



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:57 AM UTC

PDB ID : 4AMV / pdb_00004amv
Title : E.COLI GLUCOSAMINE-6P SYNTHASE IN COMPLEX WITH FRUCTOSE-6P
Authors : Mouilleron, S.; Golinelli-Pimpaneau, B.
Deposited on : 2012-03-14
Resolution : 2.05 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

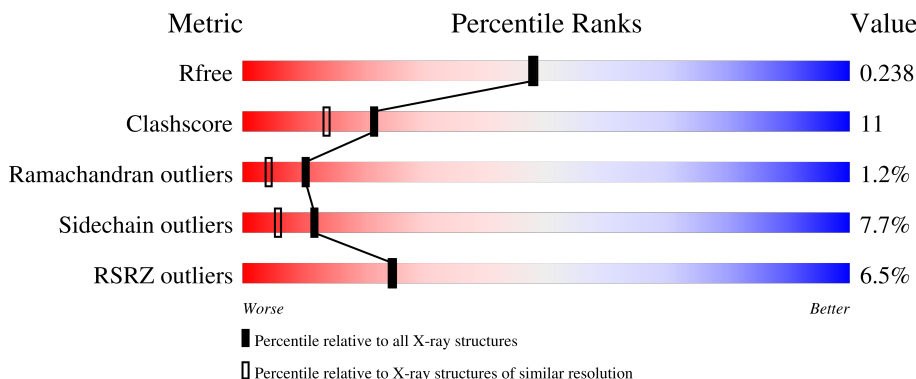
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	609	
1	B	609	
1	C	609	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	F6R	B	1609	X	-	-	-
2	F6R	C	1609	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14225 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.

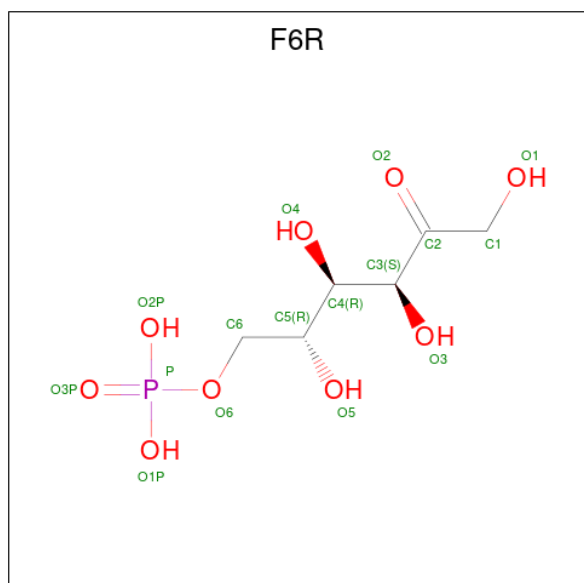
- Molecule 1 is a protein called GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINO-TRANSFERASE [ISOMER IZING].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4679	2945	823	894	17			
1	B	608	Total	C	N	O	S	0	0	0
			4198	2618	740	825	15			
1	C	608	Total	C	N	O	S	0	0	0
			4606	2897	812	880	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	LYS	ARG	conflict	UNP P17169
B	421	LYS	ARG	conflict	UNP P17169
C	421	LYS	ARG	conflict	UNP P17169

- Molecule 2 is FRUCTOSE -6-PHOSPHATE (CCD ID: F6R) (formula: $C_6H_{13}O_9P$).



