ILE:HG12	2.10	0.52
1:A:155:SER:HA	1:A:208:ASN:HD22	1.74	0.52
1:B:393:ILE:O	1:B:396:ARG:HB3	2.08	0.52
1:A:122:SER:HA	1:A:178:SER:OG	2.10	0.52
1:A:324:ILE:HG23	1:A:328:LEU:HD23	1.90	0.52
1:B:491:MET:O	1:B:495:MET:HG3	2.09	0.52
1:B:319:LEU:HB3	1:B:320:PHE:CE1	2.45	0.52
1:A:451:LYS:O	1:A:455:MET:HG2	2.09	0.52
1:B:687:MET:CE	1:B:704:CYS:SG	2.98	0.52
1:A:420:HIS:CD2	1:A:423:TYR:HB2	2.44	0.52
1:B:354:GLU:O	1:B:358:ARG:HG3	2.10	0.52
1:A:646:GLU:HB2	1:A:647:PHE:CD2	2.45	0.51
1:B:514:SER:OG	1:B:704:CYS:HB3	2.10	0.51
1:A:317:GLY:CA	1:A:321:GLU:O	2.57	0.51
1:B:644:ARG:CD	1:B:646:GLU:OE1	2.58	0.51
1:A:387:ALA:HA	1:A:427:PHE:HE1	1.76	0.51
1:A:137:PHE:O	1:A:141:ARG:HD3	2.10	0.51
1:B:574:LEU:O	1:B:578:ILE:HG12	2.11	0.51
1:A:418:LYS:HG2	1:A:444:LEU:HD21	1.92	0.51
1:B:674:VAL:HB	1:B:858:VAL:HG22	1.92	0.51
1:B:763:LYS:CG	1:B:772:ILE:HD11	2.41	0.51
1:B:531:LEU:HD21	1:B:582:ILE:HD11	1.91	0.51
1:A:307:ARG:HB2	1:A:334:PHE:HB3	1.93	0.51
1:A:763:LYS:CG	1:A:772:ILE:HD11	2.39	0.51
1:A:224:CYS:HA	1:A:409:THR:O	2.11	0.51
1:B:306:VAL:HG11	1:B:334:PHE:CE2	2.46	0.50
1:A:235:ASN:HA	1:A:261:TRP:NE1	2.25	0.50
1:B:782:PHE:CD1	1:B:786:PHE:CE1	2.99	0.50
1:A:33:ASP:O	1:A:37:ILE:HG12	2.12	0.50
1:A:69:ARG:O	1:A:70:SER:HB3	2.12	0.50
1:B:93:LEU:HD12	1:B:93:LEU:N	2.26	0.50
1:A:655:VAL:HG12	1:A:656:ASN:O	2.12	0.50
1:B:278:ASP:O	1:B:281:ILE:HG22	2.11	0.50
1:A:414:GLY:HA2	3:A:1002:BG6:O6	2.11	0.50
1:A:787:LEU:O	1:A:791:GLU:HG3	2.11	0.50
1:B:687:MET:HE2	1:B:704:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:97:VAL:HG21	1:A:105:VAL:HG22	1.93	0.50
1:A:93:LEU:N	1:A:93:LEU:HD12	2.27	0.50
1:B:786:PHE:HE2	1:B:803:ILE:HG22	1.76	0.50
1:A:646:GLU:HB2	1:A:647:PHE:HD2	1.76	0.50
1:A:67:PHE:HA	1:A:255:MET:SD	2.52	0.50
1:A:514:SER:HA	1:A:608:GLN:HE22	1.76	0.50
1:A:265:GLY:HA2	1:A:269:SER:OG	2.12	0.50
1:B:646:GLU:HB3	1:B:647:PHE:HD2	1.77	0.50
1:B:563:PRO:HG2	1:B:566:ILE:HG13	1.94	0.49
1:A:97:VAL:CG2	1:A:105:VAL:HG22	2.41	0.49
1:B:662:MET:SD	1:B:687:MET:HE3	2.53	0.49
1:B:98:ASN:O	1:B:103:GLN:O	2.30	0.49
1:A:786:PHE:CE2	1:A:807:LEU:HD11	2.48	0.49
1:A:245:ILE:HG22	1:A:245:ILE:O	2.12	0.49
