



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 4FPA / pdb_00004fpa
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 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

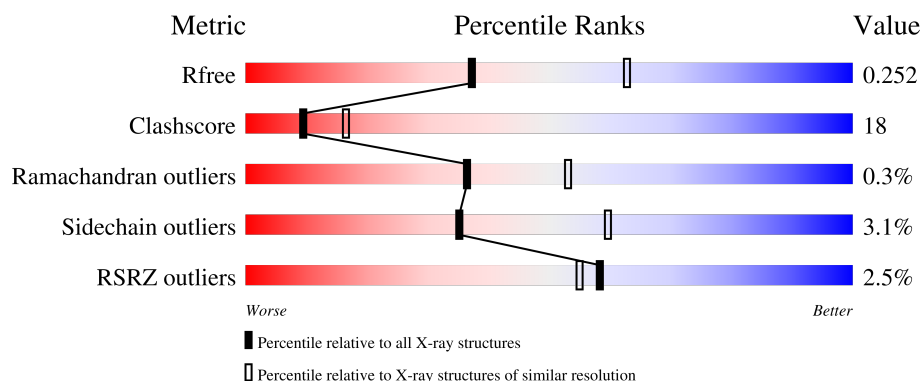
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 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	3% 66% 30% ..
1	B	917	2% 70% 27% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14391 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.

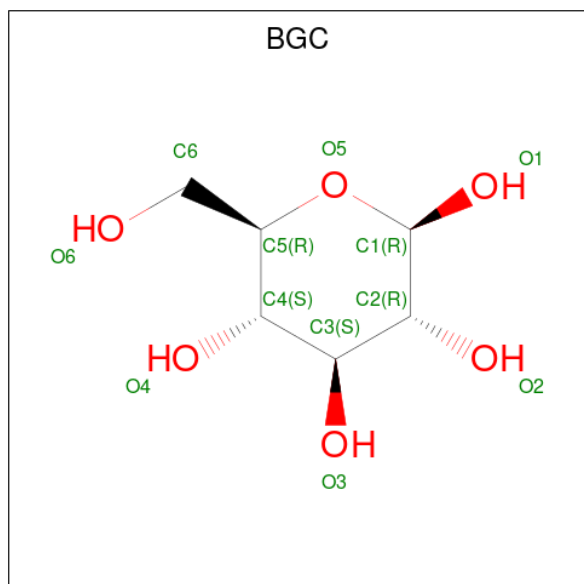
- Molecule 1 is a protein called Hexokinase-1.

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).



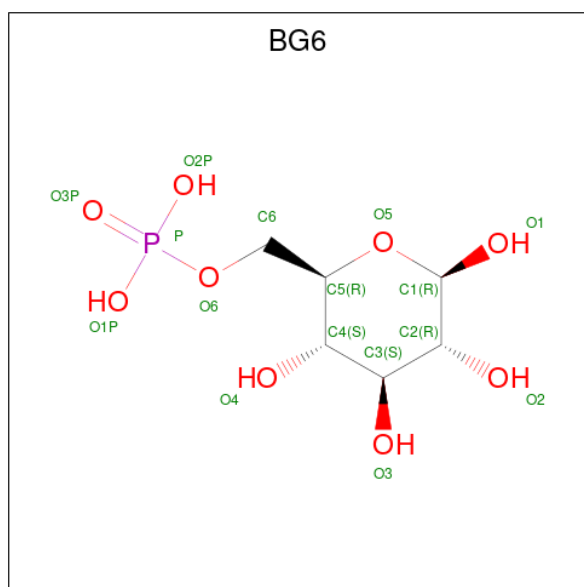
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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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 6-O-phosphono-beta-D-glucopyranose (CCD ID: BG6) (formula: $C_6H_{13}O_9P$).

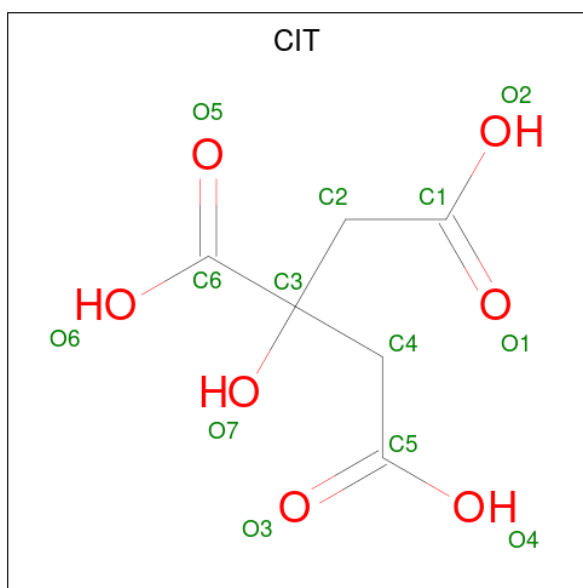


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is SODIUM ION (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		

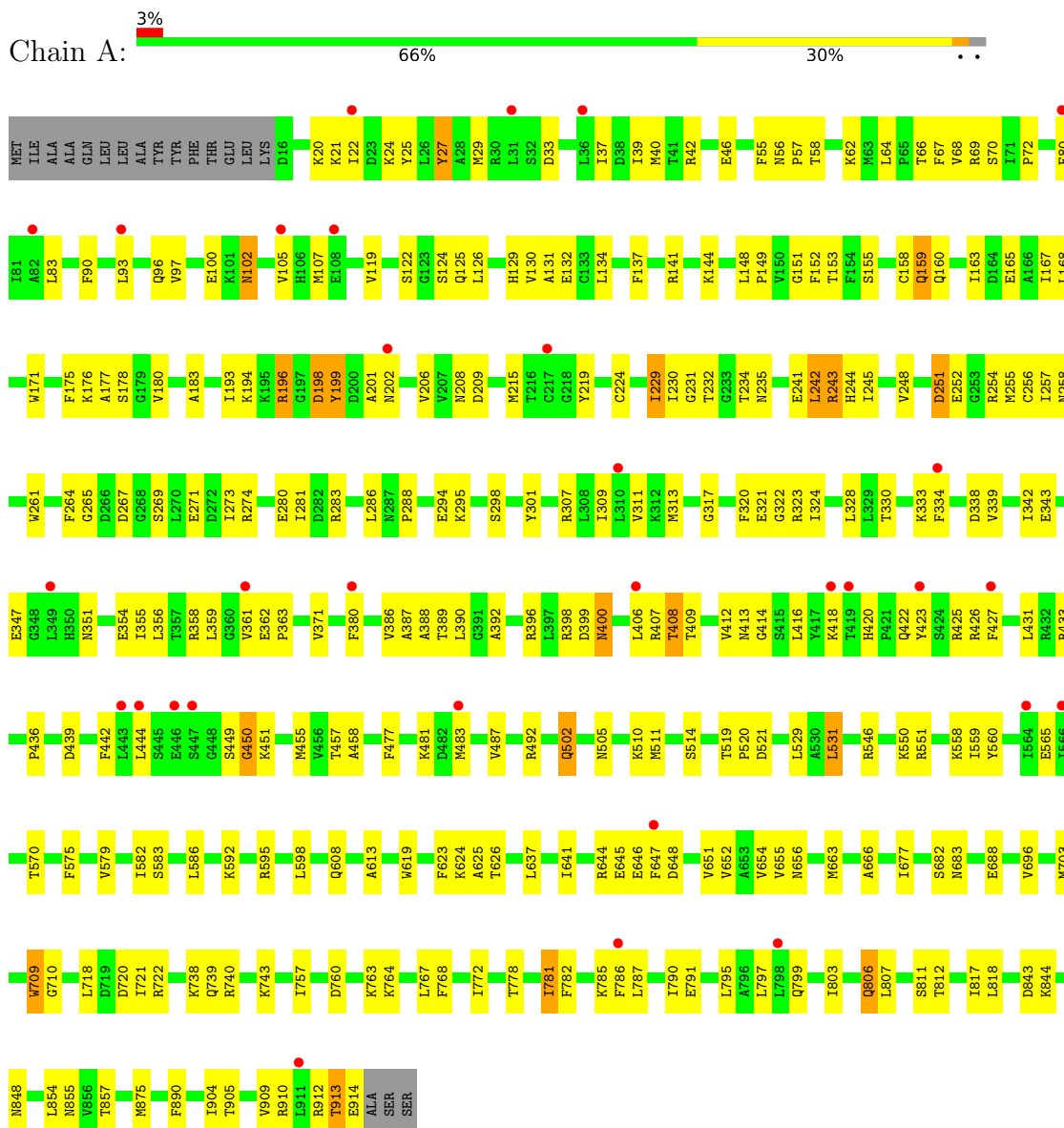
- Molecule 6 is water.