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

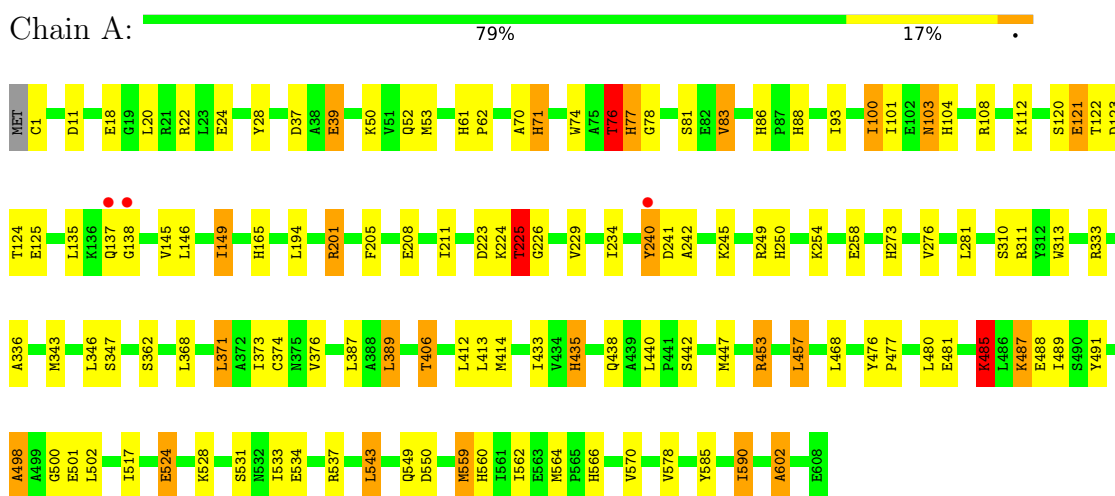
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	431	Total	O	0	0
			431	431		
3	B	53	Total	O	0	0
			53	53		
3	C	210	Total	O	0	0
			210	210		

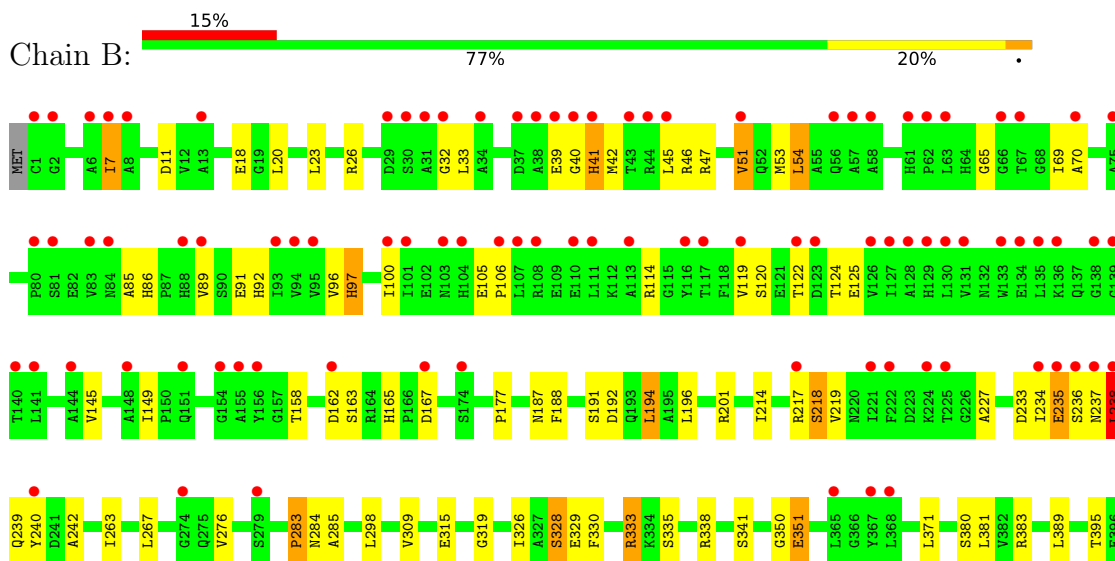
3 Residue-property plots

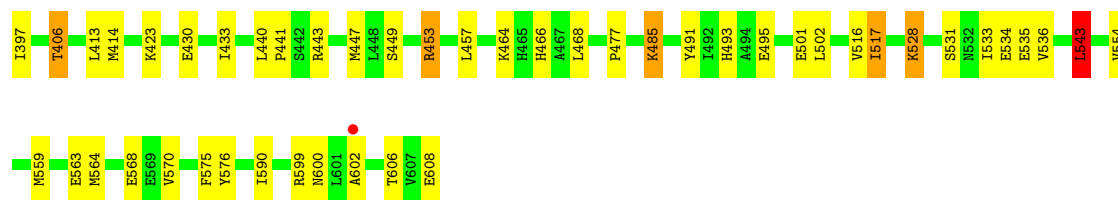
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMER IZING]