1:B:168:LEU:HD23	1:B:180:VAL:HG12	1.95	0.49
1:B:524:GLU:H	1:B:524:GLU:CD	2.16	0.49
1:B:79:ASP:HB3	1:B:148:LEU:CD2	2.43	0.49
1:A:248:VAL:HG21	1:A:255:MET:HE1	1.94	0.49
1:A:598:LEU:HD23	1:A:598:LEU:C	2.33	0.48
1:A:356:LEU:HD23	1:A:359:LEU:HD12	1.94	0.48
1:A:412:VAL:HG12	1:A:413:ASN:N	2.27	0.48
1:A:163:ILE:HG13	1:A:163:ILE:O	2.13	0.48
1:A:141:ARG:HD2	1:A:141:ARG:N	2.28	0.48
1:B:79:ASP:HB3	1:B:148:LEU:HD22	1.96	0.48
1:A:242:LEU:C	1:A:244:HIS:H	2.16	0.48
1:B:677:ILE:O	1:B:682:SER:HA	2.14	0.48
1:A:782:PHE:CD1	1:A:786:PHE:CE1	3.02	0.48
1:A:637:LEU:O	1:A:641:ILE:HG13	2.14	0.48
1:B:136:ASP:C	1:B:136:ASP:OD1	2.51	0.48
1:A:198:ASP:HB3	1:A:199:TYR:HD2	1.79	0.48
1:B:518:ARG:HH12	1:B:521:ASP:CA	2.25	0.48
1:B:523:THR:OG1	1:B:910:ARG:NH1	2.47	0.48
1:B:669:GLU:OE2	1:B:671:THR:N	2.40	0.48
1:B:342:ILE:O	1:B:372:GLN:HG3	2.13	0.47
1:B:66:THR:CG2	1:B:68:VAL:H	2.25	0.47
1:A:320:PHE:O	1:A:322:GLY:N	2.40	0.47
1:A:608:GLN:HG2	1:A:613:ALA:O	2.15	0.47
1:B:654:VAL:HG13	1:B:654:VAL:O	2.13	0.47
1:A:905:THR:O	1:A:909:VAL:HG23	2.14	0.47
1:A:321:GLU:N	1:A:321:GLU:OE1	2.47	0.47
1:B:58:THR:CG2	1:B:58:THR:O	2.63	0.47
1:A:66:THR:O	1:A:67:PHE:HB2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:786:PHE:CE2	1:B:807:LEU:HD11	2.49	0.47
1:B:671:THR:OG1	1:B:857:THR:HG23	2.15	0.47
1:B:271:GLU:OE2	1:B:274:ARG:HD3	2.14	0.47
1:A:83:LEU:O	1:A:153:THR:HB	2.15	0.47
1:A:66:THR:HG23	1:A:68:VAL:H	1.79	0.47
1:B:598:LEU:HD23	1:B:598:LEU:C	2.35	0.47
1:B:796:ALA:O	1:B:799:GLN:HB3	2.14	0.47
1:B:640:ALA:N	1:B:643:ARG:HH21	2.13	0.47
1:B:420:HIS:CD2	1:B:423:TYR:H	2.26	0.47
1:A:519:THR:HB	1:A:520:PRO:HD2	1.96	0.47
1:A:390:LEU:HD23	1:A:431:LEU:HD22	1.98	0.46
1:B:689:GLU:N	1:B:689:GLU:OE1	2.48	0.46
1:A:416:LEU:HD21	1:A:423:TYR:CE2	2.49	0.46
1:A:654:VAL:O	1:A:654:VAL:HG13	2.15	0.46
1:B:664:THR:HG23	1:B:899:LYS:HB3	1.98	0.46
1:B:797:LEU:HD21	1:B:817:ILE:HD13	1.97	0.46
1:A:652:VAL:HG21	1:A:909:VAL:HG22	1.97	0.46
1:B:810:ASN:N	1:B:810:ASN:ND2	2.63	0.46
1:A:529:LEU:HD11	1:A:586:LEU:HD21	1.97	0.46
1:A:56:ASN:N	1:A:57:PRO:CD	2.77	0.46
1:B:101:LYS:C	1:B:103:GLN:N	2.68	0.46
