



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:25 PM UTC

PDB ID : 4FOI / pdb_00004foi
Title : Crystal Structure of recombinant human Hexokinase type I mutant D413N with Glucose 1,6-bisphosphate
Authors : Shen, L.; Honzatko, R.B.
Deposited on : 2012-06-20
Resolution : 2.40 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

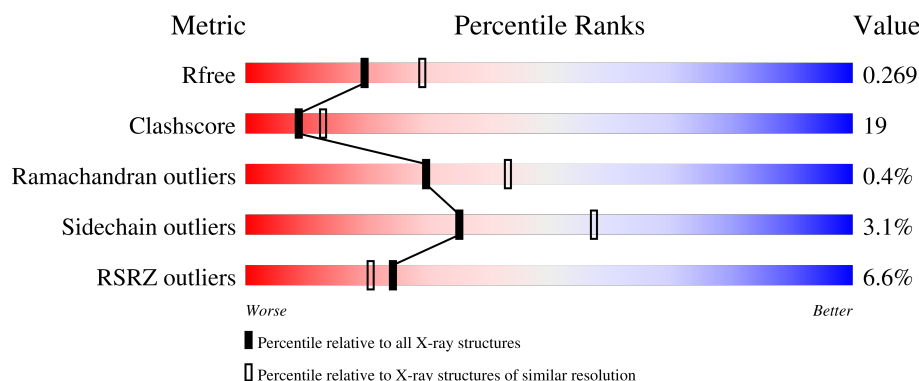
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	6% 67% 29% ..
1	B	917	7% 72% 23% ...

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14495 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.

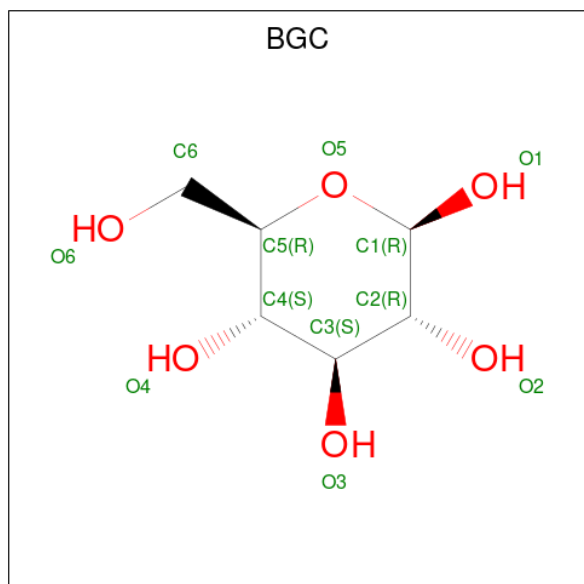
- Molecule 1 is a protein called Hexokinase-1.

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



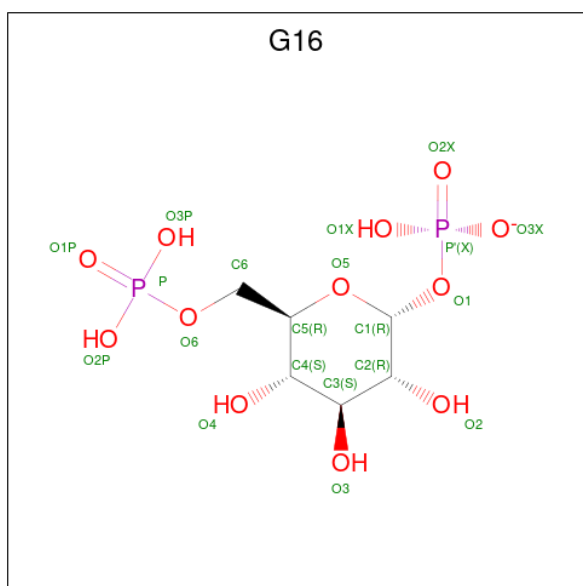
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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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 1,6-di-O-phosphono-alpha-D-glucopyranose (CCD ID: G16) (formula: $C_6H_{13}O_{12}P_2$).

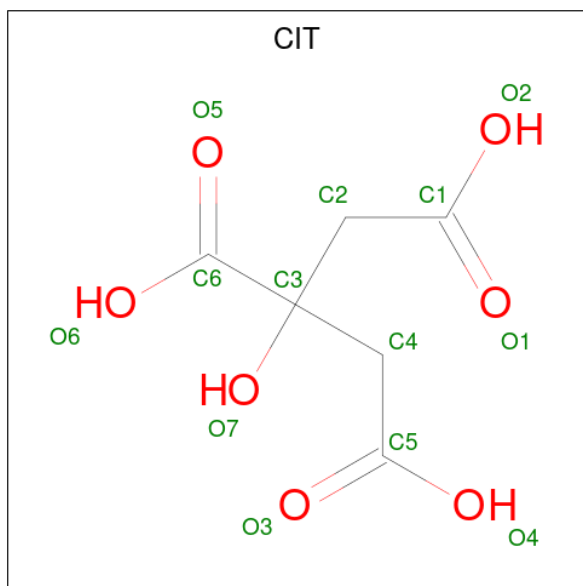


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is CITRIC ACID (CCD ID: 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		

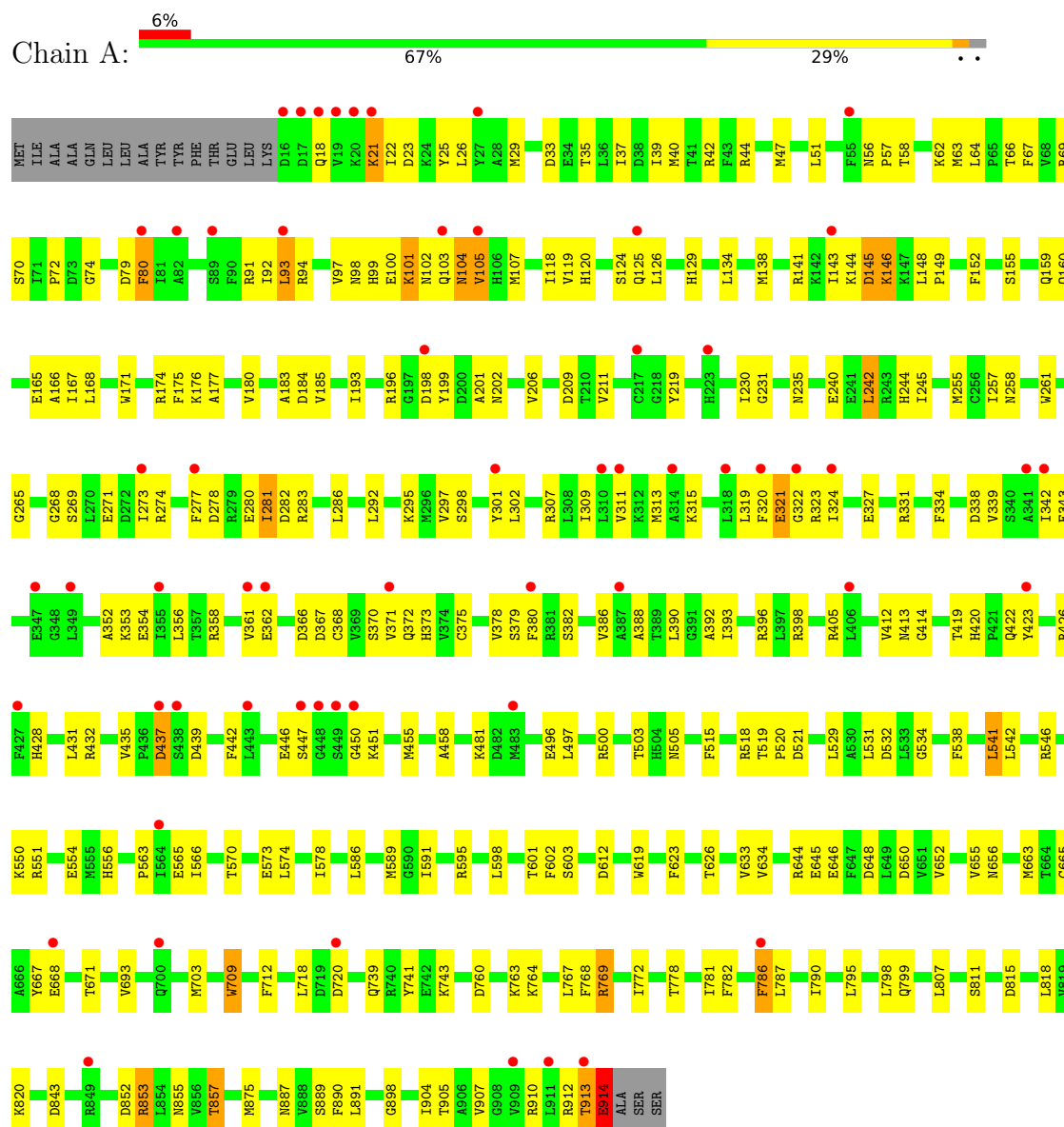
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	130	Total	O	0	0
			130	130		
6	B	143	Total	O	0	0
			143	143		

3 Residue-property plots

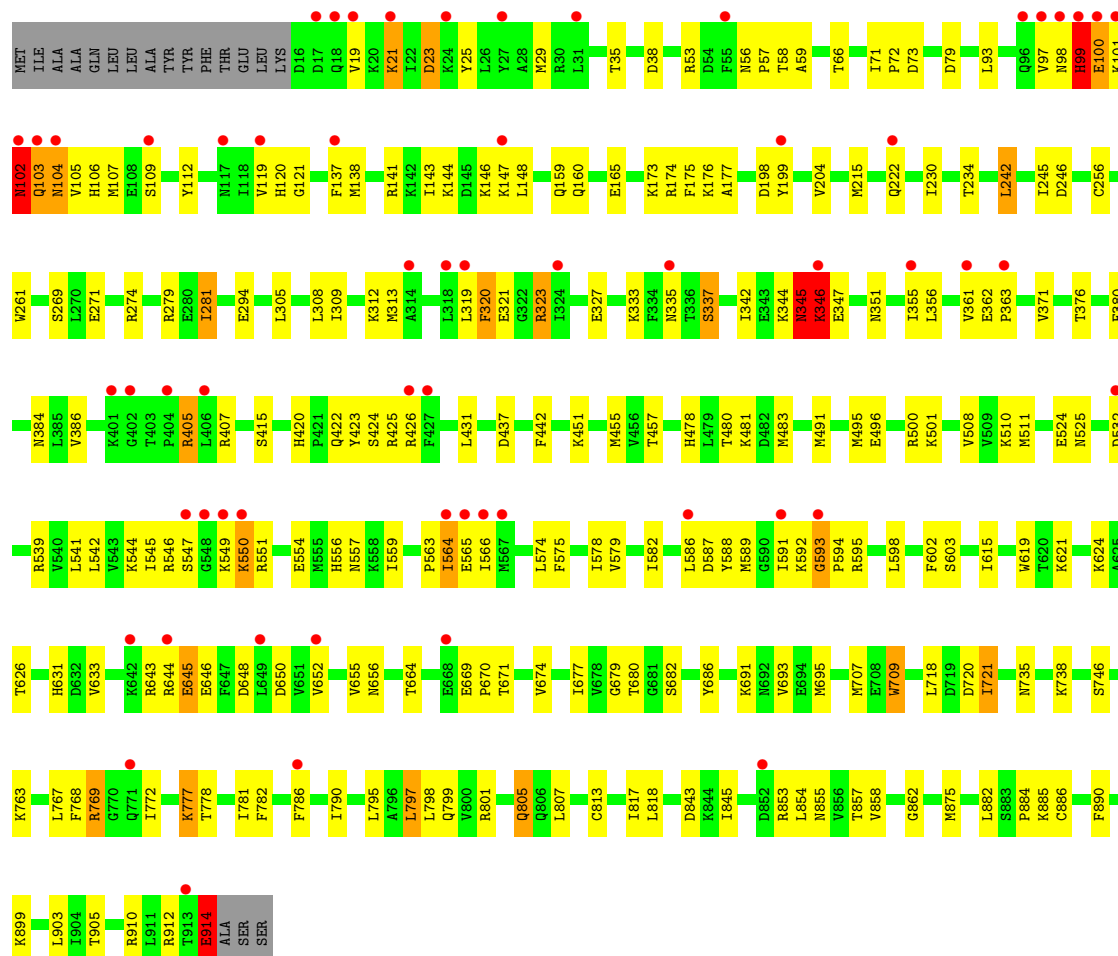
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hexokinase-1