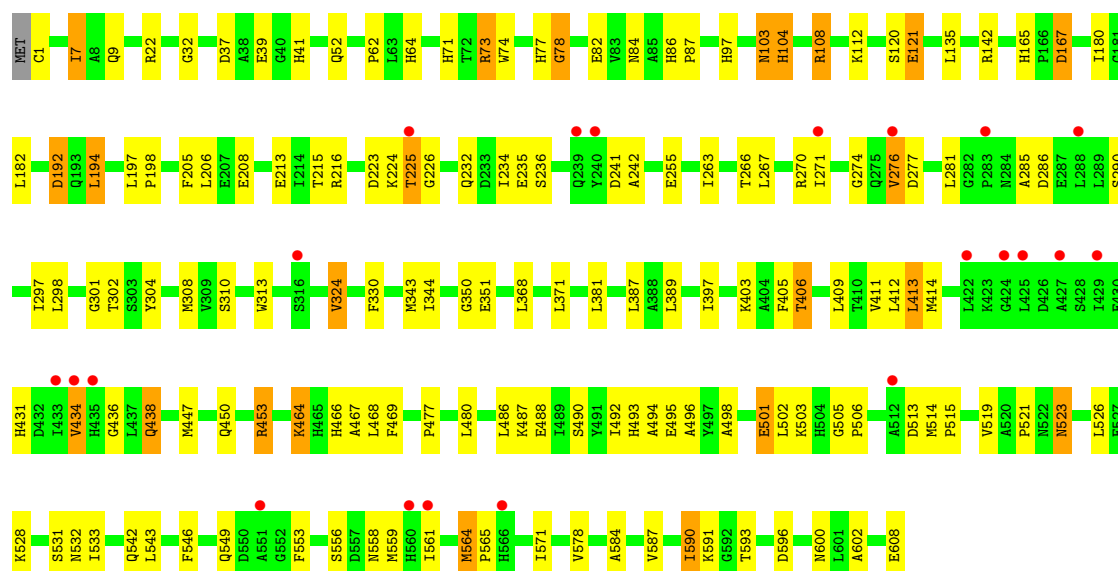
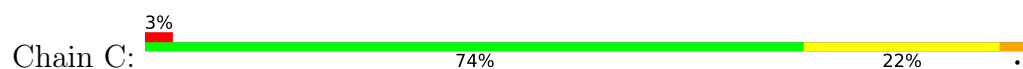


- Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMER IZING]





• Molecule 1: GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMER IZING]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.20Å 109.68Å 176.33Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	15.00 – 2.05 15.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-2.05) 98.3 (15.00-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.206 , 0.240 0.205 , 0.238	Depositor DCC
R_{free} test set	7769 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: F6R