1:B:342:ILE:CG2	1:B:342:ILE:O	2.63	0.46
1:A:583:SER:OG	1:A:592:LYS:NZ	2.49	0.46
1:A:785:LYS:HB2	6:A:1159:HOH:O	2.15	0.46
1:B:769:ARG:HH22	1:B:811:SER:HA	1.81	0.46
1:A:408:THR:OG1	1:A:409:THR:N	2.49	0.46
1:A:90:PHE:CZ	1:A:130:VAL:HG13	2.51	0.46
1:B:165:GLU:HG3	1:B:184:ASP:OD2	2.16	0.46
1:A:24:LYS:O	1:A:27:TYR:CB	2.63	0.46
1:A:64:LEU:HD13	1:A:158:CYS:O	2.16	0.46
1:B:856:VAL:HG22	1:B:857:THR:N	2.31	0.46
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.51	0.46
1:A:339:VAL:O	1:A:343:GLU:HG3	2.16	0.45
1:B:376:THR:O	1:B:380:PHE:HB2	2.16	0.45
1:B:691:LYS:HG3	1:B:692:ASN:N	2.31	0.45
1:A:425:ARG:NH1	5:A:1007:CIT:O2	2.50	0.45
1:B:320:PHE:N	1:B:320:PHE:CD1	2.85	0.45
1:A:803:ILE:O	1:A:806:GLN:HB2	2.16	0.45
1:A:799:GLN:NE2	1:B:58:THR:CB	2.78	0.45
1:A:398:ARG:CB	1:A:398:ARG:HH11	2.27	0.45
1:A:193:ILE:O	1:A:194:LYS:C	2.55	0.45
1:B:181:GLU:HG3	6:B:1189:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:195:LYS:HG2	1:B:195:LYS:O	2.17	0.45
1:B:595:ARG:NE	1:B:648:ASP:OD2	2.50	0.45
1:B:539:ARG:HG3	1:B:541:LEU:HD11	1.99	0.45
1:B:589:MET:CE	1:B:589:MET:HA	2.46	0.45
1:B:659:VAL:HG22	1:B:704:CYS:SG	2.56	0.45
1:B:320:PHE:C	1:B:322:GLY:H	2.19	0.45
1:B:718:LEU:C	1:B:720:ASP:N	2.70	0.45
1:A:320:PHE:C	1:A:322:GLY:N	2.71	0.45
1:B:646:GLU:HB3	1:B:647:PHE:CD2	2.51	0.45
1:B:361:VAL:HG23	1:B:363:PRO:HD3	1.98	0.45
1:A:514:SER:HA	1:A:608:GLN:NE2	2.32	0.45
1:A:62:LYS:HB3	1:A:64:LEU:CD2	2.46	0.45
1:A:232:THR:O	1:A:298:SER:HB2	2.17	0.44
1:B:862:GLY:HA2	3:B:1004:BG6:O6	2.17	0.44
1:A:193:ILE:O	1:A:196:ARG:N	2.49	0.44
1:A:134:LEU:CD2	1:A:199:TYR:HE1	2.31	0.44
1:B:539:ARG:HB3	1:B:559:ILE:CD1	2.44	0.44
1:B:480:THR:HG23	1:B:483:MET:CE	2.47	0.44
1:A:722:ARG:CZ	1:A:740:ARG:HD3	2.46	0.44
1:B:330:THR:HB	1:B:333:LYS:HG3	1.98	0.44
1:A:168:LEU:CD2	1:A:180:VAL:HG12	2.48	0.44
1:B:204:VAL:HG12	1:B:457:THR:HG23	2.00	0.44
1:A:323:ARG:NH2	1:A:362:GLU:O	2.51	0.44
1:A:786:PHE:CE1	1:A:790:ILE:HG13	2.53	0.44
1:B:144:LYS:NZ	1:B:198:ASP:HB3	2.33	0.44
1:A:46:GLU:HG3	1:A:264:PHE:CE1	2.53	0.44
1:A:252:GLU:OE2	1:A:812:THR:HB	2.17	0.44
1:B:762:THR:O	1:B:770:GLY:HA2	2.17	0.44