• Molecule 1: Hexokinase-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.38Å 120.77Å 120.59Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	35.41 – 2.40 35.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.41-2.40) 98.5 (35.41-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.247 , 0.273 0.244 , 0.269	Depositor DCC
R_{free} test set	4603 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k 0.000 for -h,l,k 0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14495	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: NA, BGC, CIT, G16

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	0.33	1/7138 (0.0%)	0.77	5/9606 (0.1%)
1	B	0.33	1/7138 (0.0%)	0.77	4/9606 (0.0%)
All	All	0.33	2/14276 (0.0%)	0.77	9/19212 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	914	GLU	C-O	7.95	1.39	1.23
1	B	914	GLU	C-O	5.73	1.35	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	914	GLU	CA-C-O	21.06	156.60	120.80
1	B	914	GLU	CA-C-O	16.78	149.32	120.80
1	B	99	HIS	N-CA-C	7.89	123.41	112.04
1	B	345	ASN	N-CA-C	7.73	121.21	111.24
1	A	435	VAL	CA-C-N	6.49	125.92	118.85
1	A	435	VAL	C-N-CA	6.49	125.92	118.85
1	B	173	LYS	CB-CA-C	-5.62	110.11	116.63
1	A	450	GLY	N-CA-C	5.57	119.38	112.64
1	A	145	ASP	N-CA-C	-5.22	103.25	110.35

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	ASN	Peptide
1	B	345	ASN	Peptide
1	B	99	HIS	Peptide