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

3 Residue-property plots [i](#)

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



V860	D861	G862	D895	K899	L903	I904	V907	R910	L911	E914	ALA	SER	SER	R727	N735	K738	D760	F761	T762	K763	K764	L767	F768	R769	G770	G771	I772	K777	T778	I781	F782	F786	L795	A796	L797	L798	Q799	I803	L804	Q805	Q806	L807	N810	S811	T812	C813	I817	L818	D843	R849	D852	L854	N855	V856	T857	V858	G859	M511	L512	P513	S514	R518	D521	G522	T523	E524	L531	G534	R539	V540	L541	T545	N557	K558	I559	P563	I564	E565	G567	E574	F575	I578	V579	I582	S583	D587	Y588	M589	K592	R595	L598	F602	S603	F604	P605	G614	W619	K624	R381	V386	I393	R396	M400	R405	L406	R407	K418	T419	H420	P421	Q422	Y423	S424	R425	R426	F427	L431	P436	D437	F442	L443	L444	S449	T457	L463	E471	H476	L479	T480	M483	R490	M491	E494	M495	K501	M505	K510	R125	L134	G135	D136	F137	M138	K142	I143	K144	D145	K146	L148	F152	T153	F154	Q160	E165	A166	I167	L168	V180	T58	E181	G182	A183	D184	V185	I193	K194	K195	D198	A201	V204	G212	M215	I230	C256	W261	G265	D266	D267	G268	S269	L270	E271	R274	D278	E279	E280	I281	R283	V306	K312	E316	L319	F320	E321	G322	R323	I324	T325	T330	K333	F334	I342	E347	G348	N351	A352	R353	I355	L356	T357	R358	L359	G360	V361	E362	P363	D366	V369	S370	V371	Q372	T376	F380	D17	Q18	V19	M29	T35	D38	M56	P57	T58	A59	T66	F67	V68	I71	P72	D73	E76	D79	L83	D84	L93	R94	N98	H99	E100	K101	N102	Q103	N104	M107	S122
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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) 98.8 (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 0.235 , 0.252	Depositor DCC
R_{free} test set	4185 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k 0.000 for -h,l,k 0.019 for h,-k,-l	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.

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 [i](#)

5.1 Standard geometry [i](#)

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

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%)	0.76	1/9606 (0.0%)
1	B	0.32	0/7138	0.74	0/9606
All	All	0.33	1/14276 (0.0%)	0.75	1/19212 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	ALA	C-O	5.71	1.30	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ASP	N-CA-C	-5.24	105.98	114.09

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7032	0	7092	255	0
1	B	7032	0	7092	261	0
2	A	24	0	24	2	0
2	B	24	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	A	77	0	0	4	0
6	B	108	0	0	6	0
All	All	14391	0	14286	511	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 18.