1:B:71:ILE:HB	1:B:72:PRO:HD2	2.00	0.44
1:A:39:ILE:HD11	1:A:273:ILE:HG12	2.00	0.44
1:A:80:PHE:CE2	1:A:458:ALA:HA	2.53	0.44
1:B:280:GLU:HG3	1:B:283:ARG:NH2	2.32	0.44
1:A:119:VAL:O	1:A:119:VAL:HG12	2.18	0.44
1:A:718:LEU:C	1:A:720:ASP:N	2.70	0.43
1:A:323:ARG:HH21	1:A:362:GLU:HB2	1.80	0.43
1:A:797:LEU:HD21	1:A:817:ILE:HG12	2.00	0.43
1:B:614:GLY:O	1:B:632:ASP:HA	2.18	0.43
1:A:251:ASP:N	1:A:251:ASP:OD1	2.51	0.43
1:A:595:ARG:CD	1:A:648:ASP:OD2	2.67	0.43
1:B:579:VAL:HG21	1:B:640:ALA:CB	2.48	0.43
1:B:420:HIS:CD2	1:B:423:TYR:HB2	2.53	0.43
1:A:406:LEU:HD12	1:A:407:ARG:H	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:HIS:CD2	1:A:396:ARG:NH2	2.85	0.43
1:B:146:LYS:HB2	1:B:148:LEU:HG	2.00	0.43
1:A:677:ILE:HG21	2:A:1003:BGC:C6	2.48	0.43
1:A:477:PHE:CZ	1:A:757:ILE:HD11	2.53	0.43
1:B:101:LYS:O	1:B:103:GLN:CG	2.66	0.43
1:A:148:LEU:HA	1:A:149:PRO:HD3	1.82	0.43
1:B:386:VAL:HG12	1:B:427:PHE:CE1	2.54	0.43
1:A:413:ASN:ND2	3:A:1002:BG6:O1	2.45	0.43
1:A:519:THR:HB	1:A:666:ALA:HB1	2.00	0.43
1:B:154:PHE:CE2	1:B:185:VAL:HG11	2.54	0.43
1:B:644:ARG:HD3	1:B:646:GLU:HB2	2.01	0.43
1:A:677:ILE:O	1:A:682:SER:HA	2.19	0.43
1:B:655:VAL:HG12	1:B:656:ASN:O	2.19	0.43
1:A:400:ASN:HD22	1:A:400:ASN:HA	1.60	0.43
1:B:907:VAL:HG12	1:B:907:VAL:O	2.19	0.43
1:B:640:ALA:HA	1:B:643:ARG:HE	1.84	0.42
1:B:101:LYS:O	1:B:103:GLN:HG3	2.19	0.42
1:A:25:TYR:C	1:A:27:TYR:H	2.21	0.42
1:B:640:ALA:CA	1:B:643:ARG:HH21	2.31	0.42
1:B:323:ARG:NH2	1:B:362:GLU:HB2	2.33	0.42
1:A:449:SER:O	1:A:450:GLY:C	2.58	0.42
1:A:912:ARG:C	1:A:914:GLU:N	2.72	0.42
1:A:274:ARG:NH1	6:A:1156:HOH:O	2.52	0.42
1:B:84:ASP:HA	1:B:153:THR:HB	2.01	0.42
1:A:199:TYR:CD2	1:A:199:TYR:N	2.87	0.42
1:B:541:LEU:HG	1:B:557:ASN:CB	2.48	0.42
1:A:330:THR:HB	1:A:333:LYS:HG3	2.01	0.42
1:A:55:PHE:C	1:A:57:PRO:HD2	2.39	0.42
1:B:640:ALA:HB2	1:B:643:ARG:NH2	2.35	0.42
1:A:677:ILE:HG21	2:A:1003:BGC:H6C1	2.00	0.42
1:A:492:ARG:CZ	1:A:844:LYS:HG3	2.49	0.42
1:B:420:HIS:CD2	1:B:422:GLN:H	2.38	0.42
1:A:644:ARG:O	1:A:645:GLU:HB3	2.20	0.42
1:A:433:ARG:O	1:A:436:PRO:HD3	2.19	0.42
1:A:230:ILE:HD13	1:A:386:VAL:HG21	2.00	0.42