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	276	0
1	B	7032	0	7092	257	0
2	A	24	0	24	0	0
2	B	24	0	24	2	0
3	A	40	0	20	2	0
3	B	40	0	20	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	13	0	5	0	0
5	B	13	0	5	1	0
6	A	130	0	0	8	0
6	B	143	0	0	14	0
All	All	14495	0	14282	532	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 (532) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:HIS:N	1:B:100:GLU:HB3	1.29	1.47
1:A:496:GLU:HG3	1:A:500:ARG:NH1	1.13	1.45
1:B:323:ARG:NH1	1:B:362:GLU:HB2	1.38	1.34
1:A:496:GLU:CG	1:A:500:ARG:HH12	1.39	1.32
1:A:94:ARG:NH1	1:A:143:ILE:HD11	1.57	1.17
1:B:159:GLN:HG2	6:B:1204:HOH:O	1.44	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:PRO:HG2	1:B:566:ILE:HD12	1.25	1.11
1:B:595:ARG:HD2	1:B:648:ASP:OD2	1.50	1.10
1:B:103:GLN:OE1	1:B:103:GLN:HA	1.51	1.10
1:A:361:VAL:HB	6:A:1192:HOH:O	1.52	1.09
1:A:668:GLU:HG3	6:A:1204:HOH:O	0.90	1.07
1:A:101:LYS:HD2	1:A:101:LYS:N	1.66	1.05
1:A:595:ARG:HD2	1:A:648:ASP:OD2	1.53	1.04
1:B:99:HIS:N	1:B:100:GLU:CB	2.21	1.03
1:A:176:LYS:HE2	6:A:1216:HOH:O	1.58	1.02
1:A:496:GLU:CG	1:A:500:ARG:NH1	2.09	1.01
1:B:99:HIS:H	1:B:100:GLU:CB	1.74	0.99
1:B:564:ILE:H	1:B:564:ILE:CD1	1.74	0.98
1:A:565:GLU:HG3	1:A:566:ILE:N	1.80	0.96
1:B:564:ILE:HD12	1:B:564:ILE:N	1.81	0.95
1:B:335:ASN:OD1	6:B:1150:HOH:O	1.85	0.95
1:A:98:ASN:OD1	1:A:101:LYS:HD3	1.65	0.95
1:B:345:ASN:N	1:B:346:LYS:HB3	1.82	0.95
1:B:563:PRO:CG	1:B:566:ILE:HD12	1.96	0.94
1:B:323:ARG:NH1	1:B:362:GLU:CB	2.30	0.93
1:B:797:LEU:HD11	1:B:817:ILE:HD11	1.49	0.93
1:A:913:THR:HG22	1:A:913:THR:O	1.65	0.93
1:B:795:LEU:HD11	1:B:799:GLN:HG2	1.51	0.92
1:B:323:ARG:HH12	1:B:362:GLU:HB2	1.37	0.89
1:B:323:ARG:HH11	1:B:362:GLU:HB2	1.20	0.89
1:B:564:ILE:H	1:B:564:ILE:HD12	1.34	0.89
1:A:97:VAL:HG22	1:A:105:VAL:HA	1.55	0.88
1:B:103:GLN:HG3	1:B:106:HIS:HB2	1.54	0.88
1:B:345:ASN:N	1:B:346:LYS:CB	2.36	0.88
1:A:343:GLU:HG3	1:A:420:HIS:CE1	2.10	0.87
1:B:99:HIS:H	1:B:100:GLU:HB3	1.06	0.87
1:A:591:ILE:HG22	1:A:591:ILE:O	1.74	0.87
1:B:321:GLU:CG	1:B:323:ARG:NH2	2.38	0.86
1:A:143:ILE:HG21	1:A:148:LEU:CD1	2.05	0.86
1:B:431:LEU:HD22	1:B:442:PHE:HZ	1.40	0.86
1:A:563:PRO:HG2	1:A:566:ILE:HD12	1.56	0.86
1:B:591:ILE:O	1:B:591:ILE:HG22	1.74	0.85
1:A:94:ARG:CZ	1:A:143:ILE:HD11	2.07	0.85
1:A:51:LEU:HD21	1:A:257:ILE:HD13	1.58	0.85
1:A:767:LEU:HG	1:A:818:LEU:HD23	1.57	0.85
1:B:563:PRO:HG2	1:B:566:ILE:CD1	2.07	0.85
1:B:102:ASN:HA	1:B:104:ASN:N	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:N	1:A:101:LYS:CD	2.40	0.83
1:A:518:ARG:HH21	1:A:910:ARG:HH22	1.26	0.83
1:B:768:PHE:HA	1:B:769:ARG:NH2	1.94	0.83
1:B:650:ASP:OD2	1:B:912:ARG:NH2	2.12	0.83
1:A:143:ILE:HG21	1:A:148:LEU:HD12	1.59	0.82
1:A:320:PHE:CG	1:A:361:VAL:HG11	2.14	0.82
1:B:420:HIS:HD2	1:B:423:TYR:H	1.24	0.82
1:B:99:HIS:CA	1:B:100:GLU:HB3	2.10	0.81
1:A:518:ARG:HH21	1:A:910:ARG:NH2	1.80	0.80
1:B:98:ASN:HB2	1:B:100:GLU:HG2	1.64	0.80
1:A:763:LYS:HG3	1:A:772:ILE:HD11	1.65	0.79
1:B:323:ARG:HH11	1:B:362:GLU:CB	1.92	0.79
1:A:820:LYS:NZ	6:A:1198:HOH:O	1.67	0.79
1:A:160:GLN:HG2	1:A:165:GLU:O	1.83	0.78
1:A:565:GLU:CG	1:A:566:ILE:N	2.46	0.78
1:A:380:PHE:HD2	1:A:426:ARG:HD3	1.49	0.77
1:A:79:ASP:OD1	1:A:148:LEU:HD22	1.82	0.77
1:B:356:LEU:HD11	1:B:371:VAL:HG21	1.65	0.77
1:B:321:GLU:HG3	1:B:323:ARG:NH2	1.99	0.77
1:A:143:ILE:HG22	1:A:143:ILE:O	1.82	0.77
1:A:431:LEU:HD23	1:A:442:PHE:HZ	1.47	0.76
1:B:103:GLN:OE1	1:B:103:GLN:CA	2.33	0.76
1:A:281:ILE:HD12	6:A:1229:HOH:O	1.85	0.75
1:B:321:GLU:CG	1:B:323:ARG:HH21	2.00	0.74
1:A:343:GLU:HG3	1:A:420:HIS:HE1	1.52	0.74
1:A:107:MET:HE1	1:A:451:LYS:HB2	1.69	0.74
1:A:380:PHE:CD2	1:A:426:ARG:HD3	2.23	0.73
1:A:145:ASP:O	1:A:146:LYS:CB	2.37	0.72
1:A:320:PHE:CD1	1:A:361:VAL:HG11	2.24	0.72
1:B:344:LYS:HB3	1:B:346:LYS:HG2	1.71	0.71
1:A:40:MET:HG3	1:A:388:ALA:O	1.91	0.71
1:B:778:THR:O	1:B:781:ILE:HG12	1.91	0.71
1:A:100:GLU:C	1:A:101:LYS:HD2	2.15	0.70
1:B:103:GLN:O	1:B:104:ASN:C	2.34	0.70
1:B:546:ARG:O	1:B:551:ARG:HA	1.92	0.70
1:B:508:VAL:HG22	6:B:1242:HOH:O	1.91	0.70
1:B:405:ARG:HB3	1:B:405:ARG:HH11	1.56	0.70
1:B:321:GLU:CB	1:B:323:ARG:HH21	2.05	0.69
1:A:309:ILE:O	1:A:313:MET:HG3	1.91	0.69
1:B:346:LYS:HG3	1:B:347:GLU:HG2	1.75	0.69
1:B:160:GLN:HG2	1:B:165:GLU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ARG:NH2	1:A:815:ASP:OD2	2.25	0.69
1:A:437:ASP:OD1	1:A:437:ASP:N	2.25	0.68
1:B:595:ARG:CD	1:B:648:ASP:OD2	2.36	0.68
1:B:674:VAL:HB	1:B:858:VAL:HG22	1.76	0.68
1:A:145:ASP:O	1:A:146:LYS:HG3	1.92	0.68
1:B:797:LEU:CD1	1:B:817:ILE:HD11	2.23	0.67
1:B:344:LYS:C	1:B:346:LYS:HB3	2.19	0.67
1:A:159:GLN:HB3	1:A:167:ILE:HB	1.74	0.67
1:A:420:HIS:HD2	1:A:423:TYR:N	1.92	0.67
1:A:913:THR:O	1:A:913:THR:CG2	2.38	0.67
1:B:344:LYS:HB3	1:B:346:LYS:HB3	1.76	0.67
1:B:598:LEU:HD23	1:B:598:LEU:C	2.20	0.67
1:B:21:LYS:NZ	1:B:21:LYS:HB3	2.09	0.67
1:B:102:ASN:HA	1:B:104:ASN:H	1.58	0.67
1:B:602:PHE:CE2	1:B:633:VAL:HG11	2.30	0.66
1:B:914:GLU:C	1:B:914:GLU:OE1	2.39	0.66
1:A:591:ILE:O	1:A:591:ILE:CG2	2.43	0.66
1:B:405:ARG:HD2	1:B:437:ASP:HB3	1.77	0.66
1:B:345:ASN:H	1:B:346:LYS:CB	2.09	0.66
1:A:786:PHE:CD2	1:A:807:LEU:HD11	2.31	0.66
1:A:145:ASP:O	1:A:146:LYS:HB2	1.95	0.66
1:B:644:ARG:C	1:B:645:GLU:HG3	2.20	0.66
1:A:245:ILE:HG12	1:A:257:ILE:HD11	1.75	0.66
1:B:588:TYR:HD2	1:B:589:MET:HE3	1.61	0.65
1:B:98:ASN:HB2	1:B:100:GLU:CG	2.25	0.65
1:B:524:GLU:O	1:B:547:SER:HB3	1.96	0.65
1:B:588:TYR:CD2	1:B:589:MET:HE3	2.32	0.65
1:B:174:ARG:NH1	6:B:1177:HOH:O	2.29	0.65
1:A:913:THR:O	1:A:914:GLU:CD	2.40	0.65
1:A:565:GLU:CG	1:A:566:ILE:H	2.10	0.65
1:B:345:ASN:H	1:B:346:LYS:HB2	1.62	0.64
1:B:575:PHE:O	1:B:579:VAL:HG23	1.97	0.64
1:B:415:SER:HB2	6:B:1239:HOH:O	1.98	0.64
1:A:798:LEU:HD23	1:A:798:LEU:C	2.23	0.64
1:B:813:CYS:O	1:B:817:ILE:HG12	1.98	0.64
1:A:420:HIS:HD2	1:A:423:TYR:H	1.46	0.63
1:B:565:GLU:OE1	1:B:565:GLU:N	2.20	0.63
1:B:782:PHE:HD1	1:B:786:PHE:CE1	2.16	0.63
1:B:345:ASN:N	1:B:346:LYS:HB2	2.12	0.63
1:A:786:PHE:CZ	1:A:790:ILE:HG13	2.34	0.63
1:B:159:GLN:CG	6:B:1204:HOH:O	2.20	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:HB2	1:B:351:ASN:ND2	2.14	0.63
1:A:356:LEU:HD11	1:A:371:VAL:HG21	1.81	0.62
1:A:768:PHE:HE1	1:A:811:SER:HB3	1.65	0.62
1:B:346:LYS:CE	1:B:346:LYS:HA	2.29	0.62
1:B:321:GLU:HB2	1:B:323:ARG:HH21	1.64	0.62
1:A:496:GLU:CD	1:A:500:ARG:HH12	2.06	0.62
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.13	0.62
1:B:650:ASP:CG	1:B:912:ARG:HH22	2.07	0.62
1:A:176:LYS:CE	6:A:1216:HOH:O	2.30	0.62
1:B:79:ASP:HB3	1:B:148:LEU:HD22	1.82	0.61
1:B:98:ASN:C	1:B:100:GLU:HB3	2.20	0.61
1:B:346:LYS:HA	1:B:346:LYS:HE3	1.81	0.61
1:A:143:ILE:HG21	1:A:148:LEU:HD11	1.82	0.61
1:A:320:PHE:HB3	1:A:361:VAL:CG1	2.30	0.61
1:B:320:PHE:C	1:B:323:ARG:HH21	2.07	0.61
1:A:56:ASN:N	1:A:57:PRO:HD2	2.14	0.61
1:B:420:HIS:HD2	1:B:423:TYR:N	1.97	0.61
1:B:420:HIS:CD2	1:B:423:TYR:H	2.13	0.61
1:A:144:LYS:HD3	1:A:199:TYR:HB3	1.81	0.61
1:A:176:LYS:HG3	1:A:286:LEU:HG	1.83	0.61
1:A:361:VAL:HG12	1:A:362:GLU:N	2.15	0.61
1:B:772:ILE:HG22	1:B:777:LYS:HD2	1.83	0.61
1:A:529:LEU:HD11	1:A:586:LEU:HD21	1.83	0.61
1:B:541:LEU:HG	1:B:557:ASN:HB3	1.83	0.60
1:A:143:ILE:O	1:A:145:ASP:O	2.19	0.60
1:B:587:ASP:OD1	1:B:592:LYS:HD2	2.01	0.60
1:A:268:GLY:HA2	1:A:271:GLU:HG2	1.82	0.60
1:A:778:THR:HB	1:A:781:ILE:HD13	1.83	0.60
1:A:167:ILE:HD12	1:A:167:ILE:N	2.17	0.60
1:B:346:LYS:HG3	1:B:347:GLU:H	1.66	0.60
1:B:644:ARG:HD3	1:B:646:GLU:OE1	2.02	0.59
1:A:143:ILE:O	1:A:143:ILE:CG2	2.48	0.59
1:B:491:MET:O	1:B:495:MET:HG3	2.01	0.59
1:B:361:VAL:O	1:B:363:PRO:HD3	2.01	0.59
1:A:795:LEU:HD11	1:A:799:GLN:HG2	1.83	0.59
1:B:344:LYS:HB3	1:B:346:LYS:CG	2.31	0.59
1:B:564:ILE:H	1:B:564:ILE:HD13	1.64	0.59
1:B:102:ASN:HB2	1:B:104:ASN:ND2	2.17	0.59
1:B:59:ALA:HB1	6:B:1110:HOH:O	2.03	0.59
1:B:767:LEU:HG	1:B:818:LEU:HD23	1.85	0.59
1:B:875:MET:HE1	1:B:890:PHE:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:N	1:A:93:LEU:HD12	2.18	0.59
1:A:320:PHE:O	1:A:323:ARG:HG3	2.02	0.58
1:B:431:LEU:HD22	1:B:442:PHE:CZ	2.31	0.58
1:A:119:VAL:HG13	1:A:175:PHE:CD1	2.38	0.58
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.36	0.58
1:B:335:ASN:ND2	1:B:337:SER:HB2	2.18	0.58
1:B:735:ASN:HB2	1:B:738:LYS:HE3	1.84	0.58
1:A:145:ASP:O	1:A:146:LYS:CG	2.52	0.58
1:A:104:ASN:O	1:A:105:VAL:C	2.47	0.58
1:A:315:LYS:HA	1:A:324:ILE:HD11	1.86	0.58
1:B:582:ILE:O	1:B:586:LEU:HG	2.03	0.58
1:A:786:PHE:CE2	1:A:790:ILE:HD11	2.40	0.57
1:A:570:THR:OG1	1:A:573:GLU:HG3	2.04	0.57
1:A:652:VAL:HB	1:A:905:THR:HG23	1.87	0.57
1:B:99:HIS:CA	1:B:100:GLU:CB	2.80	0.57
1:A:428:HIS:O	1:A:432:ARG:HG2	2.04	0.57
1:A:497:LEU:O	1:A:503:THR:HG23	2.05	0.57
1:A:798:LEU:HD23	1:A:798:LEU:O	2.05	0.57
1:B:621:LYS:HE2	2:B:1003:BGC:O5	2.04	0.57
1:A:307:ARG:O	1:A:311:VAL:HG23	2.05	0.57
1:B:351:ASN:O	1:B:355:ILE:HG12	2.05	0.56
1:B:619:TRP:CD1	1:B:624:LYS:HA	2.41	0.56
1:B:693:VAL:HG12	1:B:693:VAL:O	2.05	0.56
1:A:21:LYS:HB2	1:A:21:LYS:NZ	2.20	0.56
1:A:302:LEU:HD22	1:A:378:VAL:HG12	1.87	0.56
1:A:570:THR:HA	1:A:626:THR:OG1	2.06	0.56
1:A:98:ASN:CG	1:A:101:LYS:HD3	2.30	0.56
1:B:574:LEU:O	1:B:578:ILE:HG12	2.06	0.56
1:A:105:VAL:HG11	1:A:451:LYS:HE2	1.87	0.56
1:A:168:LEU:HD23	1:A:180:VAL:HG12	1.87	0.56
1:B:425:ARG:HH22	5:B:1007:CIT:H22	1.71	0.56
1:B:686:TYR:CD2	1:B:845:ILE:HD11	2.41	0.56
1:A:171:TRP:NE1	1:A:177:ALA:H	2.03	0.55
1:A:375:CYS:O	1:A:379:SER:HB3	2.06	0.55
1:B:578:ILE:O	1:B:582:ILE:HG13	2.05	0.55
1:B:542:LEU:HD11	1:B:544:LYS:HE3	1.86	0.55
1:A:875:MET:HE1	1:A:890:PHE:CE2	2.41	0.55
1:B:525:ASN:HA	1:B:545:ILE:O	2.06	0.55
1:B:98:ASN:ND2	1:B:100:GLU:HG3	2.22	0.55
1:A:853:ARG:HH11	1:A:853:ARG:HG2	1.72	0.55
1:A:58:THR:OG1	1:B:799:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ILE:HD13	1:B:903:LEU:HD23	1.89	0.54
1:A:912:ARG:O	1:A:914:GLU:N	2.37	0.54
1:B:346:LYS:HG3	1:B:347:GLU:N	2.21	0.54
1:A:760:ASP:O	1:A:764:LYS:HG2	2.07	0.54
1:B:313:MET:CB	1:B:319:LEU:HD12	2.37	0.54
1:A:98:ASN:OD1	1:A:101:LYS:CD	2.47	0.54
1:A:446:GLU:HG3	1:A:447:SER:N	2.23	0.54
1:B:98:ASN:HD21	1:B:101:LYS:HB2	1.73	0.54
1:A:307:ARG:NH2	1:A:331:ARG:HA	2.23	0.54
1:B:405:ARG:CD	1:B:437:ASP:HB3	2.38	0.54
1:B:643:ARG:O	1:B:645:GLU:CG	2.56	0.54
1:B:29:MET:HE1	1:B:309:ILE:HD11	1.88	0.54
1:A:25:TYR:CD2	1:A:313:MET:HE3	2.42	0.54
1:A:398:ARG:NH1	1:A:398:ARG:HB3	2.23	0.54
1:A:413:ASN:ND2	1:A:414:GLY:H	2.05	0.54
1:B:323:ARG:HH11	1:B:362:GLU:CG	2.20	0.54
1:B:344:LYS:HB3	1:B:346:LYS:CB	2.36	0.54
1:B:58:THR:HG22	1:B:58:THR:O	2.06	0.54
1:A:165:GLU:HG3	1:A:184:ASP:OD2	2.08	0.53
1:A:671:THR:OG1	1:A:857:THR:HG23	2.08	0.53
1:A:767:LEU:CG	1:A:818:LEU:HD23	2.35	0.53
1:B:644:ARG:C	1:B:645:GLU:CG	2.78	0.53
1:A:496:GLU:HG3	1:A:500:ARG:HH11	1.51	0.53
1:B:321:GLU:HG2	1:B:323:ARG:NH2	2.21	0.53
1:A:240:GLU:HB3	1:A:257:ILE:HD12	1.90	0.53
1:B:361:VAL:HG12	1:B:362:GLU:N	2.23	0.53
1:A:342:ILE:O	1:A:372:GLN:HG3	2.08	0.53
1:B:591:ILE:O	1:B:591:ILE:CG2	2.47	0.53
1:A:563:PRO:HG2	1:A:566:ILE:CD1	2.34	0.53
1:A:39:ILE:HD11	1:A:273:ILE:HG12	1.90	0.53
1:A:283:ARG:HD2	1:B:559:ILE:O	2.09	0.53
1:B:198:ASP:HB3	1:B:199:TYR:HD1	1.74	0.53
1:B:313:MET:HB2	1:B:319:LEU:HD12	1.91	0.53
1:A:72:PRO:HG3	1:A:455:MET:HB3	1.90	0.53
1:A:297:VAL:HG13	1:A:382:SER:OG	2.08	0.53
1:A:505:ASN:HB2	6:A:1205:HOH:O	2.08	0.53
1:B:281:ILE:HG13	1:B:305:LEU:HD13	1.90	0.52
1:A:321:GLU:HB2	1:A:323:ARG:NH1	2.24	0.52
1:A:718:LEU:C	1:A:720:ASP:N	2.66	0.52
1:A:414:GLY:HA2	3:A:1002:G16:O6	2.09	0.52
1:B:679:GLY:O	1:B:746:SER:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HA	1:A:47:MET:HE2	1.92	0.52
1:A:598:LEU:C	1:A:598:LEU:HD23	2.34	0.52
1:A:26:LEU:HD22	1:A:29:MET:CE	2.39	0.52
1:B:346:LYS:CG	1:B:347:GLU:H	2.21	0.52
1:A:94:ARG:CZ	1:A:143:ILE:CD1	2.84	0.52
1:A:107:MET:HE1	1:A:451:LYS:CB	2.39	0.52
1:B:782:PHE:CD1	1:B:786:PHE:CE1	2.97	0.52
1:B:539:ARG:HG3	1:B:541:LEU:HD11	1.92	0.51
1:B:541:LEU:HG	1:B:557:ASN:CB	2.40	0.51
1:A:166:ALA:HB3	1:A:185:VAL:HG22	1.92	0.51
1:B:347:GLU:HB2	1:B:351:ASN:HD21	1.74	0.51
1:A:91:ARG:HG2	1:A:92:ILE:N	2.24	0.51
1:B:664:THR:HG23	1:B:899:LYS:HD3	1.92	0.51