All (511) 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:687:MET:HE1	1:B:704:CYS:HB2	1.24	1.17
1:A:132:GLU:HG3	1:A:196:ARG:NH2	1.62	1.15
1:B:480:THR:N	1:B:483:MET:HE3	1.61	1.13
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: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	0.83	1.00
1:A:795:LEU:HD11	1:A:799:GLN:HG2	1.44	0.99
1:B:29:MET:HE2	1:B:381:ARG:CZ	2.02	0.90
1:B:795:LEU:HD11	1:B:799:GLN:HG2	1.53	0.90
1:B:687:MET:HE1	1:B:704:CYS:CB	2.02	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:HG23	1:A:913:THR:O	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:A:505:ASN:HB2	6:A:1158:HOH:O	1.79	0.82
1:B:735:ASN:HB2	1:B:738:LYS:HE3	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:662:MET:HE1	1:B:687:MET:HE3	1.63	0.79
1:A:323:ARG:NH2	1:A:362:GLU:HB2	1.98	0.79
1:B:539:ARG:CZ	1:B:559:ILE:HD11	2.13	0.78
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:NH1	1:B:853:ARG:HB3	2.00	0.77
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:22:ILE:HD12	1:A:313:MET:HE1	1.67	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:A:209:ASP:CG	1:A:229:ILE:HD12	2.11	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:687:MET:CE	1:B:704:CYS:HB2	2.13	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:A:107:MET:HE1	1:A:451:LYS:HB2	1.71	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:A:502:GLN:OE1	1:A:502:GLN:N	2.17	0.71
1:B:853:ARG:HB3	1:B:853:ARG:HH11	1.54	0.71
1:A:483:MET:HE2	1:A:721:ILE:HG21	1.72	0.71
1:B:688:GLU:OE1	1:B:689:GLU:OE1	2.07	0.71
1:B:589:MET:HE2	1:B:589:MET:HA	1.72	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:ILE:HD13	1:A:42:ARG:HH21	1.57	0.69
1:A:57:PRO:HG2	1:B:799:GLN:HE21	1.58	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:159:GLN:HB3	1:A:167:ILE:HB	1.75	0.68
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.25	0.68
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.07	0.68
1:A:398:ARG:HH11	1:A:398:ARG:HB3	1.59	0.68
1:A:799:GLN:NE2	1:B:58:THR:HB	2.08	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
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:A:875:MET:HE1	1:A:890:PHE:CE2	2.30	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:A:241:GLU:O	1:A:245:ILE:HD12	1.95	0.66
1:B:772:ILE:HG22	1:B:777:LYS:HD2	1.78	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:101:LYS:C	1:B:103:GLN:H	2.04	0.66
1:A:778:THR:HB	1:A:781:ILE:HD13	1.75	0.66
1:B:98:ASN:HB3	1:B:103:GLN:HB2	1.78	0.66
1:B:142:LYS:HA	1:B:142:LYS:HE2	1.78	0.66
1:B:564:ILE:HG23	1:B:565:GLU:H	1.60	0.66
1:B:760:ASP:O	1:B:764:LYS:HG2	1.96	0.66
1:A:245:ILE:HG12	1:A:257:ILE:HD11	1.77	0.66
1:B:425:ARG:HH22	5:B:1007:CIT:H42	1.61	0.66
1:A:280:GLU:HG3	1:A:283:ARG:NH2	2.11	0.65
1:A:309:ILE:O	1:A:313:MET:HG3	1.96	0.65
1:A:913:THR:O	1:A:913:THR:CG2	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:CD2	1:B:442:PHE:HZ	2.10	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:NH1	2.13	0.64
1:B:405:ARG:HB3	1:B:405:ARG:HH11	1.63	0.64
1:B:18:GLN:HE22	1:B:366:ASP:C	2.06	0.63
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:912:ARG:C	1:A:914:GLU:H	2.06	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:134:LEU:O	1:B:138:MET:HG3	1.99	0.62
1:B:810:ASN:HD22	1:B:810:ASN:N	1.97	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:A:361:VAL:C	1:A:363:PRO:HD3	2.24	0.62
1:B:813:CYS:O	1:B:817:ILE:HG12	1.98	0.62
1:A:420:HIS:HD2	1:A:423:TYR:N	1.98	0.61
1:B:426:ARG:HE	5:B:1007:CIT:H22	1.65	0.61
1:A:66:THR:CG2	1:A:256:CYS:HB3	2.30	0.61
1:A:799:GLN:HE22	1:B:58:THR:HB	1.65	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: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:768:PHE:CE1	1:B:811:SER:HB3	2.37	0.60
1:A:558:LYS:HD3	1:A:560:TYR:OH	2.01	0.60
1:B:782:PHE:HD1	1:B:786:PHE:CE1	2.19	0.60
1:A:483:MET:HE2	1:A:721:ILE:CG2	2.31	0.60
1:A:696:VAL:HG21	1:A:703:MET:HE1	1.84	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:763:LYS:HG3	1:B:772:ILE:HD11	1.83	0.59
1:B:768:PHE:HE1	1:B:811:SER:HB3	1.65	0.59
1:B:66:THR:HG23	1:B:68:VAL:H	1.68	0.59
1:B:76:GLU:CD	1:B:76:GLU:H	2.10	0.59
1:A:910:ARG:O	1:A:914:GLU:HB2	2.02	0.59
1:B:662:MET:CE	1:B:687:MET:HE3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLU:HG3	6:B:1161:HOH:O	2.02	0.59
1:A:320:PHE:C	1:A:322:GLY:H	2.10	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: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:502:GLN:H	1:A:502:GLN:CD	2.09	0.57
1:A:171:TRP:NE1	1:A:177:ALA:H	2.02	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:673:GLU:CD	1:B:849:ARG:HH22	2.13	0.57
1:B:619:TRP:CD1	1:B:624:LYS:HA	2.40	0.57
1:B:56:ASN:N	1:B:57:PRO:HD2	2.19	0.57
1:B:605:PRO:HB3	1:B:708:GLU:HG3	1.87	0.57
1:A:595:ARG:HD2	1:A:648:ASP:OD2	2.05	0.56
1:B:426:ARG:NH2	5:B:1007:CIT:H41	2.04	0.56
1:A:389:THR:O	1:A:392:ALA:HB3	2.05	0.56
1:B:265:GLY:HA2	1:B:269:SER:HB3	1.87	0.56
1:A:235:ASN:HA	1:A:261:TRP:CD1	2.40	0.56
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: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:A:307:ARG:O	1:A:311:VAL:HG23	2.05	0.55
1:B:420:HIS:HD2	1:B:423:TYR:N	2.02	0.55
1:A:155:SER:HA	1:A:208:ASN:ND2	2.20	0.55
1:A:688:GLU:OE1	1:A:848:ASN:ND2	2.38	0.55
1:A:760:ASP:O	1:A:764:LYS:HG2	2.05	0.55
1:B:230:ILE:HD11	1:B:386:VAL:HG11	1.87	0.55
1:B:724:HIS:HA	1:B:727:ARG:NH1	2.21	0.55
1:A:171:TRP:HB3	1:A:175:PHE:O	2.06	0.55
1:B:342:ILE:O	1:B:342:ILE:HG22	2.06	0.55
1:A:126:LEU:O	1:A:129:HIS:HB3	2.07	0.55
1:B:565:GLU:HG2	1:B:566:ILE:H	1.70	0.55
1:B:565:GLU:CG	1:B:566:ILE:N	2.70	0.55
1:A:558:LYS:HD3	1:A:560:TYR:CZ	2.42	0.54
1:B:101:LYS:O	1:B:103:GLN:N	2.40	0.54
1:A:420:HIS:HD2	1:A:423:TYR:H	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:380:PHE:HD2	1:A:426:ARG:HD3	1.72	0.54
1:B:602:PHE:CE2	1:B:633:VAL:HG11	2.42	0.54
1:A:242:LEU:C	1:A:244:HIS:H	2.16	0.53
1:A:244:HIS:HD2	1:A:396:ARG:NH2	2.06	0.53
1:A:608:GLN:OE1	1:A:654:VAL:HG13	2.08	0.53
1:B:418:LYS:HG2	1:B:444:LEU:HD21	1.90	0.53
1:B:479:LEU:HA	1:B:483:MET:CE	2.38	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:B:524:GLU:CD	1:B:524:GLU:H	2.16	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:134:LEU:HD23	1:A:199:TYR:HE1	1.71	0.53
1:A:598:LEU:C	1:A:598:LEU:HD23	2.33	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:136:ASP:OD1	1:B:136:ASP:C	2.51	0.53
1:A:351:ASN:O	1:A:355:ILE:HG12	2.10	0.52
1:B:735:ASN:HB2	1:B:738:LYS:CE	2.33	0.52
1:A:155:SER:HA	1:A:208:ASN:HD22	1.74	0.52
1:A:122:SER:HA	1:A:178:SER:OG	2.10	0.52
1:B:393:ILE:O	1:B:396:ARG:HB3	2.08	0.52
1:A:324:ILE:HG23	1:A:328:LEU:HD23	1.90	0.52
1:B:319:LEU:HB3	1:B:320:PHE:CE1	2.45	0.52
1:B:491:MET:O	1:B:495:MET:HG3	2.09	0.52
1:A:451:LYS:O	1:A:455:MET:HG2	2.09	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:B:687:MET:CE	1:B:704:CYS:SG	2.98	0.52
1:A:646:GLU:HB2	1:A:647:PHE:CD2	2.45	0.51
1:B:101:LYS:C	1:B:103:GLN:N	2.68	0.51
1:B:598:LEU:HD23	1:B:598:LEU:C	2.35	0.51
1:A:317:GLY:CA	1:A:321:GLU:O	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:MET:HE2	1:B:381:ARG:NH1	2.24	0.51
1:B:514:SER:OG	1:B:704:CYS:HB3	2.10	0.51
1:A:387:ALA:HA	1:A:427:PHE:HE1	1.76	0.51
1:A:619:TRP:NE1	1:A:625:ALA:H	2.08	0.51
1:B:480:THR:HG23	1:B:483:MET:HE2	1.92	0.51
1:B:644:ARG:CD	1:B:646:GLU:OE1	2.58	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:531:LEU:HD21	1:B:582:ILE:HD11	1.91	0.51
1:B:763:LYS:CG	1:B:772:ILE:HD11	2.41	0.51
1:A:307:ARG:HB2	1:A:334:PHE:HB3	1.93	0.51
1:A:224:CYS:HA	1:A:409:THR:O	2.11	0.51
1:A:763:LYS:CG	1:A:772:ILE:HD11	2.39	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: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:B:479:LEU:HA	1:B:483:MET:HE3	1.94	0.50
1:B:782:PHE:CD1	1:B:786:PHE:CE1	2.99	0.50
1:A:22:ILE:CD1	1:A:313:MET:HE1	2.37	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:A:93:LEU:N	1:A:93:LEU:HD12	2.27	0.50
1:A:97:VAL:HG21	1:A:105:VAL:HG22	1.93	0.50
1:A:646:GLU:HB2	1:A:647:PHE:HD2	1.76	0.50
1:B:786:PHE:HE2	1:B:803:ILE:HG22	1.76	0.50
1:A:67:PHE:HA	1:A:255:MET:SD	2.52	0.50
1:A:265:GLY:HA2	1:A:269:SER:OG	2.12	0.50
1:A:514:SER:HA	1:A:608:GLN:HE22	1.76	0.50
1:B:646:GLU:HB3	1:B:647:PHE:HD2	1.77	0.50
1:A:193:ILE:O	1:A:194:LYS:C	2.55	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:98:ASN:O	1:B:103:GLN:O	2.30	0.49
1:B:320:PHE:C	1:B:322:GLY:H	2.19	0.49
1:A:25:TYR:CD2	1:A:313:MET:HE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:MET:HE3	1:B:707:MET:HE3	1.94	0.49
1:B:662:MET:SD	1:B:687:MET:HE3	2.52	0.49
1:A:245:ILE:HG22	1:A:245:ILE:O	2.12	0.49
1:A:786:PHE:CE2	1:A:807:LEU:HD11	2.48	0.49
1:B:168:LEU:HD23	1:B:180:VAL:HG12	1.95	0.49
1:B:79:ASP:HB3	1:B:148:LEU:CD2	2.43	0.49
1:A:320:PHE:C	1:A:322:GLY:N	2.71	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:718:LEU:C	1:A:720:ASP:N	2.70	0.48
1:A:141:ARG:N	1:A:141:ARG:HD2	2.28	0.48
1:B:79:ASP:HB3	1:B:148:LEU:HD22	1.96	0.48
1:B:677:ILE:O	1:B:682:SER:HA	2.14	0.48