1:B:66:THR:HG23	1:B:68:VAL:HG23	2.02	0.42
1:A:258:ASN:OD1	1:A:258:ASN:C	2.57	0.42
1:B:167:ILE:HA	1:B:183:ALA:O	2.20	0.42
1:B:579:VAL:HG21	1:B:640:ALA:HB3	2.01	0.42
1:A:619:TRP:CD1	1:A:624:LYS:HA	2.55	0.42
1:B:587:ASP:OD1	1:B:592:LYS:HE2	2.19	0.42
1:A:420:HIS:CD2	1:A:422:GLN:H	2.37	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:595:ARG:NE	1:A:648:ASP:OD2	2.52	0.42
1:A:231:GLY:O	1:A:232:THR:C	2.58	0.42
1:B:501:LYS:HB3	1:B:695:MET:SD	2.60	0.42
1:A:134:LEU:HD23	1:A:199:TYR:CE1	2.52	0.42
1:B:640:ALA:HA	1:B:643:ARG:NE	2.34	0.42
1:B:854:LEU:HD12	1:B:855:ASN:H	1.82	0.42
1:B:356:LEU:HD23	1:B:359:LEU:HD12	2.02	0.41
1:B:604:PHE:HB3	1:B:605:PRO:HD2	2.01	0.41
1:B:510:LYS:HA	1:B:510:LYS:HD3	1.92	0.41
1:B:94:ARG:NH1	1:B:143:ILE:HG21	2.35	0.41
1:B:325:THR:HG21	1:B:360:GLY:HA3	2.00	0.41
1:A:105:VAL:HG11	1:A:451:LYS:HE2	2.02	0.41
1:A:20:LYS:O	1:A:24:LYS:HG3	2.20	0.41
1:A:492:ARG:HD2	1:A:492:ARG:O	2.21	0.41
1:A:710:GLY:O	1:A:739:GLN:HA	2.21	0.41
1:A:347:GLU:HB3	1:A:351:ASN:ND2	2.35	0.41
1:B:72:PRO:HD3	1:B:215:MET:CE	2.50	0.41
1:A:151:GLY:HA3	1:A:457:THR:OG1	2.19	0.41
1:B:73:ASP:OD1	1:B:73:ASP:C	2.59	0.41
1:B:431:LEU:HD22	1:B:442:PHE:CZ	2.43	0.41
1:A:854:LEU:HD12	1:A:855:ASN:N	2.36	0.41
1:A:167:ILE:HA	1:A:183:ALA:O	2.21	0.41
1:B:476:HIS:CD2	6:B:1194:HOH:O	2.74	0.41
1:B:518:ARG:HH22	1:B:521:ASP:CG	2.22	0.41
1:A:786:PHE:CE2	1:A:790:ILE:HD11	2.56	0.41
1:A:72:PRO:HG3	1:A:455:MET:HB3	2.01	0.41
1:B:545:ILE:HD13	1:B:903:LEU:HD23	2.02	0.41
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.56	0.41
1:B:312:LYS:O	1:B:316:GLU:HG3	2.20	0.41
1:B:342:ILE:HG23	1:B:352:ALA:HB2	2.02	0.41
1:B:330:THR:HB	1:B:333:LYS:CG	2.50	0.41
1:B:663:MET:HG3	1:B:904:ILE:HD11	2.02	0.41
1:A:356:LEU:HB3	1:A:363:PRO:HG3	2.03	0.41
1:B:98:ASN:CB	1:B:103:GLN:HB2	2.47	0.41
1:B:786:PHE:HZ	1:B:804:LEU:CD2	2.34	0.41
1:B:193:ILE:HD13	1:B:201:ALA:CB	2.50	0.41
1:B:361:VAL:O	1:B:363:PRO:HD3	2.21	0.41
1:B:83:LEU:HD21	1:B:134:LEU:HD13	2.02	0.41
1:B:94:ARG:O	1:B:107:MET:HA	2.21	0.41
1:B:83:LEU:HB2	1:B:152:PHE:CD1	2.56	0.41
1:B:400:ASN:HD22	1:B:400:ASN:HA	1.70	0.41