1:A:26:LEU:HD22	1:A:29:MET:HE3	1.92	0.51
1:B:786:PHE:CD2	1:B:807:LEU:HD11	2.45	0.51
1:B:798:LEU:O	1:B:798:LEU:HD23	2.10	0.51
1:A:145:ASP:C	1:A:146:LYS:HG3	2.35	0.51
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.46	0.51
1:B:21:LYS:HB3	1:B:21:LYS:HZ3	1.75	0.51
1:B:71:ILE:HA	1:B:215:MET:SD	2.51	0.51
1:B:119:VAL:CG1	1:B:175:PHE:HA	2.41	0.51
1:A:18:GLN:HE22	1:A:366:ASP:HB3	1.74	0.51
1:B:103:GLN:O	1:B:105:VAL:N	2.44	0.51
1:B:198:ASP:HB3	1:B:199:TYR:CD1	2.46	0.51
1:B:320:PHE:O	1:B:323:ARG:NH2	2.44	0.51
1:B:655:VAL:HG12	1:B:656:ASN:O	2.11	0.51
1:B:644:ARG:NE	1:B:646:GLU:OE1	2.44	0.51
1:A:258:ASN:C	1:A:258:ASN:OD1	2.53	0.50
1:A:66:THR:O	1:A:67:PHE:HB2	2.11	0.50
1:B:56:ASN:N	1:B:57:PRO:HD2	2.26	0.50
1:B:910:ARG:O	1:B:914:GLU:HB3	2.12	0.50
1:B:98:ASN:ND2	1:B:101:LYS:HB2	2.25	0.50
1:B:279:ARG:HD2	6:B:1218:HOH:O	2.11	0.50
1:B:588:TYR:CD2	1:B:589:MET:CE	2.94	0.50
1:A:574:LEU:O	1:A:578:ILE:HG12	2.10	0.50
1:B:242:LEU:HD12	1:B:245:ILE:HD12	1.93	0.50
1:B:79:ASP:HB3	1:B:148:LEU:CD2	2.41	0.50
1:B:320:PHE:O	1:B:323:ARG:HB2	2.12	0.50
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.11	0.50
1:B:495:MET:HE3	1:B:707:MET:HE3	1.93	0.50
1:B:269:SER:HB3	6:B:1230:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:ILE:HA	1:B:631:HIS:O	2.12	0.49
1:A:98:ASN:HB3	1:A:103:GLN:OE1	2.13	0.49
1:A:645:GLU:O	1:A:645:GLU:HG2	2.13	0.49
1:B:35:THR:O	1:B:38:ASP:HB3	2.12	0.49
1:B:798:LEU:HD23	1:B:798:LEU:C	2.38	0.49
1:A:786:PHE:O	1:A:790:ILE:HG12	2.12	0.49
1:B:451:LYS:NZ	6:B:1238:HOH:O	2.45	0.49
1:B:643:ARG:O	1:B:645:GLU:HG2	2.13	0.49
1:A:541:LEU:HD22	1:A:898:GLY:HA3	1.93	0.49
1:B:549:LYS:HD2	1:B:550:LYS:HB2	1.93	0.49
1:B:671:THR:OG1	1:B:857:THR:HG23	2.13	0.49
1:B:320:PHE:O	1:B:321:GLU:HB2	2.13	0.49
1:B:107:MET:HE1	1:B:451:LYS:HB2	1.95	0.49
1:A:852:ASP:C	1:A:853:ARG:HD2	2.38	0.49
1:B:380:PHE:CD2	1:B:426:ARG:HD3	2.48	0.49
1:B:644:ARG:CD	1:B:646:GLU:OE1	2.61	0.49
1:A:339:VAL:O	1:A:343:GLU:HG2	2.13	0.48
1:A:612:ASP:O	1:A:634:VAL:HG21	2.13	0.48
1:B:541:LEU:HD12	1:B:541:LEU:N	2.28	0.48
1:B:854:LEU:HD12	1:B:855:ASN:N	2.28	0.48
1:A:22:ILE:HD11	1:A:370:SER:HB3	1.94	0.48
1:A:79:ASP:OD1	1:A:148:LEU:CD2	2.57	0.48
1:A:152:PHE:HB3	1:A:206:VAL:HG22	1.95	0.48
1:B:234:THR:HG22	1:B:294:GLU:HG3	1.94	0.48
1:A:69:ARG:O	1:A:70:SER:HB3	2.14	0.48
1:B:105:VAL:HG11	1:B:451:LYS:HE2	1.94	0.48
1:B:320:PHE:CG	1:B:361:VAL:HG11	2.48	0.48
1:A:62:LYS:O	1:A:63:MET:C	2.57	0.48
1:A:390:LEU:HD23	1:A:431:LEU:HD22	1.96	0.48
1:B:143:ILE:HD12	1:B:148:LEU:HD12	1.96	0.48
1:B:786:PHE:O	1:B:790:ILE:HG22	2.13	0.48
1:B:73:ASP:OD1	1:B:73:ASP:C	2.57	0.48
1:A:35:THR:O	1:A:39:ILE:HG12	2.14	0.48
1:A:39:ILE:HD13	1:A:42:ARG:HH21	1.78	0.48
1:A:230:ILE:HD11	1:A:386:VAL:HG11	1.96	0.48
1:B:420:HIS:CD2	1:B:423:TYR:HB2	2.49	0.48
1:B:138:MET:HE2	1:B:144:LYS:HA	1.95	0.47
1:A:124:SER:O	1:A:125:GLN:C	2.57	0.47
1:B:335:ASN:HD22	1:B:337:SER:HB2	1.78	0.47
1:B:480:THR:OG1	1:B:483:MET:HG3	2.14	0.47
1:B:524:GLU:CD	1:B:524:GLU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PHE:C	1:B:323:ARG:NH2	2.72	0.47
1:A:80:PHE:CZ	1:A:458:ALA:HB2	2.50	0.47
1:A:412:VAL:HG12	1:A:413:ASN:N	2.28	0.47
1:B:691:LYS:HB2	6:B:1213:HOH:O	2.14	0.47
1:B:786:PHE:CD1	1:B:786:PHE:C	2.92	0.47
1:A:601:THR:HA	1:A:655:VAL:O	2.14	0.47
1:B:93:LEU:HG	1:B:109:SER:HB2	1.96	0.47
1:B:102:ASN:HA	1:B:103:GLN:C	2.39	0.47
1:A:144:LYS:NZ	1:A:198:ASP:OD2	2.44	0.47
1:A:398:ARG:HB3	1:A:398:ARG:HH11	1.79	0.47
1:B:71:ILE:HB	1:B:72:PRO:HD2	1.97	0.47
1:A:667:TYR:CE2	1:A:668:GLU:OE2	2.67	0.47
1:B:327:GLU:O	1:B:333:LYS:HG3	2.15	0.47
1:A:265:GLY:HA2	1:A:269:SER:HB2	1.96	0.47
1:A:278:ASP:O	1:A:281:ILE:HG22	2.15	0.47
1:A:361:VAL:CG1	1:A:362:GLU:N	2.77	0.47
1:A:29:MET:HE1	1:A:309:ILE:CD1	2.45	0.47
1:A:353:LYS:HA	1:A:368:CYS:SG	2.55	0.47
1:B:718:LEU:C	1:B:720:ASP:N	2.71	0.47
1:A:144:LYS:HZ3	1:A:198:ASP:CG	2.23	0.46
1:A:145:ASP:C	1:A:146:LYS:CG	2.87	0.46
1:A:338:ASP:O	1:A:342:ILE:HD13	2.14	0.46
1:A:405:ARG:NE	1:A:439:ASP:OD2	2.47	0.46
1:A:240:GLU:CB	1:A:257:ILE:HD12	2.46	0.46
1:B:549:LYS:HD2	1:B:550:LYS:N	2.30	0.46
1:B:669:GLU:OE2	1:B:670:PRO:HD2	2.15	0.46
1:B:669:GLU:CD	1:B:670:PRO:HD2	2.40	0.46
1:A:33:ASP:O	1:A:37:ILE:HG12	2.16	0.46
1:B:478:HIS:HB2	6:B:1227:HOH:O	2.16	0.46
1:A:307:ARG:HB2	1:A:334:PHE:HB3	1.98	0.46
1:A:66:THR:HG21	1:A:211:VAL:HG21	1.97	0.46
1:A:155:SER:HB3	1:A:209:ASP:OD2	2.16	0.46
1:A:393:ILE:O	1:A:396:ARG:HB3	2.16	0.46
1:A:320:PHE:CB	1:A:361:VAL:HG11	2.45	0.45
1:A:168:LEU:CD2	1:A:180:VAL:HG12	2.46	0.45
1:A:515:PHE:HA	1:A:703:MET:SD	2.56	0.45
1:A:518:ARG:NH2	1:A:907:VAL:HG22	2.31	0.45
1:A:518:ARG:HH22	1:A:907:VAL:HG22	1.81	0.45
1:A:619:TRP:HB3	1:A:623:PHE:O	2.16	0.45
1:A:782:PHE:CD1	1:A:786:PHE:CE1	3.04	0.45
1:A:913:THR:O	1:A:914:GLU:OE2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HD11	1:B:386:VAL:HG11	1.97	0.45
1:B:550:LYS:HD2	1:B:550:LYS:HA	1.66	0.45
1:A:25:TYR:HD2	1:A:313:MET:HE3	1.79	0.45
1:A:367:ASP:O	1:A:371:VAL:HG23	2.17	0.45
1:B:772:ILE:CG2	1:B:777:LYS:HD2	2.47	0.45
1:A:231:GLY:O	1:A:298:SER:HB2	2.17	0.45
1:A:342:ILE:O	1:A:342:ILE:CG2	2.65	0.45
1:A:354:GLU:O	1:A:358:ARG:HG3	2.17	0.45
1:A:419:THR:O	1:A:420:HIS:C	2.59	0.45
1:A:541:LEU:N	1:A:541:LEU:HD12	2.31	0.45
1:A:663:MET:HG3	1:A:904:ILE:HD11	1.99	0.45
1:A:565:GLU:HG3	1:A:566:ILE:H	1.67	0.45
1:A:202:ASN:C	1:A:202:ASN:ND2	2.72	0.45
1:A:718:LEU:C	1:A:720:ASP:H	2.23	0.45
1:B:323:ARG:HB2	1:B:323:ARG:HE	1.62	0.45
1:B:854:LEU:HD12	1:B:855:ASN:H	1.82	0.45
1:A:655:VAL:HG12	1:A:656:ASN:O	2.17	0.45
1:A:62:LYS:HB3	1:A:64:LEU:HD21	1.98	0.45
1:A:546:ARG:O	1:A:551:ARG:HA	2.17	0.45
1:B:53:ARG:HB3	1:B:246:ASP:HB3	1.99	0.45
1:B:146:LYS:HB2	1:B:148:LEU:HG	1.99	0.45
1:B:593:GLY:N	1:B:594:PRO:CD	2.80	0.45
1:A:23:ASP:OD1	1:A:373:HIS:NE2	2.39	0.44
1:B:376:THR:O	1:B:380:PHE:HB2	2.16	0.44
1:B:738:LYS:HE3	6:B:1107:HOH:O	2.17	0.44
1:A:134:LEU:O	1:A:138:MET:HG3	2.17	0.44
1:A:196:ARG:C	1:A:198:ASP:N	2.74	0.44
1:A:196:ARG:C	1:A:198:ASP:H	2.25	0.44
1:B:261:TRP:CD1	1:B:261:TRP:C	2.95	0.44
1:B:882:LEU:C	1:B:884:PRO:HD3	2.42	0.44
1:A:119:VAL:HG13	1:A:175:PHE:CG	2.52	0.44
1:B:801:ARG:O	1:B:805:GLN:HB2	2.17	0.44
1:A:853:ARG:HH11	1:A:853:ARG:CG	2.29	0.44
1:B:271:GLU:OE2	1:B:274:ARG:HD3	2.18	0.44
1:B:323:ARG:HH11	1:B:362:GLU:HG3	1.82	0.44
1:A:554:GLU:OE2	1:A:556:HIS:HE1	2.01	0.44
1:B:121:GLY:O	1:B:177:ALA:HA	2.18	0.44
1:A:602:PHE:CE2	1:A:633:VAL:HG11	2.53	0.44
1:A:798:LEU:C	1:A:798:LEU:CD2	2.89	0.44
1:A:152:PHE:O	1:A:206:VAL:HA	2.18	0.44
1:A:786:PHE:CD1	1:A:786:PHE:C	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:O	1:B:23:ASP:HB2	2.17	0.44
1:A:56:ASN:N	1:A:57:PRO:CD	2.80	0.43
1:A:320:PHE:HB3	1:A:361:VAL:HG11	1.96	0.43
1:B:105:VAL:HG12	1:B:107:MET:HE2	2.00	0.43
1:B:112:TYR:OH	1:B:137:PHE:HB2	2.18	0.43
1:A:327:GLU:N	1:A:327:GLU:OE1	2.51	0.43
1:A:709:TRP:C	1:A:709:TRP:CD1	2.95	0.43
1:B:451:LYS:O	1:B:455:MET:HG2	2.18	0.43
1:B:677:ILE:O	1:B:682:SER:HA	2.18	0.43
1:A:104:ASN:HD22	1:A:104:ASN:HA	1.58	0.43
1:A:422:GLN:O	1:A:426:ARG:HG3	2.17	0.43
1:B:281:ILE:HG12	1:B:308:LEU:HD12	2.00	0.43
1:A:405:ARG:HG3	1:A:437:ASP:O	2.18	0.43
1:A:739:GLN:O	1:A:743:LYS:HG3	2.18	0.43
1:B:147:LYS:O	1:B:147:LYS:HG2	2.19	0.43
1:B:644:ARG:O	1:B:645:GLU:HG3	2.18	0.43
1:A:277:PHE:CE1	1:A:309:ILE:HA	2.53	0.43
1:A:420:HIS:CD2	1:A:422:GLN:H	2.36	0.43
1:B:718:LEU:HD22	1:B:721:ILE:HD11	2.00	0.43
1:B:603:SER:HB2	2:B:1003:BGC:H4	2.01	0.43
1:A:21:LYS:HB2	1:A:21:LYS:HZ3	1.82	0.43
1:A:67:PHE:HA	1:A:255:MET:HE2	1.99	0.43
1:A:118:ILE:CG2	1:A:126:LEU:HA	2.49	0.43
1:A:176:LYS:HD2	1:A:286:LEU:HG	2.01	0.43
1:A:242:LEU:C	1:A:244:HIS:H	2.25	0.43
1:B:709:TRP:CD1	1:B:709:TRP:C	2.96	0.43
1:A:650:ASP:OD2	1:A:912:ARG:NH2	2.51	0.43
1:B:345:ASN:CA	1:B:346:LYS:CB	2.96	0.43
1:A:143:ILE:HD13	1:A:148:LEU:HD11	2.00	0.43
1:A:280:GLU:HG3	1:A:283:ARG:NH2	2.33	0.43
1:A:532:ASP:O	1:A:538:PHE:HA	2.19	0.43
1:A:193:ILE:HD13	1:A:201:ALA:HB3	2.00	0.43
1:B:25:TYR:OH	1:B:312:LYS:HG3	2.19	0.43
1:B:763:LYS:HG3	1:B:772:ILE:HD11	2.00	0.43
1:B:222:GLN:HA	1:B:222:GLN:NE2	2.34	0.42
1:B:321:GLU:HB2	1:B:323:ARG:NH2	2.31	0.42
1:A:274:ARG:NH1	1:A:292:LEU:HD22	2.34	0.42
1:A:519:THR:HB	1:A:520:PRO:HD2	2.00	0.42
1:A:667:TYR:CD2	1:A:668:GLU:HG2	2.54	0.42
1:A:80:PHE:CE2	1:A:458:ALA:HA	2.54	0.42
1:B:532:ASP:HB3	1:B:539:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:LEU:C	1:B:720:ASP:H	2.27	0.42
1:A:763:LYS:CG	1:A:772:ILE:HD11	2.43	0.42
1:B:66:THR:OG1	1:B:256:CYS:HB3	2.18	0.42
1:A:235:ASN:HA	1:A:261:TRP:CD1	2.55	0.42
1:B:361:VAL:CG1	1:B:362:GLU:N	2.82	0.42
1:B:420:HIS:CD2	1:B:422:GLN:H	2.37	0.42
1:B:853:ARG:HA	1:B:885:LYS:O	2.20	0.42
1:A:167:ILE:N	1:A:167:ILE:CD1	2.83	0.42
1:A:74:GLY:O	1:A:99:HIS:HD2	2.03	0.42
1:A:141:ARG:N	1:A:141:ARG:HD2	2.35	0.42
1:A:589:MET:HA	1:A:589:MET:HE2	2.02	0.42
3:A:1002:G16:O3P	3:A:1002:G16:H5	2.20	0.42
1:B:104:ASN:H	1:B:104:ASN:ND2	2.18	0.42
1:B:320:PHE:O	1:B:323:ARG:NE	2.53	0.42
1:B:679:GLY:O	1:B:680:THR:C	2.62	0.42
1:B:342:ILE:O	1:B:342:ILE:HG22	2.20	0.42
1:B:652:VAL:HB	1:B:905:THR:HG23	2.02	0.42
1:B:763:LYS:CG	1:B:772:ILE:HD11	2.50	0.42
1:A:534:GLY:HA3	1:A:603:SER:HB2	2.02	0.42
1:A:811:SER:HB2	1:A:815:ASP:HB2	2.01	0.42
1:B:120:HIS:NE2	1:B:174:ARG:O	2.52	0.42
1:B:554:GLU:OE2	1:B:556:HIS:HE1	2.03	0.42
1:B:589:MET:HE2	1:B:589:MET:HA	2.01	0.42
1:A:143:ILE:C	1:A:145:ASP:O	2.62	0.42
1:A:521:ASP:C	1:A:521:ASP:OD1	2.63	0.42
1:A:166:ALA:HB3	1:A:185:VAL:CG2	2.50	0.41
1:A:320:PHE:HB3	1:A:361:VAL:HG13	2.00	0.41
1:B:501:LYS:CB	1:B:695:MET:SD	3.08	0.41
1:A:44:ARG:HA	1:A:47:MET:CE	2.50	0.41
1:A:44:ARG:HG2	1:A:392:ALA:HB1	2.02	0.41
1:A:202:ASN:C	1:A:202:ASN:HD22	2.29	0.41
1:A:644:ARG:HG2	1:A:646:GLU:HG3	2.02	0.41
1:B:176:LYS:HB3	6:B:1206:HOH:O	2.20	0.41
1:A:811:SER:HB2	1:A:815:ASP:CB	2.51	0.41
1:A:79:ASP:CG	1:A:148:LEU:HD22	2.45	0.41
1:A:120:HIS:NE2	1:A:174:ARG:O	2.52	0.41
1:A:420:HIS:CD2	1:A:423:TYR:HB2	2.56	0.41
1:B:105:VAL:HG11	1:B:451:LYS:HG3	2.01	0.41
1:A:342:ILE:CG2	1:A:372:GLN:HG3	2.51	0.41
1:B:342:ILE:O	1:B:342:ILE:CG2	2.68	0.41
1:B:346:LYS:CG	1:B:347:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:GLY:HA2	3:B:1004:G16:O6	2.20	0.41
1:B:496:GLU:OE2	1:B:500:ARG:NH1	2.44	0.41
1:A:148:LEU:HA	1:A:149:PRO:HD3	1.90	0.41
1:A:26:LEU:HD21	1:A:309:ILE:CG2	2.51	0.41
1:A:281:ILE:HG23	1:A:282:ASP:N	2.36	0.41
1:A:520:PRO:HD3	1:A:663:MET:CE	2.51	0.41
1:A:595:ARG:HG3	1:A:648:ASP:O	2.21	0.41
1:A:665:CYS:HB3	1:A:891:LEU:HD23	2.03	0.41
1:A:693:VAL:HA	6:A:1207:HOH:O	2.21	0.41
1:A:767:LEU:HG	1:A:818:LEU:CD2	2.41	0.41
1:B:510:LYS:O	1:B:511:MET:C	2.64	0.41
1:B:545:ILE:HD13	1:B:903:LEU:CD2	2.50	0.41
1:A:62:LYS:HB3	1:A:64:LEU:CD2	2.51	0.41
1:A:319:LEU:O	1:A:321:GLU:O	2.39	0.41
1:A:786:PHE:CD1	1:A:787:LEU:N	2.89	0.41
1:A:342:ILE:HG13	1:A:352:ALA:HB2	2.02	0.40
1:A:356:LEU:CD1	1:A:371:VAL:HG21	2.49	0.40
1:B:384:ASN:HD22	1:B:384:ASN:HA	1.67	0.40
1:B:884:PRO:C	1:B:886:CYS:H	2.28	0.40
1:A:101:LYS:O	1:A:102:ASN:CB	2.70	0.40
1:A:167:ILE:HA	1:A:183:ALA:O	2.22	0.40
1:A:219:TYR:C	1:A:219:TYR:CD1	2.99	0.40
1:B:141:ARG:O	1:B:143:ILE:HG23	2.22	0.40
1:B:204:VAL:CG2	1:B:457:THR:HG23	2.52	0.40
1:A:321:GLU:HB3	1:A:322:GLY:H	1.53	0.40
1:B:97:VAL:HA	1:B:104:ASN:O	2.21	0.40
1:B:405:ARG:HB3	1:B:405:ARG:NH1	2.29	0.40
1:B:564:ILE:O	1:B:565:GLU:C	2.64	0.40
1:A:126:LEU:O	1:A:129:HIS:HB3	2.21	0.40
1:A:353:LYS:CA	1:A:368:CYS:SG	3.10	0.40
1:A:712:PHE:HB3	1:A:741:TYR:HB2	2.03	0.40
1:A:855:ASN:OD1	1:A:887:ASN:HB3	2.21	0.40
1:A:857:THR:HA	1:A:889:SER:O	2.21	0.40
1:B:98:ASN:O	1:B:101:LYS:O	2.39	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%)	849 (95%)	45 (5%)	3 (0%)	36	50
1	B	897/917 (98%)	856 (95%)	37 (4%)	4 (0%)	30	43
All	All	1794/1834 (98%)	1705 (95%)	82 (5%)	7 (0%)	30	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	GLU
1	B	104	ASN
1	B	346	LYS
1	A	146	LYS
1	A	913	THR
1	A	105	VAL
1	B	593	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%)	753 (97%)	21 (3%)	39	62
1	B	774/788 (98%)	747 (96%)	27 (4%)	32	53
All	All	1548/1576 (98%)	1500 (97%)	48 (3%)	35	57