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	1.29	12/4760 (0.3%)	1.26	25/6448 (0.4%)
1	B	1.09	12/4258 (0.3%)	1.09	12/5780 (0.2%)
1	C	1.08	8/4685 (0.2%)	1.13	12/6353 (0.2%)
All	All	1.16	32/13703 (0.2%)	1.16	49/18581 (0.3%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	ASP	C-O	19.99	1.49	1.24
1	B	167	ASP	C-N	18.30	1.56	1.33
1	B	39	GLU	C-N	-17.45	1.11	1.33
1	B	39	GLU	N-CA	14.82	1.65	1.46
1	B	42	MET	N-CA	14.26	1.63	1.46
1	B	41	HIS	C-N	13.61	1.51	1.33
1	B	39	GLU	C-O	9.49	1.36	1.24
1	A	76	THR	C-O	9.11	1.31	1.23
1	B	40	GLY	C-N	-7.93	1.22	1.33
1	A	435	HIS	CE1-NE2	7.47	1.40	1.32
1	A	435	HIS	CG-CD2	7.30	1.43	1.35
1	B	41	HIS	CA-C	6.88	1.61	1.52
1	B	41	HIS	N-CA	6.81	1.54	1.46
1	A	149	ILE	CA-CB	6.78	1.57	1.54
1	A	440	LEU	N-CA	-6.25	1.40	1.46
1	C	41	HIS	CG-CD2	6.20	1.42	1.35
1	C	104	HIS	CG-CD2	6.18	1.42	1.35
1	A	485	LYS	C-O	6.11	1.31	1.24
1	C	64	HIS	CG-CD2	6.08	1.42	1.35
1	C	64	HIS	ND1-CE1	5.84	1.38	1.32
1	A	560	HIS	ND1-CE1	5.82	1.38	1.32
1	B	92	HIS	CG-CD2	5.79	1.42	1.35
1	A	560	HIS	CG-CD2	5.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	ASP	N-CA	5.65	1.52	1.46
1	B	40	GLY	N-CA	-5.60	1.36	1.45
1	A	71	HIS	ND1-CE1	5.52	1.38	1.32
1	A	578	VAL	CA-C	5.29	1.57	1.52
1	C	167	ASP	CG-OD2	5.16	1.35	1.25
1	C	32	GLY	N-CA	5.13	1.51	1.45
1	A	476	TYR	C-O	-5.12	1.19	1.24
1	C	165	HIS	CG-ND1	-5.09	1.32	1.38
1	A	273	HIS	CG-CD2	5.04	1.41	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ASP	O-C-N	10.24	134.94	122.35
1	A	61	HIS	CA-C-N	-9.53	110.97	120.31
1	A	61	HIS	C-N-CA	-9.53	110.97	120.31
1	B	39	GLU	CA-C-N	-8.76	110.17	122.00
1	B	39	GLU	C-N-CA	-8.76	110.17	122.00
1	A	476	TYR	CA-C-N	-7.20	112.39	119.87
1	A	476	TYR	C-N-CA	-7.20	112.39	119.87
1	A	240	TYR	CA-C-N	7.05	129.73	120.28
1	A	240	TYR	C-N-CA	7.05	129.73	120.28
1	B	39	GLU	O-C-N	6.92	132.53	122.43
1	A	498	ALA	N-CA-C	-6.74	99.84	109.96
1	B	40	GLY	CA-C-O	6.70	126.49	118.86
1	C	7	ILE	CB-CA-C	6.61	117.94	110.41
1	A	376	VAL	N-CA-C	6.57	114.65	108.15
1	C	498	ALA	N-CA-C	-6.54	100.60	110.28
1	A	406	THR	OG1-CB-CG2	6.50	122.29	109.30
1	C	182	LEU	CA-C-N	-6.45	116.69	122.43
1	C	182	LEU	C-N-CA	-6.45	116.69	122.43
1	A	406	THR	N-CA-CB	-6.45	100.37	110.30
1	A	414	MET	CG-SD-CE	-6.42	86.79	100.90
1	A	333	ARG	CG-CD-NE	-6.23	98.30	112.00
1	A	241	ASP	N-CA-CB	-6.09	101.17	110.12
1	A	201	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	A	406	THR	CA-CB-CG2	6.05	120.78	110.50
1	A	500	GLY	N-CA-C	-5.84	106.55	115.66
1	B	41	HIS	CA-C-O	-5.82	112.19	120.51
1	B	165	HIS	CA-C-N	5.66	126.73	120.45
1	B	165	HIS	C-N-CA	5.66	126.73	120.45
1	C	216	ARG	CB-CA-C	-5.58	100.30	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ALA	N-CA-C	5.57	118.12	111.71
1	C	73	ARG	N-CA-C	5.56	118.29	109.50
1	A	1	CYS	CA-CB-SG	-5.53	101.67	114.40
1	C	564	MET	CA-C-N	-5.51	112.95	119.84
1	C	564	MET	C-N-CA	-5.51	112.95	119.84
1	C	37	ASP	CA-C-N	5.42	127.55	120.28
1	C	37	ASP	C-N-CA	5.42	127.55	120.28
1	B	543	LEU	N-CA-C	5.40	118.42	109.46
1	C	532	ASN	N-CA-C	5.25	117.75	111.71
1	B	41	HIS	O-C-N	5.21	129.52	122.59
1	A	18	GLU	N-CA-C	-5.19	105.70	111.36
1	B	97	HIS	N-CA-C	5.18	117.12	108.99
1	A	336	ALA	N-CA-C	-5.15	100.34	108.73
1	A	165	HIS	CA-C-N	5.12	125.80	120.12
1	A	165	HIS	C-N-CA	5.12	125.80	120.12
1	A	602	ALA	N-CA-C	-5.09	101.51	108.38
1	B	227	ALA	N-CA-C	5.09	117.42	110.24
1	A	590	ILE	CB-CA-C	-5.08	105.28	112.14
1	A	241	ASP	N-CA-C	5.08	116.81	111.28
1	A	442	SER	CB-CA-C	-5.02	102.46	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4679	0	4689	100	1
1	B	4198	0	3877	92	0
1	C	4606	0	4563	124	1
2	A	16	0	8	0	0
2	B	16	0	11	0	0
2	C	16	0	11	0	0
3	A	431	0	0	10	0
3	B	53	0	0	6	0
3	C	210	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14225	0	13159	288	1