1:A:551:ARG:NH1	1:A:551:ARG:HG3	2.35	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:531:LEU:HD21	1:A:582:ILE:HD11	2.02	0.40
1:B:490:ARG:O	1:B:494:GLU:HG2	2.20	0.40
1:A:243:ARG:NH1	1:A:244:HIS:HE1	2.18	0.40
1:B:709:TRP:C	1:B:709:TRP:CD1	2.94	0.40
1:B:806:GLN:HB3	1:B:806:GLN:HE21	1.56	0.40
1:B:531:LEU:HD13	1:B:598:LEU:HD11	2.03	0.40
1:A:637:LEU:HD23	1:A:651:VAL:HG21	2.01	0.40
1:A:338:ASP:O	1:A:342:ILE:HD13	2.21	0.40
1:A:520:PRO:HD3	1:A:663:MET:CE	2.52	0.40
1:A:46:GLU:HG3	1:A:264:PHE:HE1	1.86	0.40
1:B:767:LEU:CG	1:B:818:LEU:HD23	2.47	0.40
1:A:152:PHE:O	1:A:206:VAL:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	897/917 (98%)	840 (94%)	55 (6%)	2 (0%)	56	77
1	B	897/917 (98%)	845 (94%)	49 (6%)	3 (0%)	50	71
All	All	1794/1834 (98%)	1685 (94%)	104 (6%)	5 (0%)	50	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	ASN
1	B	102	ASN
1	A	243	ARG
1	A	450	GLY
1	B	436	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%)	749 (97%)	25 (3%)	51	76
1	B	774/788 (98%)	756 (98%)	18 (2%)	63	86
All	All	1548/1576 (98%)	1505 (97%)	43 (3%)	56	81

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	21	LYS
1	A	27	TYR
1	A	96	GLN
1	A	102	ASN
1	A	159	GLN
1	A	196	ARG
1	A	198	ASP
1	A	199	TYR
1	A	202	ASN
1	A	254	ARG
1	A	261	TRP
1	A	320	PHE
1	A	400	ASN
1	A	407	ARG
1	A	408	THR
1	A	481	LYS
1	A	502	GLN
1	A	531	LEU
1	A	565	GLU
1	A	709	TRP
1	A	810	ASN
1	A	843	ASP
1	A	857	THR
1	A	913	THR
1	B	66	THR
1	B	99	HIS
1	B	202	ASN
1	B	261	TRP

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Mol	Chain	Res	Type
1	B	320	PHE
1	B	321	GLU
1	B	380	PHE
1	B	407	ARG
1	B	424	SER
1	B	437	ASP
1	B	463	LEU
1	B	709	TRP
1	B	769	ARG
1	B	798	LEU
1	B	805	GLN
1	B	806	GLN
1	B	810	ASN
1	B	843	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	104	ASN
1	A	125	GLN
1	A	159	GLN
1	A	202	ASN
1	A	244	HIS
1	A	345	ASN
1	A	351	ASN
1	A	384	ASN
1	A	400	ASN
1	A	420	HIS
1	A	466	GLN
1	A	506	ASN
1	A	577	HIS
1	A	700	GLN
1	A	771	GLN
1	A	805	GLN
1	A	806	GLN
1	A	810	ASN
1	A	887	ASN
1	B	98	ASN
1	B	104	ASN
1	B	202	ASN
1	B	244	HIS

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Mol	Chain	Res	Type