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	80	PHE
1	A	93	LEU
1	A	101	LYS
1	A	104	ASN
1	A	242	LEU
1	A	281	ILE
1	A	321	GLU
1	A	437	ASP
1	A	481	LYS
1	A	531	LEU
1	A	541	LEU
1	A	542	LEU
1	A	550	LYS
1	A	709	TRP
1	A	769	ARG
1	A	786	PHE
1	A	843	ASP
1	A	853	ARG
1	A	857	THR
1	A	914	GLU
1	B	21	LYS
1	B	23	ASP
1	B	99	HIS
1	B	102	ASN
1	B	103	GLN
1	B	242	LEU
1	B	281	ILE
1	B	320	PHE
1	B	323	ARG
1	B	337	SER
1	B	346	LYS
1	B	405	ARG
1	B	407	ARG
1	B	424	SER
1	B	481	LYS
1	B	550	LYS
1	B	564	ILE
1	B	626	THR
1	B	645	GLU
1	B	709	TRP
1	B	721	ILE
1	B	769	ARG

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Mol	Chain	Res	Type
1	B	777	LYS
1	B	797	LEU
1	B	805	GLN
1	B	843	ASP
1	B	914	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	104	ASN
1	A	125	GLN
1	A	129	HIS
1	A	159	GLN
1	A	202	ASN
1	A	222	GLN
1	A	223	HIS
1	A	345	ASN
1	A	384	ASN
1	A	400	ASN
1	A	413	ASN
1	A	420	HIS
1	A	466	GLN
1	A	556	HIS
1	A	631	HIS
1	A	771	GLN
1	A	805	GLN
1	A	832	GLN
1	A	848	ASN
1	A	877	GLN
1	A	887	ASN
1	B	96	GLN
1	B	102	ASN
1	B	104	ASN
1	B	202	ASN
1	B	222	GLN
1	B	350	HIS
1	B	351	ASN
1	B	384	ASN
1	B	400	ASN
1	B	420	HIS
1	B	466	GLN