1:B:718:LEU:C	1:B:720:ASP:N	2.70	0.48
1:A:637:LEU:O	1:A:641:ILE:HG13	2.14	0.48
1:A:782:PHE:CD1	1:A:786:PHE:CE1	3.02	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:A:25:TYR:C	1:A:27:TYR:H	2.21	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: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:66:THR:CG2	1:B:68:VAL:H	2.25	0.47
1:A:25:TYR:HD2	1:A:313:MET:HE3	1.79	0.47
1:A:29:MET:HE1	1:A:309:ILE:CD1	2.44	0.47
1:B:654:VAL:HG13	1:B:654:VAL:O	2.13	0.47
1:A:449:SER:O	1:A:450:GLY:C	2.58	0.47
1:A:905:THR:O	1:A:909:VAL:HG23	2.14	0.47
1:A:912:ARG:C	1:A:914:GLU:N	2.72	0.47
1:A:321:GLU:N	1:A:321:GLU:OE1	2.47	0.47
1:A:55:PHE:C	1:A:57:PRO:HD2	2.39	0.47
1:A:83:LEU:O	1:A:153:THR:HB	2.15	0.47
1:B:58:THR:O	1:B:58:THR:CG2	2.63	0.47
1:B:271:GLU:OE2	1:B:274:ARG:HD3	2.14	0.47
1:B:671:THR:OG1	1:B:857:THR:HG23	2.15	0.47
1:B:786:PHE:CE2	1:B:807:LEU:HD11	2.49	0.47
1:A:66:THR:HG23	1:A:68:VAL:H	1.79	0.47
1:A:258:ASN:C	1:A:258:ASN:OD1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:ALA:O	1:B:799:GLN:HB3	2.14	0.47
1:A:519:THR:HB	1:A:520:PRO:HD2	1.96	0.47
1:B:420:HIS:CD2	1:B:423:TYR:H	2.26	0.47
1:B:640:ALA:N	1:B:643:ARG:HH21	2.13	0.47
1:A:231:GLY:O	1:A:232:THR:C	2.58	0.46
1:A:390:LEU:HD23	1:A:431:LEU:HD22	1.98	0.46
1:A:416:LEU:HD21	1:A:423:TYR:CE2	2.49	0.46
1:A:654:VAL:HG13	1:A:654:VAL:O	2.15	0.46
1:B:664:THR:HG23	1:B:899:LYS:HB3	1.98	0.46
1:B:689:GLU:OE1	1:B:689:GLU:N	2.48	0.46
1:A:652:VAL:HG21	1:A:909:VAL:HG22	1.97	0.46
1:B:797:LEU:HD21	1:B:817:ILE:HD13	1.97	0.46
1:A:529:LEU:HD11	1:A:586:LEU:HD21	1.97	0.46
1:B:73:ASP:OD1	1:B:73:ASP:C	2.59	0.46
1:B:810:ASN:N	1:B:810:ASN:ND2	2.63	0.46
1:A:56:ASN:N	1:A:57:PRO:CD	2.77	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:342:ILE:O	1:B:342:ILE:CG2	2.63	0.46
1:B:769:ARG:HH22	1:B:811:SER:HA	1.81	0.46
1:A:90:PHE:CZ	1:A:130:VAL:HG13	2.51	0.46
1:B:513:PRO:HB3	1:B:703:MET:HE3	1.97	0.46
1:B:518:ARG:HH22	1:B:521:ASP:CG	2.22	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:A:248:VAL:HG21	1:A:255:MET:HE1	1.97	0.46
1:B:165:GLU:HG3	1:B:184:ASP:OD2	2.16	0.46
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.51	0.46
1:B:856:VAL:HG22	1:B:857:THR:N	2.31	0.46
1:A:66:THR:O	1:A:67:PHE:HB2	2.15	0.45
1:A:339:VAL:O	1:A:343:GLU:HG3	2.16	0.45
1:A:408:THR:OG1	1:A:409:THR:N	2.49	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:A:803:ILE:O	1:A:806:GLN:HB2	2.16	0.45
1:B:320:PHE:CD1	1:B:320:PHE:N	2.85	0.45
1:A:398:ARG:HH11	1:A:398:ARG:CB	2.27	0.45
1:A:799:GLN:NE2	1:B:58:THR:CB	2.78	0.45
1:B:709:TRP:CD1	1:B:709:TRP:C	2.94	0.45
1:B:181:GLU:HG3	6:B:1189:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LYS:O	1:B:195:LYS:HG2	2.17	0.45
1:B:539:ARG:HG3	1:B:541:LEU:HD11	1.99	0.45
1:B:595:ARG:NE	1:B:648:ASP:OD2	2.50	0.45
1:B:659:VAL:HG22	1:B:704:CYS:SG	2.56	0.45
1:A:219:TYR:CD1	1:A:219:TYR:C	2.95	0.45
1:B:361:VAL:HG23	1:B:363:PRO:HD3	1.98	0.45
1:B:646:GLU:HB3	1:B:647:PHE:CD2	2.51	0.45
1:A:62:LYS:HB3	1:A:64:LEU:CD2	2.46	0.45
1:A:514:SER:HA	1:A:608:GLN:NE2	2.32	0.45
1:A:232:THR:O	1:A:298:SER:HB2	2.17	0.44
1:A:455:MET:HE2	1:A:455:MET:HA	1.98	0.44
1:B:862:GLY:HA2	3:B:1004:BG6:O6	2.17	0.44
1:A:286:LEU:C	1:A:288:PRO:HD3	2.42	0.44
1:A:134:LEU:CD2	1:A:199:TYR:HE1	2.31	0.44
1:A:193:ILE:O	1:A:196:ARG:N	2.49	0.44
1:B:539:ARG:HB3	1:B:559:ILE:CD1	2.44	0.44
1:A:483:MET:HE3	1:A:487:VAL:HG23	1.98	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:B:480:THR:HG23	1:B:483:MET:CE	2.47	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:46:GLU:HG3	1:A:264:PHE:CE1	2.53	0.44
1:A:265:GLY:C	1:A:267:ASP:H	2.25	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:252:GLU:OE2	1:A:812:THR:HB	2.17	0.44
1:B:71:ILE:HB	1:B:72:PRO:HD2	2.00	0.44
1:B:72:PRO:HD3	1:B:215:MET:HE3	2.00	0.44
1:B:762:THR:O	1:B:770:GLY:HA2	2.17	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:A:119:VAL:O	1:A:119:VAL:HG12	2.18	0.44
1:B:280:GLU:HG3	1:B:283:ARG:NH2	2.32	0.44
1:A:251:ASP:N	1:A:251:ASP:OD1	2.51	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:595:ARG:CD	1:A:648:ASP:OD2	2.67	0.43
1:A:202:ASN:C	1:A:202:ASN:ND2	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:HIS:CD2	1:B:423:TYR:HB2	2.53	0.43
1:B:579:VAL:HG21	1:B:640:ALA:CB	2.48	0.43
1:A:244:HIS:CD2	1:A:396:ARG:NH2	2.85	0.43
1:A:406:LEU:HD12	1:A:407:ARG:H	1.84	0.43
1:A:477:PHE:CZ	1:A:757:ILE:HD11	2.53	0.43
1:A:521:ASP:OD2	1:A:521:ASP:C	2.62	0.43
1:A:677:ILE:HG21	2:A:1003:BGC:C6	2.48	0.43
1:B:146:LYS:HB2	1:B:148:LEU:HG	2.00	0.43
1:B:511:MET:HE3	1:B:705:ILE:HG21	2.00	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:A:413:ASN:ND2	3:A:1002:BG6:O1	2.45	0.43
1:A:786:PHE:CD1	1:A:786:PHE:C	2.96	0.43
1:B:386:VAL:HG12	1:B:427:PHE:CE1	2.54	0.43
1:B:589:MET:HE2	1:B:589:MET:CA	2.46	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:A:400:ASN:HD22	1:A:400:ASN:HA	1.60	0.43
1:A:677:ILE:O	1:A:682:SER:HA	2.19	0.43
1:B:347:GLU:O	1:B:348:GLY:C	2.62	0.43
1:B:644:ARG:HD3	1:B:646:GLU:HB2	2.01	0.43
1:B:655:VAL:HG12	1:B:656:ASN:O	2.19	0.43
1:B:907:VAL:HG12	1:B:907:VAL:O	2.19	0.43
1:B:29:MET:HE2	1:B:381:ARG:NH2	2.34	0.42
1:B:101:LYS:O	1:B:103:GLN:HG3	2.19	0.42
1:B:640:ALA:HA	1:B:643:ARG:HE	1.84	0.42
1:A:274:ARG:NH1	6:A:1156:HOH:O	2.52	0.42
1:A:399:ASP:O	1:A:400:ASN:C	2.61	0.42
1:B:84:ASP:HA	1:B:153:THR:HB	2.01	0.42
1:B:98:ASN:C	1:B:103:GLN:O	2.62	0.42
1:B:261:TRP:CD1	1:B:261:TRP:C	2.97	0.42
1:B:323:ARG:NH2	1:B:362:GLU:HB2	2.33	0.42
1:B:640:ALA:CA	1:B:643:ARG:HH21	2.31	0.42
1:A:199:TYR:CD2	1:A:199:TYR:N	2.87	0.42
1:A:330:THR:HB	1:A:333:LYS:HG3	2.01	0.42
1:B:541:LEU:HG	1:B:557:ASN:CB	2.48	0.42
1:A:265:GLY:C	1:A:267:ASP:N	2.76	0.42
1:A:492:ARG:CZ	1:A:844:LYS:HG3	2.49	0.42
1:A:677:ILE:HG21	2:A:1003:BGC:H6C1	2.00	0.42
1:B:405:ARG:NH1	1:B:437:ASP:C	2.77	0.42
1:B:640:ALA:HB2	1:B:643:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:O	1:A:436:PRO:HD3	2.19	0.42
1:A:644:ARG:O	1:A:645:GLU:HB3	2.20	0.42
1:B:420:HIS:CD2	1:B:422:GLN:H	2.38	0.42
1:A:29:MET:HE1	1:A:309:ILE:HD11	2.01	0.42
1:A:230:ILE:HD13	1:A:386:VAL:HG21	2.00	0.42
1:A:261:TRP:CD1	1:A:261:TRP:C	2.98	0.42
1:B:66:THR:HG23	1:B:68:VAL:HG23	2.02	0.42
1:B:29:MET:CE	1:B:381:ARG:CZ	2.86	0.42
1:B:167:ILE:HA	1:B:183:ALA:O	2.20	0.42
1:B:588:TYR:HD2	1:B:589:MET:HE3	1.85	0.42
1:A:420:HIS:CD2	1:A:422:GLN:H	2.37	0.42
1:A:595:ARG:NE	1:A:648:ASP:OD2	2.52	0.42
1:A:619:TRP:CD1	1:A:624:LYS:HA	2.55	0.42
1:B:501:LYS:HB3	1:B:695:MET:SD	2.60	0.42
1:B:579:VAL:HG21	1:B:640:ALA:HB3	2.01	0.42
1:B:587:ASP:OD1	1:B:592:LYS:HE2	2.19	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: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:B:356:LEU:HD23	1:B:359:LEU:HD12	2.02	0.41
1:B:510:LYS:HD3	1:B:510:LYS:HA	1.92	0.41
1:B:604:PHE:HB3	1:B:605:PRO:HD2	2.01	0.41
1:A:20:LYS:O	1:A:24:LYS:HG3	2.20	0.41
1:A:72:PRO:HD3	1:A:215:MET:HE3	2.01	0.41
1:A:105:VAL:HG11	1:A:451:LYS:HE2	2.02	0.41
1:A:492:ARG:HD2	1:A:492:ARG:O	2.21	0.41
1:A:151:GLY:HA3	1:A:457:THR:OG1	2.19	0.41
1:A:347:GLU:HB3	1:A:351:ASN:ND2	2.35	0.41
1:A:710:GLY:O	1:A:739:GLN:HA	2.21	0.41
1:B:72:PRO:HD3	1:B:215:MET:CE	2.50	0.41
1:A:854:LEU:HD12	1:A:855:ASN:N	2.36	0.41
1:B:16:ASP:O	1:B:16:ASP:CG	2.63	0.41
1:B:431:LEU:HD22	1:B:442:PHE:CZ	2.43	0.41
1:A:100:GLU:C	1:A:102:ASN:H	2.28	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:A:72:PRO:HG3	1:A:455:MET:HB3	2.01	0.41
1:A:202:ASN:C	1:A:202:ASN:HD22	2.27	0.41
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:PHE:CE2	1:A:790:ILE:HD11	2.56	0.41
1:B:312:LYS:O	1:B:316:GLU:HG3	2.20	0.41
1:B:320:PHE:C	1:B:322:GLY:N	2.79	0.41
1:B:545:ILE:HD13	1:B:903:LEU:HD23	2.02	0.41
1:B:662:MET:HE2	1:B:662:MET:HB3	2.00	0.41
1:A:124:SER:O	1:A:125:GLN:C	2.62	0.41
1:B:330:THR:HB	1:B:333:LYS:CG	2.50	0.41
1:B:342:ILE:HG23	1:B:352:ALA:HB2	2.02	0.41
1:B:663:MET:HG3	1:B:904:ILE:HD11	2.02	0.41
1:A:321:GLU:CD	1:A:323:ARG:HH12	2.28	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: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:718:LEU:C	1:B:720:ASP:H	2.28	0.41
1:B:786:PHE:HZ	1:B:804:LEU:CD2	2.34	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:531:LEU:HD21	1:A:582:ILE:HD11	2.02	0.40
1:A:551:ARG:NH1	1:A:551:ARG:HG3	2.35	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:806:GLN:HE21	1:B:806:GLN:HB3	1.56	0.40
1:A:338:ASP:O	1:A:342:ILE:HD13	2.21	0.40
1:A:637:LEU:HD23	1:A:651:VAL:HG21	2.01	0.40
1:B:531:LEU:HD13	1:B:598:LEU:HD11	2.03	0.40
1:B:786:PHE:CD1	1:B:786:PHE:C	2.99	0.40
1:A:46:GLU:HG3	1:A:264:PHE:HE1	1.86	0.40
1:A:510:LYS:O	1:A:511:MET:C	2.63	0.40
1:A:520:PRO:HD3	1:A:663:MET:CE	2.52	0.40
1:A:709:TRP:CD1	1:A:709:TRP:C	2.98	0.40
1:A:152:PHE:O	1:A:206:VAL:HA	2.22	0.40
1:B:767:LEU:CG	1:B:818:LEU:HD23	2.47	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%)	840 (94%)	55 (6%)	2 (0%)	43	61
1	B	897/917 (98%)	845 (94%)	49 (6%)	3 (0%)	36	53
All	All	1794/1834 (98%)	1685 (94%)	104 (6%)	5 (0%)	36	53