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 11.

All (288) 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:447:MET:HE1	1:B:564:MET:SD	1.84	1.17
1:C:270:ARG:HB3	1:C:414:MET:HE1	1.15	1.15
1:A:240:TYR:HB3	1:C:235:GLU:CG	1.81	1.10
1:A:240:TYR:HB3	1:C:235:GLU:HG2	1.29	1.05
1:A:240:TYR:CB	1:C:235:GLU:HG2	1.86	1.05
1:B:453:ARG:HG2	1:B:453:ARG:HH11	1.18	1.02
1:C:104:HIS:CE1	1:C:108:ARG:HH21	1.76	1.02
1:A:201:ARG:HH12	1:A:240:TYR:HD1	1.07	0.94
1:B:534:GLU:HG2	3:B:2005:HOH:O	1.73	0.88
1:C:596:ASP:HB2	3:C:2161:HOH:O	1.72	0.88
1:B:453:ARG:HH11	1:B:453:ARG:CG	1.86	0.88
1:B:466:HIS:HD2	1:C:493:HIS:CD2	1.91	0.88
1:C:270:ARG:CB	1:C:414:MET:HE1	2.03	0.87
1:B:466:HIS:HD2	1:C:493:HIS:HD2	1.19	0.86
1:C:103:ASN:HD22	1:C:103:ASN:H	1.23	0.85
1:B:466:HIS:CD2	1:C:493:HIS:HD2	1.97	0.83
1:B:267:LEU:CD2	1:B:414:MET:HE3	2.08	0.83
1:B:263:ILE:HD11	1:B:406:THR:HG23	1.59	0.82
1:C:593:THR:HG21	3:C:2194:HOH:O	1.80	0.82
1:A:533:ILE:HG23	1:A:543:LEU:HD22	1.61	0.81
1:A:240:TYR:HB3	1:C:235:GLU:CD	2.06	0.81
1:A:104:HIS:CE1	1:A:108:ARG:HD2	2.16	0.81
1:B:351:GLU:HG3	1:B:606:THR:CG2	2.11	0.81
1:B:351:GLU:HG3	1:B:606:THR:HG22	1.61	0.80
1:B:533:ILE:HG21	1:B:559:MET:HE1	1.64	0.80
1:A:225:THR:OG1	1:A:226:GLY:N	2.13	0.80
1:A:240:TYR:CB	1:C:235:GLU:CG	2.55	0.79
1:A:103:ASN:HD22	1:A:103:ASN:H	1.30	0.79
1:B:120:SER:OG	1:B:122:THR:HG22	1.81	0.79
1:B:453:ARG:HG2	1:B:453:ARG:NH1	1.93	0.78
1:A:281:LEU:HD21	1:A:389:LEU:HD13	1.67	0.76
1:B:493:HIS:HE1	1:C:495:GLU:OE1	1.68	0.76
1:B:267:LEU:HD23	1:B:414:MET:HE3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:THR:HG23	1:B:125:GLU:H	1.52	0.74
1:C:205:PHE:HE2	1:C:234:ILE:HD11	1.53	0.74
1:A:453:ARG:HG3	1:A:453:ARG:HH11	1.51	0.73
1:A:39:GLU:CD	1:A:39:GLU:N	2.46	0.73
1:C:194:LEU:HD21	1:C:397:ILE:HD11	1.71	0.73
1:A:11:ASP:H	1:C:9:GLN:NE2	1.87	0.72
1:C:492:ILE:HD12	3:C:2196:HOH:O	1.87	0.72
1:A:104:HIS:HE1	1:A:108:ARG:HD2	1.52	0.72