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Mol	Chain	Res	Type
1	B	506	ASN
1	B	556	HIS
1	B	799	GLN
1	B	805	GLN
1	B	806	GLN
1	B	810	ASN
1	B	832	GLN
1	B	887	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 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	B	1003	-	12,12,12	0.42	0	17,17,17	1.27	2 (11%)
2	BGC	A	1001	-	12,12,12	0.56	0	17,17,17	1.05	2 (11%)
3	G16	B	1002	-	19,20,20	0.54	0	30,31,31	0.97	1 (3%)
3	G16	A	1004	-	19,20,20	0.57	0	30,31,31	0.94	0
5	CIT	B	1007	-	12,12,12	1.06	0	17,17,17	1.42	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G16	B	1004	-	19,20,20	0.52	0	30,31,31	0.97	0
3	G16	A	1002	-	19,20,20	0.56	0	30,31,31	0.91	0
5	CIT	A	1007	-	12,12,12	1.08	0	17,17,17	1.43	1 (5%)
2	BGC	B	1001	-	12,12,12	0.33	0	17,17,17	0.85	1 (5%)
2	BGC	A	1003	-	12,12,12	0.38	0	17,17,17	1.19	2 (11%)

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	B	1003	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
3	G16	B	1002	-	-	1/11/31/31	0/1/1/1
3	G16	A	1004	-	-	1/11/31/31	0/1/1/1
5	CIT	B	1007	-	-	10/16/16/16	-
3	G16	B	1004	-	-	2/11/31/31	0/1/1/1
3	G16	A	1002	-	-	1/11/31/31	0/1/1/1
5	CIT	A	1007	-	-	2/16/16/16	-
2	BGC	B	1001	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1003	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1007	CIT	O6-C6-C3	3.75	120.33	113.14
5	B	1007	CIT	O6-C6-C3	3.68	120.20	113.14
2	A	1003	BGC	C1-O5-C5	-3.14	107.57	113.65
2	B	1003	BGC	C1-O5-C5	-3.08	107.69	113.65
2	A	1001	BGC	C1-O5-C5	-3.06	107.73	113.65
2	B	1003	BGC	O5-C1-C2	-2.94	105.13	110.30
2	A	1003	BGC	O5-C1-C2	-2.86	105.26	110.30
2	B	1001	BGC	C1-O5-C5	-2.15	109.48	113.65
2	A	1001	BGC	O5-C1-C2	-2.12	106.58	110.30
3	B	1002	G16	O5-C5-C6	2.01	110.68	106.69

There are no chirality outliers.

All (17) torsion outliers are listed below:

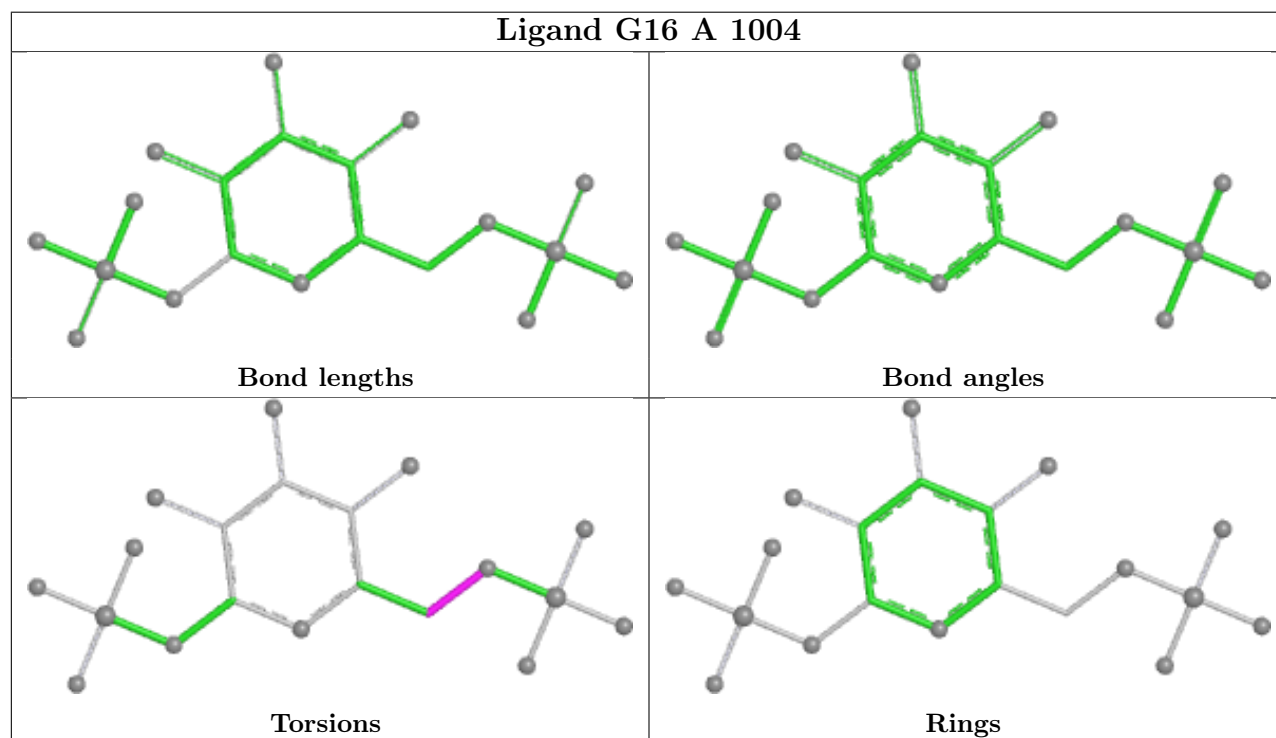
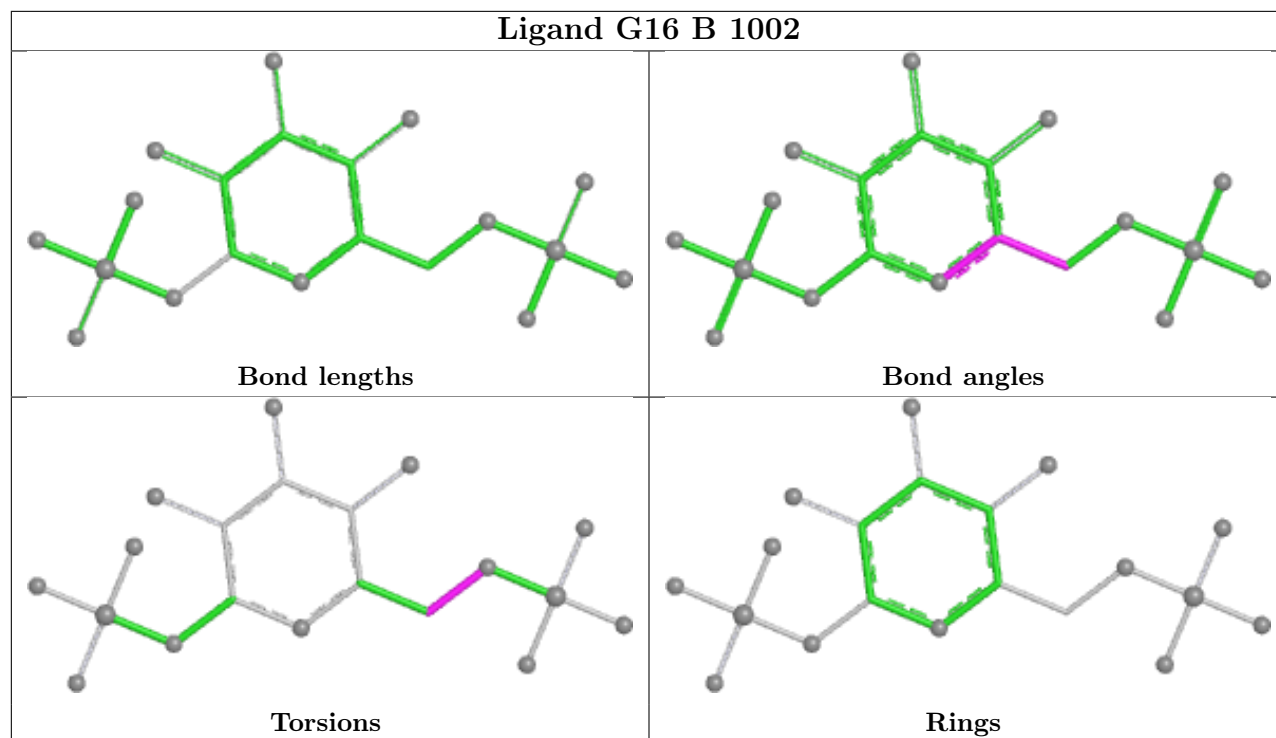
Mol	Chain	Res	Type	Atoms
5	B	1007	CIT	C2-C3-C4-C5
5	B	1007	CIT	O7-C3-C4-C5
5	B	1007	CIT	C6-C3-C4-C5
5	B	1007	CIT	O7-C3-C6-O5
5	B	1007	CIT	O7-C3-C6-O6
5	B	1007	CIT	C4-C3-C6-O5
5	B	1007	CIT	C4-C3-C6-O6
3	A	1002	G16	C5-C6-O6-P
3	B	1004	G16	C5-C6-O6-P
5	B	1007	CIT	C1-C2-C3-C6
3	A	1004	G16	C5-C6-O6-P
3	B	1002	G16	C5-C6-O6-P
5	B	1007	CIT	C1-C2-C3-O7
5	B	1007	CIT	C1-C2-C3-C4
5	A	1007	CIT	C6-C3-C4-C5
5	A	1007	CIT	C2-C3-C4-C5
3	B	1004	G16	C2-C1-O1-P'