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 [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%)	747 (96%)	27 (4%)	32	55
1	B	774/788 (98%)	753 (97%)	21 (3%)	39	64
All	All	1548/1576 (98%)	1500 (97%)	48 (3%)	35	60

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

Mol	Chain	Res	Type
1	A	21	LYS

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Mol	Chain	Res	Type
1	A	27	TYR
1	A	96	GLN
1	A	102	ASN
1	A	159	GLN
1	A	176	LYS
1	A	196	ARG
1	A	198	ASP
1	A	199	TYR
1	A	229	ILE
1	A	242	LEU
1	A	254	ARG
1	A	281	ILE
1	A	400	ASN
1	A	408	THR
1	A	481	LYS
1	A	502	GLN
1	A	531	LEU
1	A	550	LYS
1	A	559	ILE
1	A	565	GLU
1	A	709	TRP
1	A	781	ILE
1	A	806	GLN
1	A	843	ASP
1	A	857	THR
1	A	913	THR
1	B	66	THR
1	B	93	LEU
1	B	99	HIS
1	B	320	PHE
1	B	321	GLU
1	B	405	ARG
1	B	407	ARG
1	B	424	SER
1	B	437	ASP
1	B	463	LEU
1	B	531	LEU
1	B	709	TRP
1	B	764	LYS
1	B	769	ARG
1	B	777	LYS
1	B	798	LEU

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Mol	Chain	Res	Type
1	B	805	GLN
1	B	806	GLN
1	B	810	ASN
1	B	843	ASP
1	B	860	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	102	ASN
1	A	104	ASN
1	A	125	GLN
1	A	129	HIS
1	A	159	GLN
1	A	202	ASN
1	A	244	HIS
1	A	345	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	607	GLN
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	49	ASN
1	B	98	ASN
1	B	104	ASN
1	B	117	ASN
1	B	202	ASN
1	B	208	ASN
1	B	244	HIS
1	B	345	ASN
1	B	384	ASN
1	B	400	ASN
1	B	420	HIS

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Mol	Chain	Res	Type
1	B	466	GLN
1	B	502	GLN
1	B	506	ASN
1	B	557	ASN
1	B	577	HIS
1	B	631	HIS
1	B	702	GLN
1	B	771	GLN
1	B	789	GLN
1	B	799	GLN
1	B	806	GLN
1	B	810	ASN
1	B	832	GLN
1	B	848	ASN
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
5	CIT	A	1007	-	12,12,12	1.05	0	17,17,17	1.39	1 (5%)
3	BG6	B	1004	-	16,16,16	1.16	1 (6%)	23,24,24	0.88	1 (4%)
3	BG6	B	1002	-	16,16,16	1.13	1 (6%)	23,24,24	0.75	1 (4%)
2	BGC	A	1001	-	12,12,12	0.52	0	17,17,17	1.46	2 (11%)
5	CIT	B	1007	-	12,12,12	1.06	0	17,17,17	1.38	1 (5%)
2	BGC	B	1003	-	12,12,12	0.50	0	17,17,17	1.31	2 (11%)
2	BGC	A	1003	-	12,12,12	0.37	0	17,17,17	1.21	2 (11%)
3	BG6	A	1004	-	16,16,16	1.12	2 (12%)	23,24,24	1.01	1 (4%)
2	BGC	B	1001	-	12,12,12	0.38	0	17,17,17	1.38	2 (11%)
3	BG6	A	1002	-	16,16,16	1.22	2 (12%)	23,24,24	0.85	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
5	CIT	A	1007	-	-	6/16/16/16	-
3	BG6	B	1004	-	-	2/6/26/26	0/1/1/1
3	BG6	B	1002	-	-	1/6/26/26	0/1/1/1
2	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
5	CIT	B	1007	-	-	7/16/16/16	-
2	BGC	B	1003	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1003	-	-	0/2/22/22	0/1/1/1
3	BG6	A	1004	-	-	2/6/26/26	0/1/1/1
2	BGC	B	1001	-	-	2/2/22/22	0/1/1/1
3	BG6	A	1002	-	-	4/6/26/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	BG6	P-O3P	3.76	1.62	1.50
3	B	1002	BG6	P-O3P	3.56	1.61	1.50
3	B	1004	BG6	P-O3P	3.47	1.61	1.50
3	A	1004	BG6	P-O3P	3.33	1.60	1.50
3	A	1004	BG6	P-O2P	2.13	1.62	1.54
3	A	1002	BG6	P-O2P	2.07	1.62	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	BGC	C1-O5-C5	-4.26	105.41	113.65
2	B	1001	BGC	O5-C1-C2	-3.63	103.92	110.30
5	B	1007	CIT	O6-C6-C3	3.62	120.08	113.14
2	B	1001	BGC	C1-O5-C5	-3.61	106.67	113.65
5	A	1007	CIT	O6-C6-C3	3.45	119.75	113.14
2	A	1003	BGC	O5-C1-C2	-3.27	104.55	110.30
2	A	1001	BGC	O5-C1-C2	-3.19	104.69	110.30
2	B	1003	BGC	C1-O5-C5	-3.16	107.53	113.65
2	B	1003	BGC	O5-C1-C2	-3.16	104.74	110.30
3	A	1004	BG6	O1P-P-O6	3.12	114.79	106.67
3	B	1004	BG6	O1P-P-O6	2.85	114.09	106.67
2	A	1003	BGC	C1-O5-C5	-2.83	108.17	113.65
3	A	1002	BG6	O1P-P-O6	2.68	113.65	106.67
3	B	1002	BG6	O1P-P-O6	2.21	112.44	106.67

There are no chirality outliers.

All (24) torsion outliers are listed below:

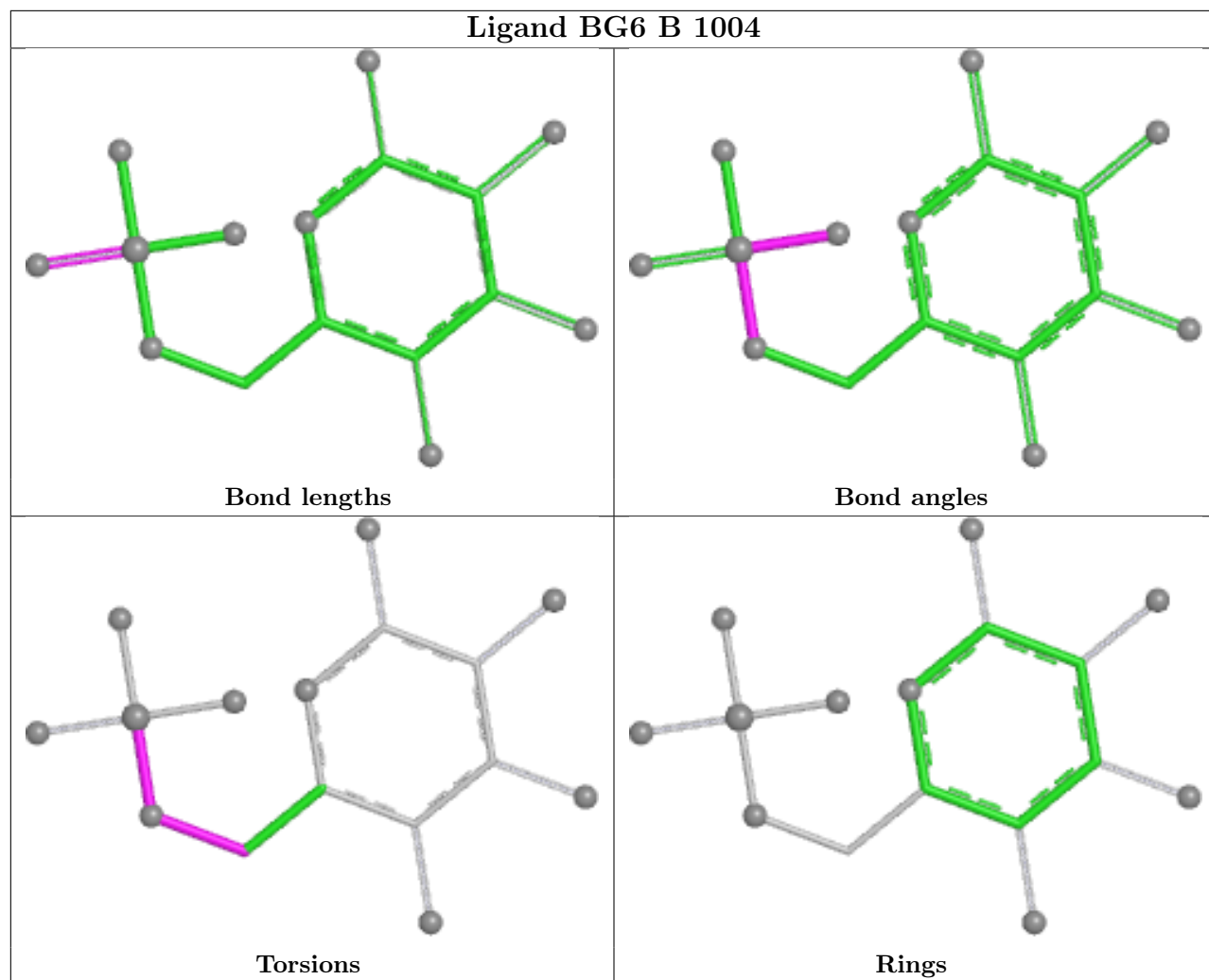
Mol	Chain	Res	Type	Atoms
3	A	1002	BG6	C6-O6-P-O3P
3	A	1004	BG6	C6-O6-P-O3P
3	B	1004	BG6	C6-O6-P-O3P
5	A	1007	CIT	O7-C3-C6-O5
5	A	1007	CIT	O7-C3-C6-O6
5	A	1007	CIT	C4-C3-C6-O5
5	A	1007	CIT	C4-C3-C6-O6
5	B	1007	CIT	C1-C2-C3-O7
5	B	1007	CIT	C1-C2-C3-C6
5	B	1007	CIT	O7-C3-C6-O5
5	B	1007	CIT	O7-C3-C6-O6
5	B	1007	CIT	C4-C3-C6-O5
5	B	1007	CIT	C4-C3-C6-O6
5	B	1007	CIT	C1-C2-C3-C4
2	B	1001	BGC	C4-C5-C6-O6
2	B	1001	BGC	O5-C5-C6-O6
3	A	1002	BG6	C5-C6-O6-P
3	B	1004	BG6	C5-C6-O6-P
5	A	1007	CIT	C2-C3-C4-C5
5	A	1007	CIT	C6-C3-C4-C5
3	B	1002	BG6	C5-C6-O6-P
3	A	1004	BG6	C5-C6-O6-P
3	A	1002	BG6	C6-O6-P-O1P
3	A	1002	BG6	C6-O6-P-O2P

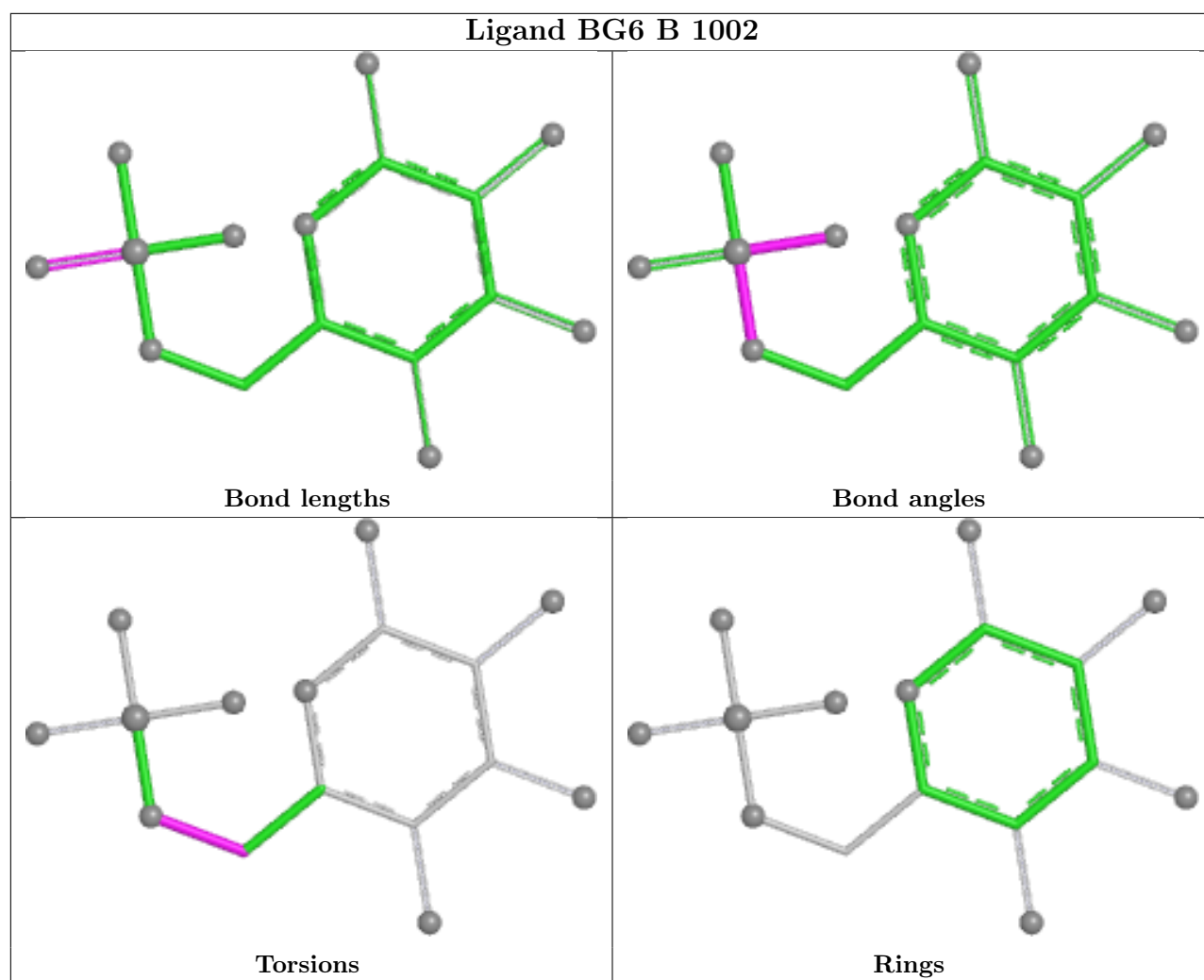
There are no ring outliers.

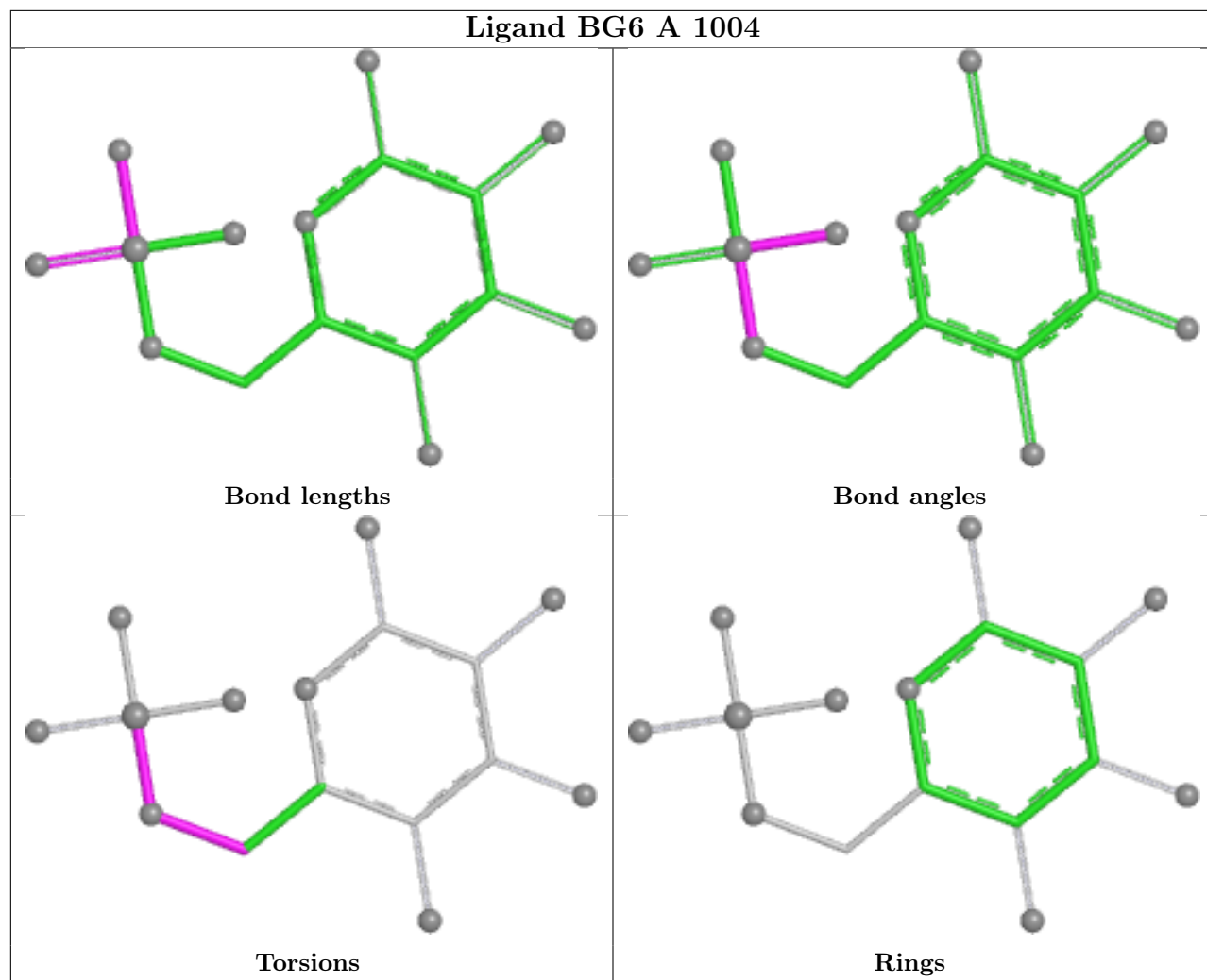
5 monomers are involved in 11 short contacts:

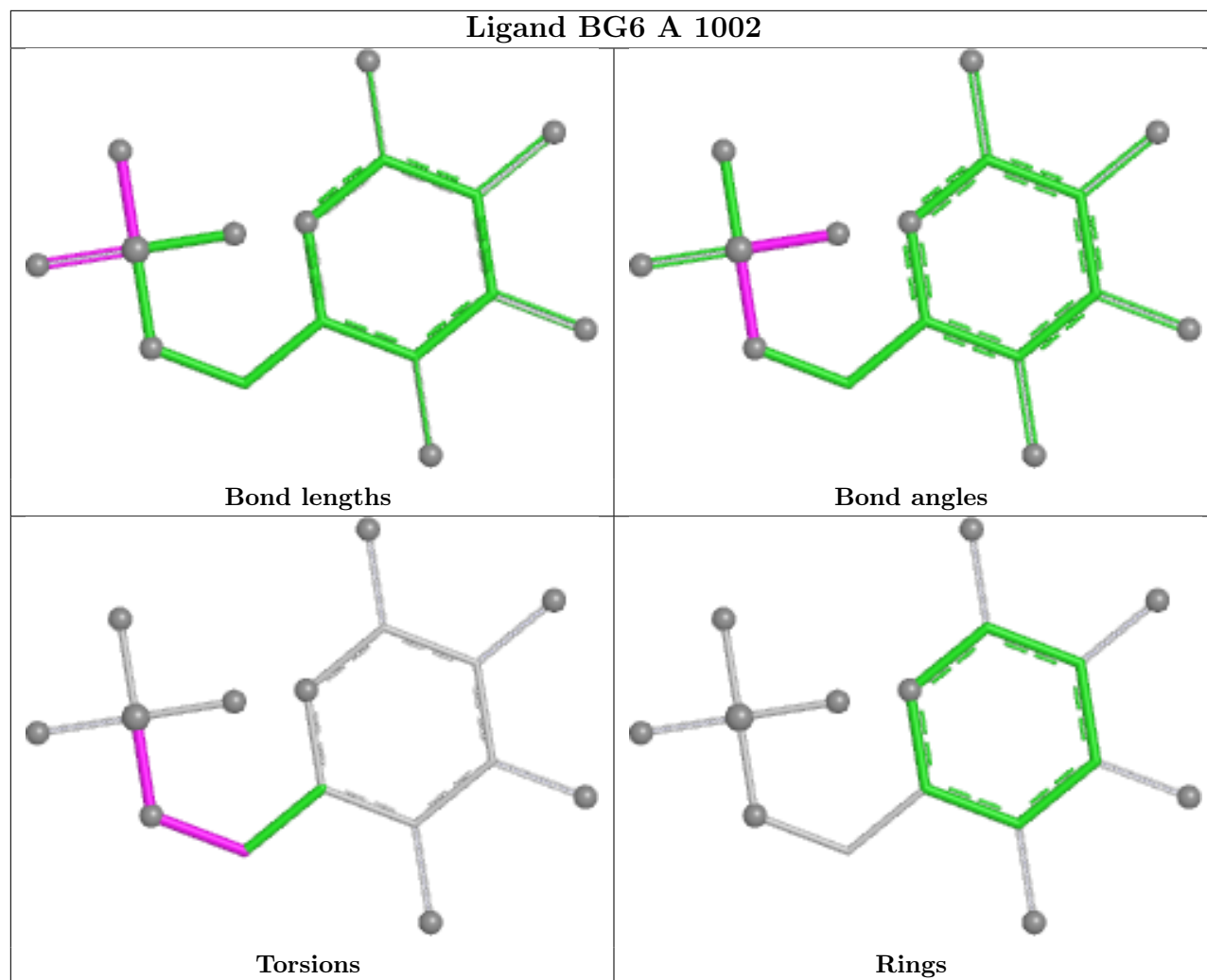
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	CIT	1	0
3	B	1004	BG6	1	0
5	B	1007	CIT	5	0
2	A	1003	BGC	2	0
3	A	1002	BG6	2	0

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 [i](#)

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%)	0.43	31 (3%) 48 44	31, 59, 85, 113	0
1	B	899/917 (98%)	0.37	14 (1%) 70 68	32, 58, 85, 112	0
All	All	1798/1834 (98%)	0.40	45 (2%) 58 55	31, 59, 85, 113	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	564	ILE	4.1
1	A	786	PHE	3.5
1	A	447	SER	3.5
1	A	911	LEU	3.4
1	B	895	ASP	3.3
1	B	18	GLN	3.2
1	A	22	ILE	3.1
1	B	99	HIS	3.0
1	B	564	ILE	3.0
1	B	786	PHE	2.9
1	B	798	LEU	2.8
1	A	443	LEU	2.8
1	A	444	LEU	2.7
1	A	93	LEU	2.6
1	A	310	LEU	2.6
1	B	689	GLU	2.6
1	A	647	PHE	2.6
1	A	36	LEU	2.6
1	A	349	LEU	2.5
1	A	217	CYS	2.4
1	A	202	ASN	2.4
1	B	911	LEU	2.4
1	A	105	VAL	2.4
1	A	427	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	418	LYS	2.3
1	B	102	ASN	2.3
1	A	406	LEU	2.3
1	B	19	VAL	2.3
1	B	406	LEU	2.3
1	A	108	GLU	2.3
1	B	518	ARG	2.2
1	B	104	ASN	2.2
1	A	483	MET	2.2
1	A	446	GLU	2.2
1	A	361	VAL	2.2
1	A	798	LEU	2.1
1	A	380	PHE	2.1
1	A	31	LEU	2.1
1	A	423	TYR	2.1
1	A	80	PHE	2.1
1	A	334	PHE	2.1
1	A	82	ALA	2.1
1	B	852	ASP	2.1
1	A	419	THR	2.0
1	A	566	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.

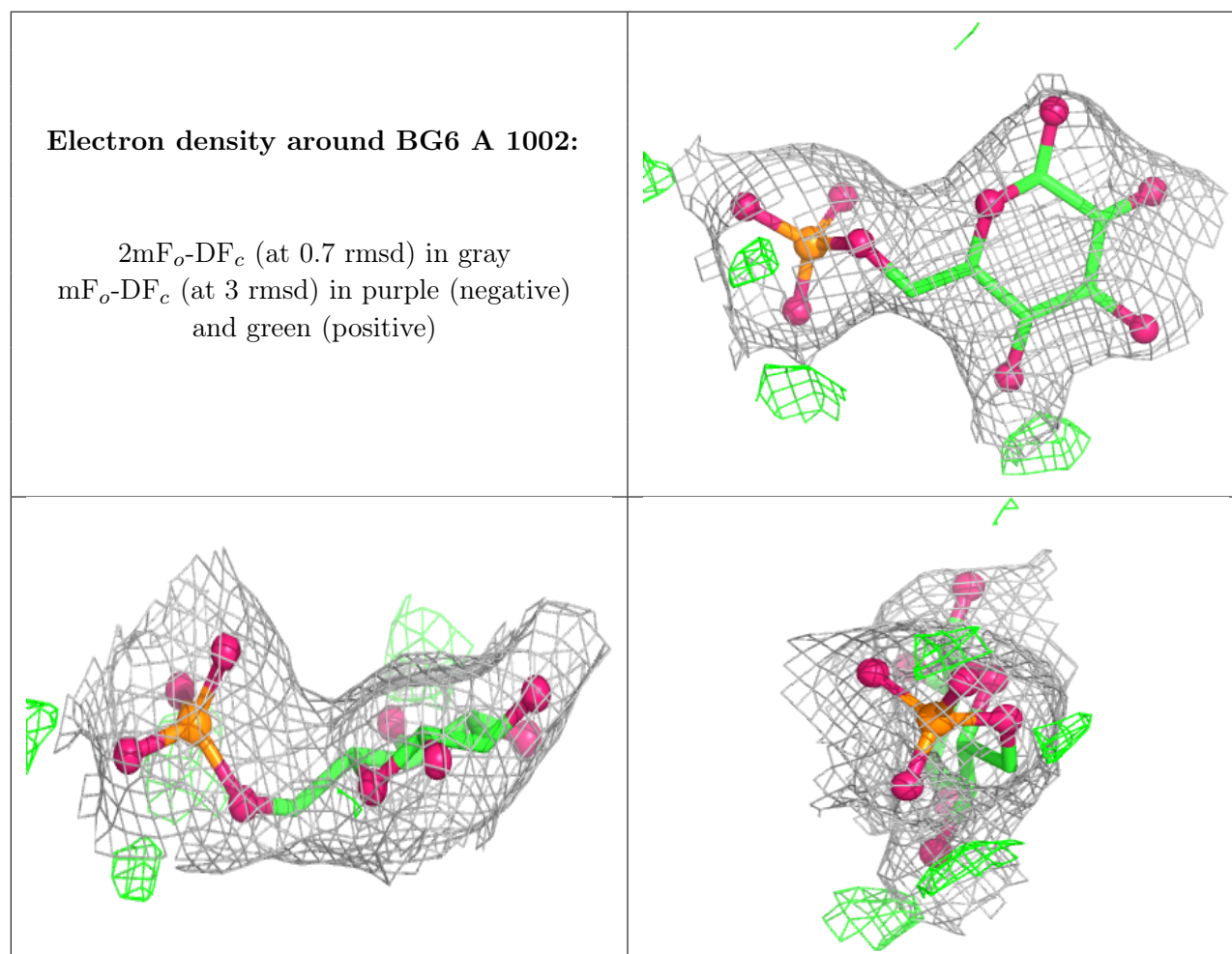
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CIT	A	1007	13/13	0.62	0.16	110,110,111,111	0
5	CIT	B	1007	13/13	0.66	0.14	106,108,108,108	0