1:A:240:TYR:CD2	1:C:235:GLU:HG3	2.25	0.72
1:B:217:ARG:O	1:B:218:SER:HB3	1.89	0.71
1:A:39:GLU:CD	1:A:39:GLU:H	1.99	0.71
1:B:47:ARG:HG2	1:B:53:MET:CG	2.21	0.71
1:C:270:ARG:HB3	1:C:414:MET:CE	2.09	0.70
1:B:430:GLU:HB3	3:B:2022:HOH:O	1.90	0.69
1:C:447:MET:HE1	1:C:564:MET:SD	2.32	0.69
1:A:201:ARG:NH1	1:A:240:TYR:CD1	2.58	0.68
1:C:108:ARG:HH22	1:C:121:GLU:HA	1.58	0.68
1:A:122:THR:HG23	1:A:125:GLU:H	1.59	0.67
1:B:350:GLY:HA2	1:B:381:LEU:HD12	1.76	0.67
1:B:491:TYR:CZ	1:B:599:ARG:HG2	2.30	0.67
1:C:453:ARG:HG2	1:C:453:ARG:HH11	1.60	0.67
1:A:201:ARG:NH1	3:A:2161:HOH:O	2.28	0.67
1:B:466:HIS:CD2	1:C:493:HIS:CD2	2.78	0.67
1:C:103:ASN:HD22	1:C:103:ASN:N	1.93	0.67
1:B:263:ILE:HD11	1:B:406:THR:CG2	2.25	0.66
1:C:180:ILE:HD12	1:C:206:LEU:HD21	1.77	0.66
1:C:71:HIS:CE1	1:C:73:ARG:HB3	2.30	0.66
1:A:205:PHE:HE2	1:A:234:ILE:HD11	1.60	0.66
1:C:546:PHE:HD2	1:C:564:MET:HE3	1.61	0.66
1:C:298:LEU:HD11	1:C:330:PHE:CD2	2.31	0.65
1:A:240:TYR:HB2	1:C:235:GLU:HG2	1.77	0.65
1:C:490:SER:HA	3:C:2194:HOH:O	1.96	0.65
1:A:11:ASP:H	1:C:9:GLN:HE22	1.44	0.65
1:C:205:PHE:CE2	1:C:234:ILE:HD11	2.31	0.65
1:A:120:SER:OG	1:A:122:THR:HG22	1.97	0.65
1:B:535:GLU:OE1	3:B:2048:HOH:O	2.13	0.65
1:C:453:ARG:HG2	1:C:453:ARG:NH1	2.12	0.65
1:B:495:GLU:OE1	1:C:493:HIS:HE1	1.79	0.65
1:A:93:ILE:HD11	1:A:135:LEU:HD12	1.79	0.64
1:A:76:THR:HG22	1:A:77:HIS:N	2.13	0.64
1:A:550:ASP:OD2	1:A:566:HIS:CE1	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ILE:CG2	1:B:559:MET:HE1	2.27	0.64
1:C:104:HIS:CE1	1:C:108:ARG:NH2	2.60	0.64
1:C:225:THR:OG1	1:C:226:GLY:N	2.30	0.64
1:C:310:SER:HB3	1:C:412:LEU:HD13	1.79	0.64
1:C:9:GLN:O	1:C:9:GLN:HG2	1.97	0.63
1:C:549:GLN:HG3	1:C:564:MET:O	1.97	0.63
1:B:145:VAL:O	1:B:149:ILE:HG12	2.00	0.62
1:A:537:ARG:HG2	1:A:543:LEU:HD13	1.81	0.62
1:B:443:ARG:NH1	1:B:568:GLU:OE1	2.31	0.62
1:B:447:MET:CE	1:B:564:MET:SD	2.76	0.62
1:A:223:ASP:O	1:A:225:THR:O	2.18	0.62
1:B:440:LEU:HB3	1:B:441:PRO:HD3	1.81	0.61