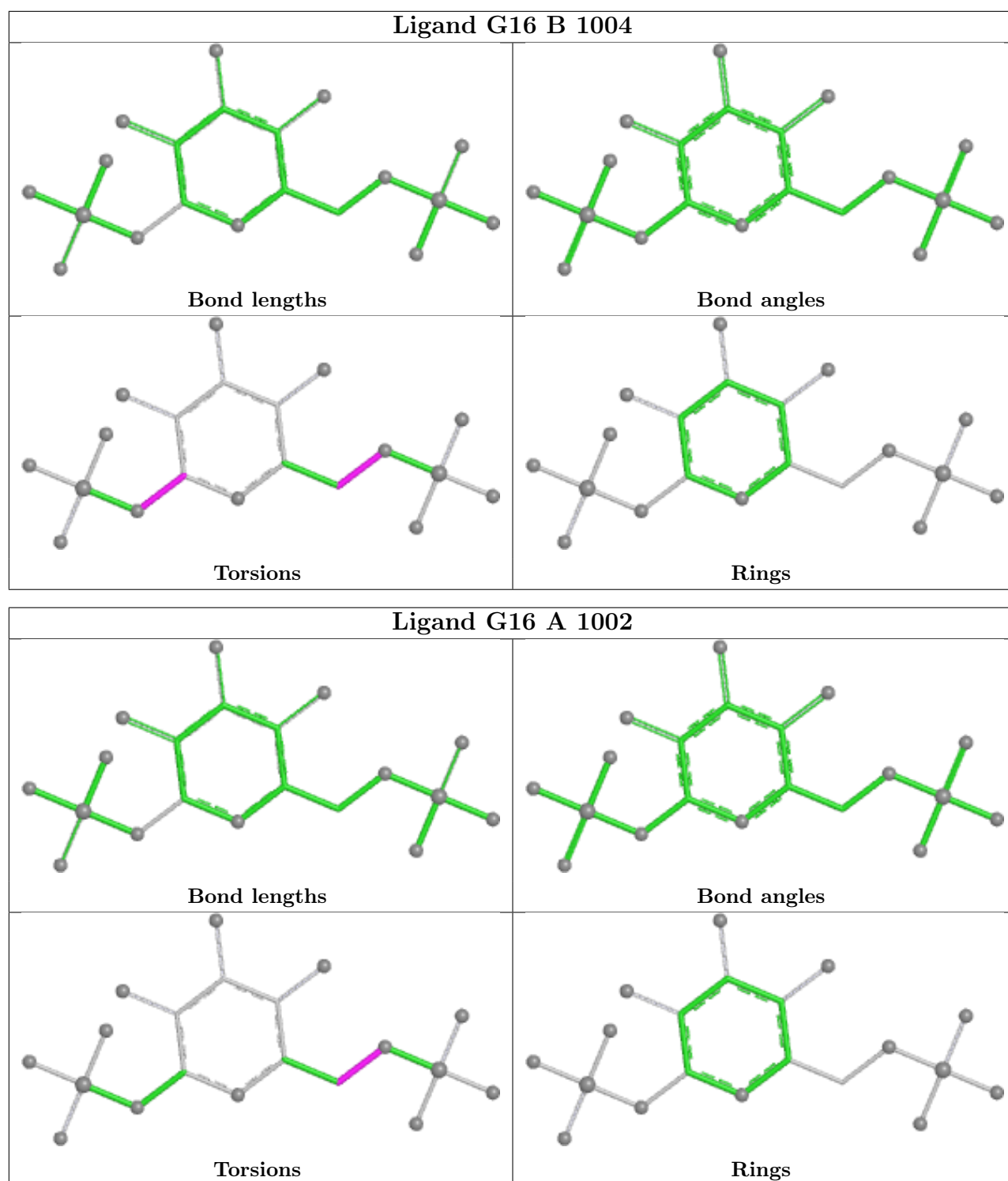
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1003	BGC	2	0
5	B	1007	CIT	1	0
3	B	1004	G16	1	0
3	A	1002	G16	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

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%)	0.66	59 (6%)	24 20	26, 51, 80, 119	0
1	B	899/917 (98%)	0.64	60 (6%)	24 20	27, 51, 80, 118	0
All	All	1798/1834 (98%)	0.65	119 (6%)	24 20	26, 51, 80, 119	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	LEU	3.9
1	B	100	GLU	3.9
1	A	105	VAL	3.7
1	B	99	HIS	3.7
1	A	786	PHE	3.6
1	A	17	ASP	3.6
1	A	277	PHE	3.5
1	A	447	SER	3.4
1	A	427	PHE	3.3
1	A	93	LEU	3.3
1	A	21	LYS	3.3
1	A	223	HIS	3.2
1	B	548	GLY	3.2
1	B	564	ILE	3.1
1	B	591	ILE	3.1
1	B	147	LYS	3.1
1	B	18	GLN	3.0
1	A	443	LEU	3.0
1	A	449	SER	3.0
1	A	314	ALA	3.0
1	A	361	VAL	3.0
1	B	19	VAL	3.0
1	B	104	ASN	3.0
1	A	318	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	720	ASP	2.9
1	B	786	PHE	2.9
1	B	101	LYS	2.9
1	B	361	VAL	2.9
1	A	27	TYR	2.9
1	B	319	LEU	2.9
1	B	199	TYR	2.8
1	B	401	LYS	2.8
1	B	335	ASN	2.8
1	A	19	VAL	2.8
1	B	586	LEU	2.8
1	A	423	TYR	2.7
1	B	137	PHE	2.7
1	A	82	ALA	2.7
1	B	565	GLU	2.7
1	B	324	ILE	2.7
1	B	566	ILE	2.7
1	A	349	LEU	2.7
1	A	911	LEU	2.7
1	B	649	LEU	2.7
1	B	913	THR	2.7
1	B	103	GLN	2.7
1	A	322	GLY	2.6
1	A	341	ALA	2.6
1	B	24	LYS	2.6
1	A	80	PHE	2.6
1	A	198	ASP	2.5
1	B	593	GLY	2.5
1	A	103	GLN	2.5
1	B	97	VAL	2.5
1	B	109	SER	2.5
1	A	437	ASP	2.5
1	B	27	TYR	2.5
1	B	550	LYS	2.4
1	B	102	ASN	2.4
1	B	117	ASN	2.4
1	A	406	LEU	2.4
1	B	644	ARG	2.4
1	B	567	MET	2.4
1	B	21	LYS	2.4
1	A	18	GLN	2.4
1	A	16	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	387	ALA	2.4
1	A	668	GLU	2.4
1	A	438	SER	2.3
1	A	273	ILE	2.3
1	B	771	GLN	2.3
1	A	311	VAL	2.3
1	B	98	ASN	2.3
1	A	347	GLU	2.3
1	A	913	THR	2.3
1	A	89	SER	2.3
1	A	371	VAL	2.3
1	A	143	ILE	2.3
1	B	406	LEU	2.3
1	A	909	VAL	2.3
1	A	700	GLN	2.3
1	A	342	ILE	2.3
1	A	483	MET	2.3
1	B	427	PHE	2.3
1	B	426	ARG	2.3
1	A	20	LYS	2.2
1	B	547	SER	2.2
1	B	17	ASP	2.2
1	A	362	GLU	2.2
1	A	301	TYR	2.2
1	B	222	GLN	2.2
1	A	448	GLY	2.2
1	A	355	ILE	2.2
1	B	642	LYS	2.2
1	A	217	CYS	2.2
1	A	849	ARG	2.1
1	B	532	ASP	2.1
1	A	125	GLN	2.1
1	B	652	VAL	2.1
1	B	31	LEU	2.1
1	B	318	LEU	2.1
1	A	564	ILE	2.1
1	B	549	LYS	2.1
1	B	852	ASP	2.1
1	A	380	PHE	2.1
1	B	119	VAL	2.1
1	B	346	LYS	2.1
1	B	96	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	55	PHE	2.0
1	B	55	PHE	2.0
1	B	314	ALA	2.0
1	A	450	GLY	2.0
1	B	402	GLY	2.0
1	A	324	ILE	2.0
1	B	363	PRO	2.0
1	B	404	PRO	2.0
1	A	320	PHE	2.0
1	B	668	GLU	2.0
1	B	355	ILE	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 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($\text{\AA}^2$)	Q<0.9
5	CIT	B	1007	13/13	0.59	0.23	102,103,104,104	0
5	CIT	A	1007	13/13	0.69	0.16	105,106,106,106	0
2	BGC	A	1001	12/12	0.82	0.12	43,46,47,49	0
3	G16	A	1002	20/20	0.88	0.11	51,53,55,55	0
2	BGC	B	1003	12/12	0.89	0.10	35,37,37,40	0
2	BGC	A	1003	12/12	0.89	0.11	33,35,35,38	0
4	NA	B	1005	1/1	0.90	0.08	53,53,53,53	0
4	NA	A	1006	1/1	0.91	0.06	54,54,54,54	0
2	BGC	B	1001	12/12	0.92	0.12	41,43,44,46	0
4	NA	A	1005	1/1	0.92	0.14	55,55,55,55	0
4	NA	B	1006	1/1	0.94	0.08	53,53,53,53	0
3	G16	B	1002	20/20	0.96	0.09	48,50,53,53	0