1	B	345	ASN
1	B	384	ASN
1	B	400	ASN
1	B	420	HIS
1	B	466	GLN
1	B	502	GLN
1	B	506	ASN
1	B	557	ASN
1	B	702	GLN
1	B	771	GLN
1	B	799	GLN
1	B	806	GLN
1	B	810	ASN
1	B	832	GLN
1	B	887	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	1001	-	12,12,12	0.49	0	17,17,17	1.52	2 (11%)
3	BG6	A	1002	-	16,16,16	1.12	2 (12%)	24,24,24	0.82	1 (4%)
2	BGC	A	1003	-	12,12,12	0.37	0	17,17,17	1.29	2 (11%)
3	BG6	A	1004	-	16,16,16	1.03	2 (12%)	24,24,24	0.96	1 (4%)
5	CIT	A	1007	-	12,12,12	0.89	0	17,17,17	1.55	1 (5%)
2	BGC	B	1001	-	12,12,12	0.35	0	17,17,17	1.45	2 (11%)
3	BG6	B	1002	-	16,16,16	1.03	1 (6%)	24,24,24	0.76	1 (4%)
2	BGC	B	1003	-	12,12,12	0.46	0	17,17,17	1.39	3 (17%)
3	BG6	B	1004	-	16,16,16	1.07	2 (12%)	24,24,24	0.82	1 (4%)
5	CIT	B	1007	-	12,12,12	0.89	0	17,17,17	1.58	1 (5%)

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	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	A	1002	-	-	0/6/26/26	0/1/1/1
2	BGC	A	1003	-	-	0/2/22/22	0/1/1/1
3	BG6	A	1004	-	-	0/6/26/26	0/1/1/1
5	CIT	A	1007	-	-	0/16/16/16	0/0/0/0
2	BGC	B	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	B	1002	-	-	0/6/26/26	0/1/1/1
2	BGC	B	1003	-	-	0/2/22/22	0/1/1/1
3	BG6	B	1004	-	-	0/6/26/26	0/1/1/1
5	CIT	B	1007	-	-	0/16/16/16	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	BG6	P-O3P	3.27	1.62	1.51
3	B	1002	BG6	P-O3P	3.08	1.61	1.51
3	B	1004	BG6	P-O3P	3.00	1.61	1.51
3	A	1004	BG6	P-O3P	2.87	1.60	1.51
3	A	1004	BG6	P-O2P	2.18	1.62	1.54
3	A	1002	BG6	P-O2P	2.13	1.62	1.54
3	B	1004	BG6	P-O2P	2.01	1.62	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1007	CIT	O6-C6-C3	4.95	120.08	112.89
5	A	1007	CIT	O6-C6-C3	4.72	119.75	112.89
2	A	1001	BGC	C1-O5-C5	-4.46	105.41	113.40
2	B	1001	BGC	O5-C1-C2	-3.83	103.92	109.86
2	B	1001	BGC	C1-O5-C5	-3.76	106.67	113.40
2	A	1003	BGC	O5-C1-C2	-3.43	104.55	109.86
2	A	1001	BGC	O5-C1-C2	-3.34	104.69	109.86
2	B	1003	BGC	O5-C1-C2	-3.30	104.74	109.86
2	B	1003	BGC	C1-O5-C5	-3.28	107.53	113.40
3	A	1004	BG6	O1P-P-O6	2.95	114.79	106.65
2	A	1003	BGC	C1-O5-C5	-2.92	108.17	113.40
3	B	1004	BG6	O1P-P-O6	2.70	114.09	106.65