1:A:223:ASP:OD1	1:A:225:THR:HG23	2.00	0.61
1:B:395:THR:HA	3:B:2017:HOH:O	2.00	0.61
1:C:350:GLY:HA2	1:C:381:LEU:HD12	1.83	0.60
1:C:492:ILE:HD11	1:C:591:LYS:HE3	1.83	0.60
1:B:194:LEU:HD21	1:B:397:ILE:HD11	1.83	0.60
1:C:223:ASP:O	1:C:225:THR:O	2.20	0.59
1:A:453:ARG:NH1	1:A:457:LEU:HD13	2.17	0.59
1:C:542:GLN:HA	1:C:558:ASN:HB3	1.84	0.59
1:A:81:SER:OG	1:A:83:VAL:HG23	2.03	0.59
1:A:564:MET:HE2	1:A:564:MET:HA	1.84	0.59
1:C:468:LEU:HD13	1:C:514:MET:SD	2.43	0.58
1:C:490:SER:CA	3:C:2194:HOH:O	2.49	0.58
1:C:180:ILE:CD1	1:C:206:LEU:HD21	2.33	0.58
1:C:301:GLY:O	1:C:304:TYR:HB3	2.03	0.58
1:A:537:ARG:CG	1:A:543:LEU:HD13	2.33	0.57
1:A:240:TYR:HB3	1:C:235:GLU:OE2	2.03	0.57
1:C:304:TYR:CE2	1:C:308:MET:HE2	2.39	0.57
1:A:52:GLN:HG3	1:A:53:MET:HE2	1.85	0.57
1:A:258:GLU:HG2	3:A:2195:HOH:O	2.05	0.57
1:B:351:GLU:CG	1:B:606:THR:HG22	2.33	0.57
1:A:346:LEU:HD23	1:A:373:ILE:HB	1.87	0.57
1:C:22:ARG:NH1	3:C:2026:HOH:O	2.38	0.57
1:C:104:HIS:NE2	1:C:108:ARG:NH2	2.48	0.57
1:B:20:LEU:HD11	1:B:70:ALA:HB1	1.87	0.56
1:B:493:HIS:HD2	1:C:466:HIS:ND1	2.03	0.56
1:C:263:ILE:O	1:C:267:LEU:HG	2.05	0.56
1:C:313:TRP:CH2	1:C:413:LEU:HD22	2.41	0.56
1:B:69:ILE:HD12	1:B:96:VAL:HG22	1.87	0.56
1:B:235:GLU:HG3	1:B:236:SER:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:HA2	1:B:54:LEU:HD11	1.87	0.56
1:C:84:ASN:HD22	1:C:120:SER:HB2	1.71	0.56
1:C:263:ILE:HD11	1:C:406:THR:HG23	1.87	0.56
1:B:464:LYS:HA	3:B:2023:HOH:O	2.05	0.55
1:A:534:GLU:OE1	3:A:2395:HOH:O	2.18	0.55
1:B:517:ILE:N	1:B:517:ILE:HD12	2.21	0.55
1:A:250:HIS:HD2	1:A:585:TYR:OH	1.89	0.55
1:A:249:ARG:NE	3:A:2182:HOH:O	2.34	0.55
1:B:447:MET:HE2	1:B:575:PHE:CE2	2.42	0.55
1:A:93:ILE:HD11	1:A:135:LEU:CD1	2.36	0.55
1:A:103:ASN:HD22	1:A:103:ASN:N	2.01	0.54
1:A:453:ARG:HH12	1:A:457:LEU:HD13	1.71	0.54
1:A:194:LEU:HG	3:A:2037:HOH:O	2.07	0.54
1:B:47:ARG:HG2	1:B:53:MET:HG2	1.88	0.54
1:C:313:TRP:CE3	1:C:413:LEU:HD13	2.41	0.54
1:A:201:ARG:NH1	1:A:240:TYR:HD1	1.91	0.54