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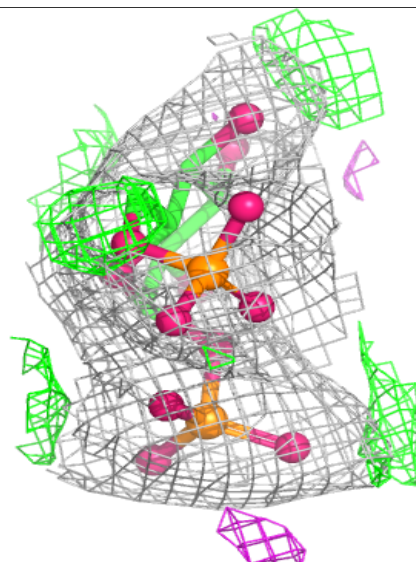
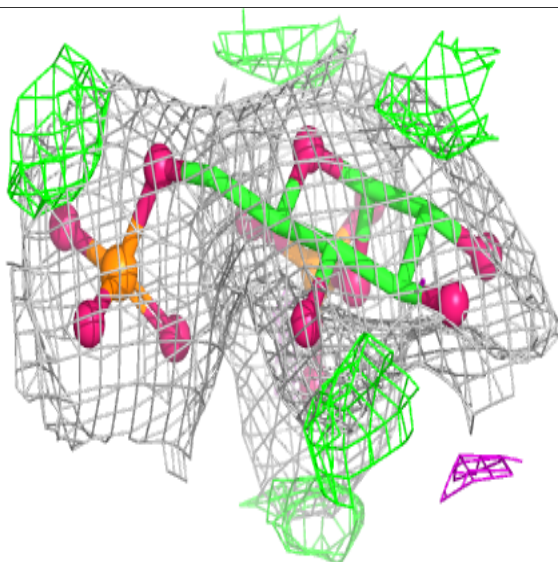
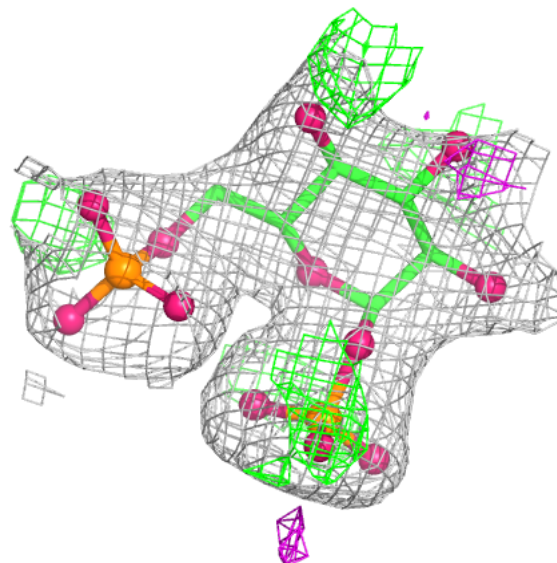
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	G16	B	1004	20/20	0.96	0.07	30,32,35,35	0
3	G16	A	1004	20/20	0.98	0.06	28,30,33,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

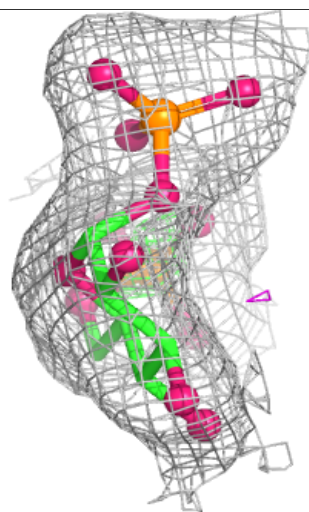
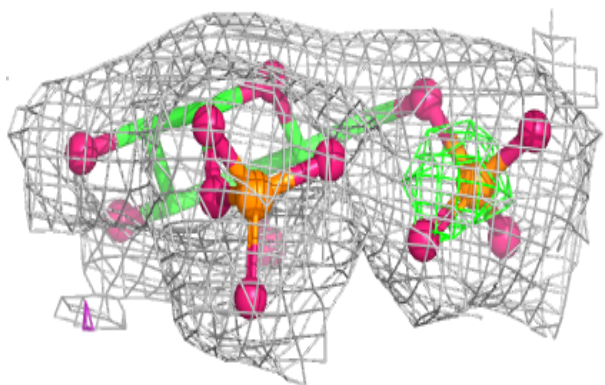
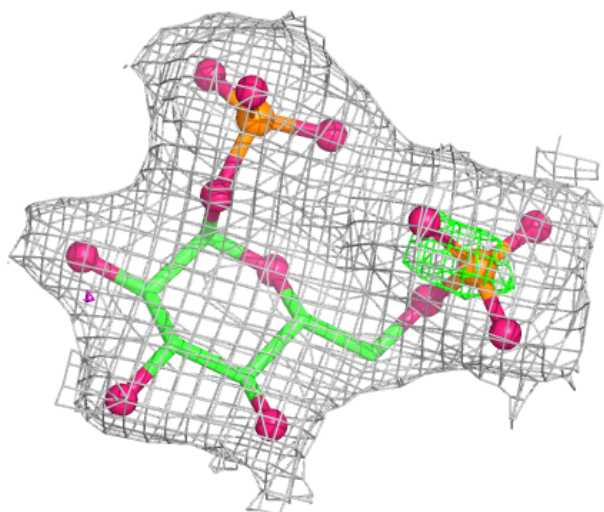
Electron density around G16 A 1002:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



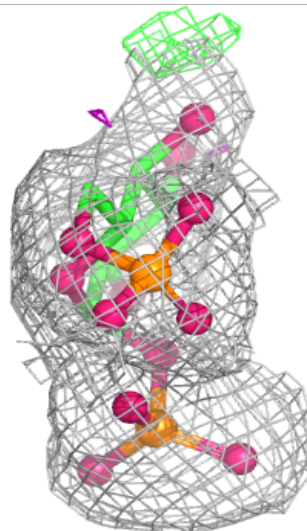
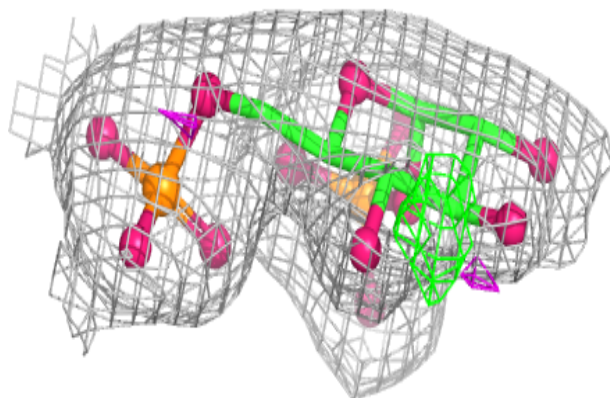
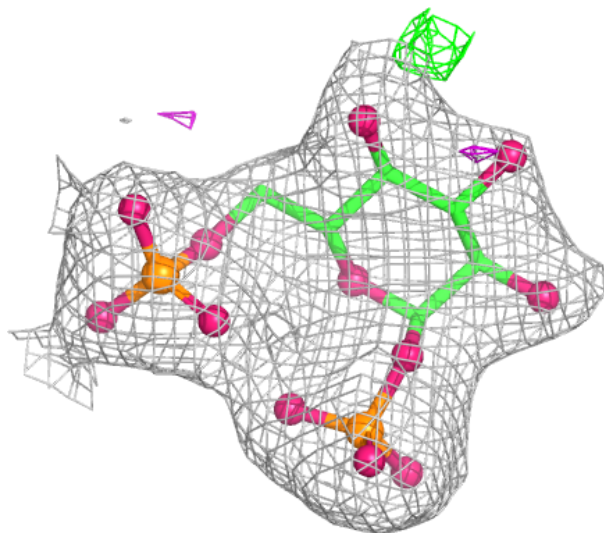
Electron density around G16 B 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



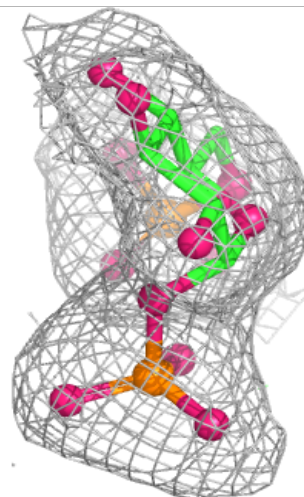
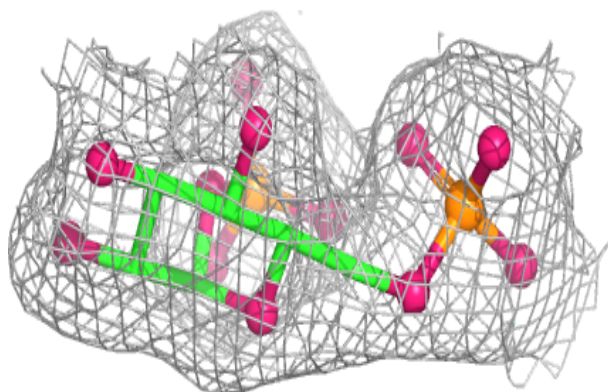
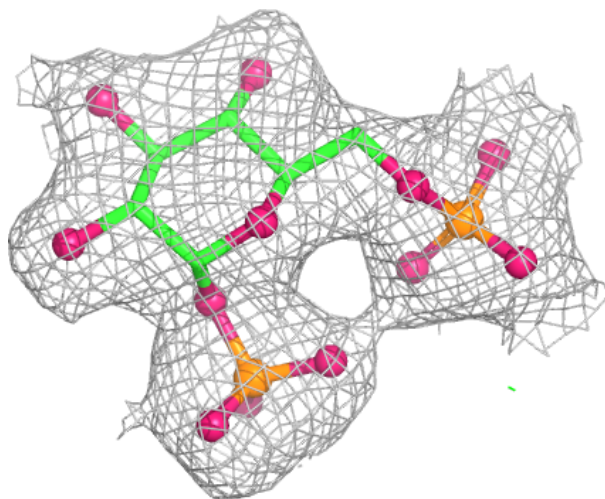
Electron density around G16 B 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G16 A 1004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.