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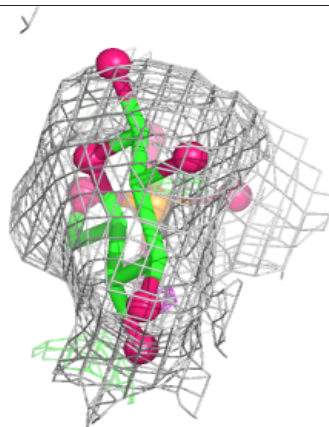
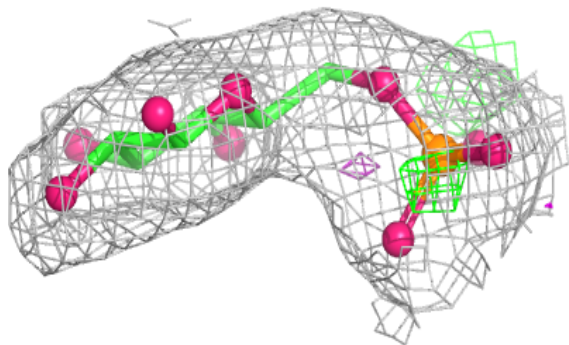
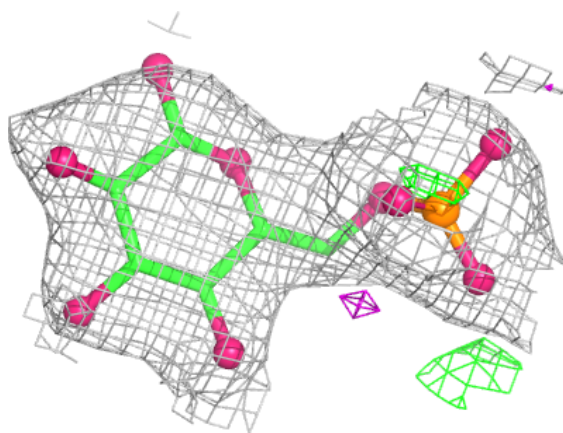
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	A	1001	12/12	0.83	0.11	50,52,53,55	0
3	BG6	A	1002	16/16	0.86	0.11	75,78,80,80	0
2	BGC	B	1003	12/12	0.89	0.08	38,39,40,42	0
2	BGC	B	1001	12/12	0.90	0.11	48,49,50,51	0
4	NA	A	1006	1/1	0.90	0.06	53,53,53,53	0
4	NA	B	1005	1/1	0.92	0.06	65,65,65,65	0
3	BG6	B	1002	16/16	0.93	0.12	71,74,75,76	0
4	NA	B	1006	1/1	0.93	0.06	52,52,52,52	0
4	NA	A	1005	1/1	0.93	0.10	63,63,63,63	0
2	BGC	A	1003	12/12	0.93	0.09	36,38,38,41	0
3	BG6	B	1004	16/16	0.96	0.08	36,43,44,45	0
3	BG6	A	1004	16/16	0.97	0.07	36,41,42,43	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.

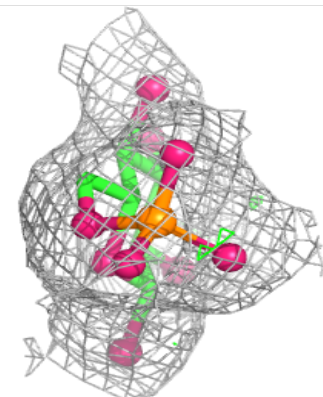
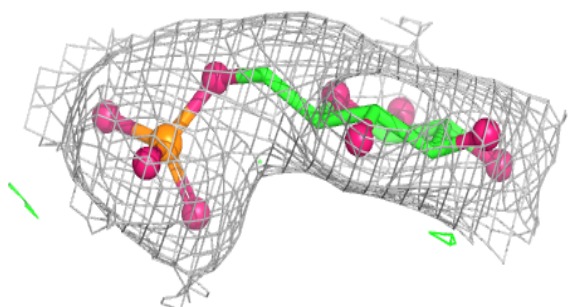
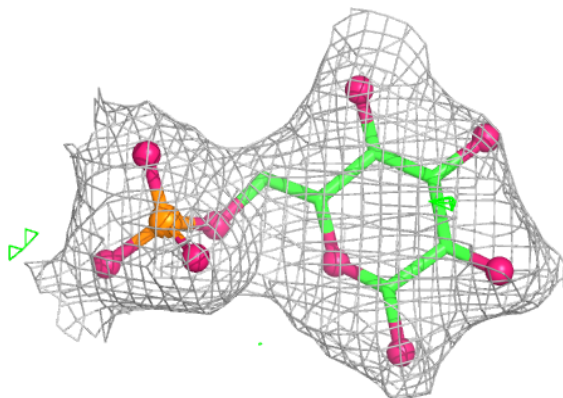


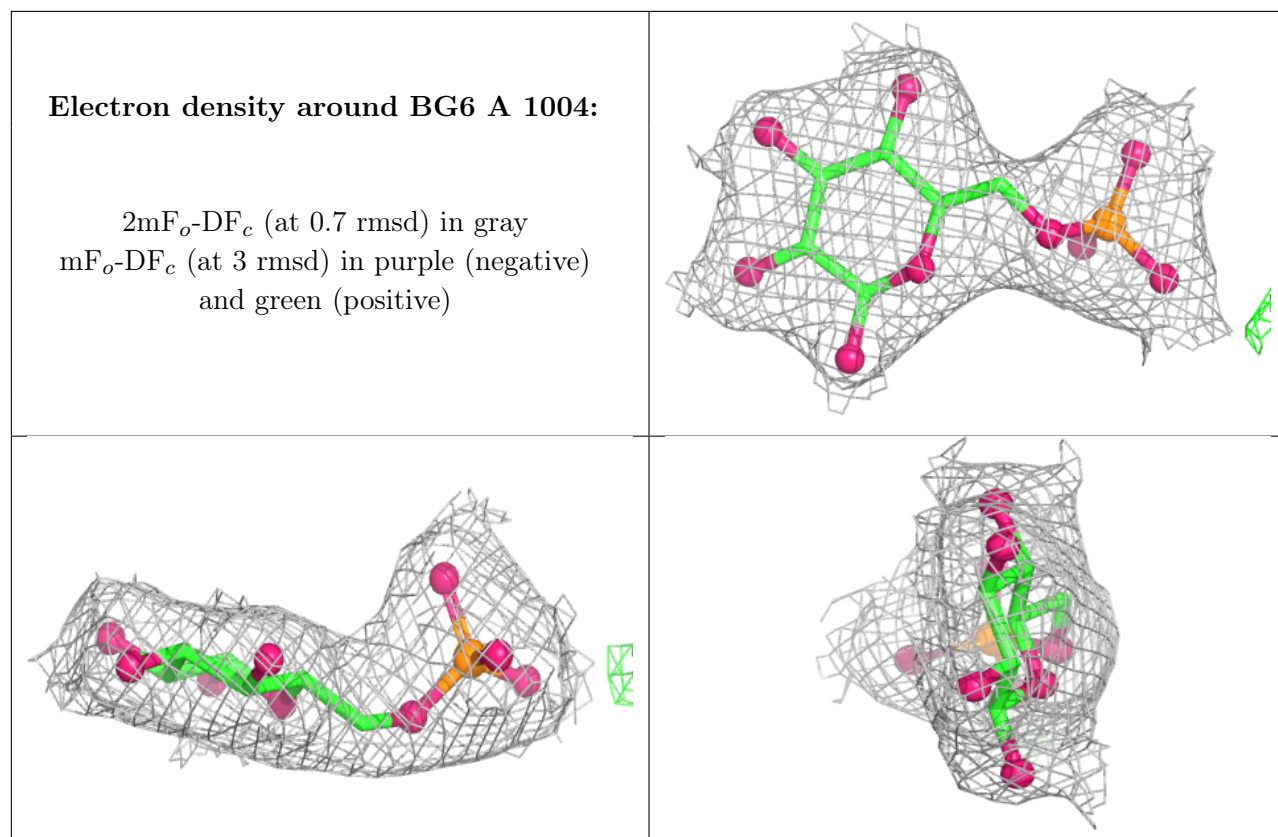
Electron density around BG6 B 1002:

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

**Electron density around BG6 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.