3	A	1002	BG6	O1P-P-O6	2.54	113.65	106.65
2	B	1003	BGC	C1-C2-C3	-2.26	106.96	110.53
3	B	1002	BG6	O1P-P-O6	2.10	112.44	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	0.23	30 (3%) 44 45	31, 59, 85, 113	0
1	B	899/917 (98%)	0.22	31 (3%) 43 44	32, 58, 85, 112	0
All	All	1798/1834 (98%)	0.22	61 (3%) 43 44	31, 59, 85, 113	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ILE	4.9
1	B	16	ASP	4.4
1	A	564	ILE	4.2
1	A	16	ASP	4.0
1	B	19	VAL	3.8
1	B	100	GLU	3.7
1	B	18	GLN	3.5
1	A	794	ARG	3.5
1	B	913	THR	3.4
1	A	786	PHE	3.3
1	A	17	ASP	3.2
1	A	310	LEU	3.2
1	A	21	LYS	3.2
1	B	237	CYS	3.1
1	A	31	LEU	3.0
1	B	786	PHE	3.0
1	B	794	ARG	2.9
1	A	229	ILE	2.9
1	B	102	ASN	2.7
1	B	101	LYS	2.6
1	A	436	PRO	2.6
1	A	443	LEU	2.5
1	B	324	ILE	2.5
1	B	17	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	210	THR	2.5
1	B	359	LEU	2.5
1	B	227	GLY	2.5
1	B	798	LEU	2.5
1	A	549	LYS	2.5
1	A	911	LEU	2.3
1	A	26	LEU	2.3
1	B	346	LYS	2.3
1	B	548	GLY	2.3
1	A	398	ARG	2.3
1	B	235	ASN	2.3
1	B	549	LYS	2.3
1	A	417	TYR	2.3
1	B	103	GLN	2.2
1	B	914	GLU	2.2
1	B	550	LYS	2.2
1	A	93	LEU	2.2
1	A	142	LYS	2.2
1	A	233	GLY	2.2
1	A	769	ARG	2.2
1	A	202	ASN	2.1
1	A	262	GLY	2.1
1	B	256	CYS	2.1
1	A	147	LYS	2.1
1	B	412	VAL	2.1
1	A	201	ALA	2.1
1	B	350	HIS	2.1
1	A	358	ARG	2.1
1	A	359	LEU	2.1
1	A	406	LEU	2.1
1	B	911	LEU	2.1
1	B	852	ASP	2.1
1	A	80	PHE	2.1
1	A	350	HIS	2.0
1	B	234	THR	2.0
1	B	229	ILE	2.0
1	B	406	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CIT	B	1007	13/13	0.26	5.47	106,108,108,108	0
2	BGC	B	1001	12/12	0.33	2.30	48,49,50,51	0
5	CIT	A	1007	13/13	0.29	1.83	110,110,111,111	0
2	BGC	A	1003	12/12	0.21	1.75	36,38,38,41	0
2	BGC	A	1001	12/12	0.32	1.65	50,52,53,55	0
2	BGC	B	1003	12/12	0.18	0.78	38,39,40,42	0
3	BG6	A	1004	16/16	0.17	0.30	36,41,42,43	0
3	BG6	B	1004	16/16	0.17	0.19	36,43,44,45	0
3	BG6	A	1002	16/16	0.20	0.10	75,78,80,80	0
3	BG6	B	1002	16/16	0.22	0.05	71,74,75,76	0
4	NA	A	1005	1/1	0.11	-1.39	63,63,63,63	0
4	NA	A	1006	1/1	0.05	-1.72	53,53,53,53	0
4	NA	B	1005	1/1	0.07	-1.81	65,65,65,65	0
4	NA	B	1006	1/1	0.05	-1.97	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.