1:B:267:LEU:HD22	1:B:414:MET:HE3	1.87	0.54
1:C:477:PRO:HA	1:C:480:LEU:HD12	1.88	0.54
1:A:74:TRP:CE3	1:A:602:ALA:HB3	2.43	0.54
1:C:453:ARG:HH11	1:C:453:ARG:CG	2.21	0.54
1:A:343:MET:HE3	1:A:362:SER:HB3	1.90	0.53
1:A:240:TYR:HE2	1:C:236:SER:O	1.90	0.53
1:C:286:ASP:O	1:C:290:SER:HB2	2.08	0.53
1:B:267:LEU:HD23	1:B:414:MET:CE	2.34	0.53
1:B:495:GLU:OE1	1:C:493:HIS:CE1	2.61	0.53
1:C:523:ASN:HB2	3:C:2200:HOH:O	2.09	0.53
1:A:28:TYR:HB2	1:A:50:LYS:HD3	1.90	0.53
1:C:86:HIS:HB3	1:C:87:PRO:HA	1.91	0.53
1:A:447:MET:HE1	1:A:564:MET:SD	2.49	0.52
1:C:142:ARG:NH1	1:C:213:GLU:OE1	2.42	0.52
1:C:447:MET:HG2	1:C:578:VAL:HB	1.91	0.52
1:C:281:LEU:HD21	1:C:389:LEU:HD13	1.90	0.52
1:C:297:ILE:HB	1:C:324:VAL:HG13	1.91	0.52
1:B:298:LEU:HD11	1:B:330:PHE:CD2	2.44	0.52
1:B:453:ARG:CG	1:B:453:ARG:NH1	2.57	0.52
1:C:103:ASN:H	1:C:103:ASN:ND2	1.99	0.52
1:B:283:PRO:C	1:B:285:ALA:H	2.18	0.51
1:C:71:HIS:HE1	1:C:73:ARG:HB3	1.75	0.51
1:A:517:ILE:HD12	1:A:517:ILE:N	2.26	0.51
1:A:537:ARG:HD2	1:A:559:MET:SD	2.50	0.51
1:B:18:GLU:OE1	1:B:18:GLU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LEU:HG	1:C:343:MET:SD	2.51	0.50
1:B:192:ASP:OD2	1:B:194:LEU:HB2	2.10	0.50
1:A:22:ARG:NH1	3:A:2037:HOH:O	2.24	0.50
1:C:274:GLY:O	1:C:431:HIS:HD2	1.94	0.50
1:A:62:PRO:HD2	3:A:2065:HOH:O	2.11	0.50
1:B:283:PRO:O	1:B:285:ALA:N	2.45	0.49
1:C:297:ILE:HA	1:C:344:ILE:O	2.13	0.49
1:C:84:ASN:ND2	1:C:120:SER:HB2	2.28	0.49
1:C:223:ASP:OD1	1:C:225:THR:HG23	2.13	0.49
1:C:270:ARG:O	1:C:277:ASP:N	2.33	0.49
1:C:513:ASP:O	1:C:515:PRO:HD3	2.13	0.49
1:A:100:ILE:C	1:A:100:ILE:HD13	2.38	0.49
1:A:100:ILE:HD13	1:A:101:ILE:C	2.38	0.49
1:A:108:ARG:HH12	1:A:121:GLU:HB3	1.78	0.49
1:B:188:PHE:HB3	1:B:196:LEU:HD22	1.93	0.49
1:B:162:ASP:C	1:B:162:ASP:OD1	2.56	0.48
1:B:32:GLY:HA3	1:B:86:HIS:O	2.13	0.48
1:C:466:HIS:NE2	3:C:2193:HOH:O	2.30	0.48
1:A:100:ILE:HD13	1:A:101:ILE:N	2.27	0.48
1:C:121:GLU:OE1	1:C:121:GLU:N	2.44	0.48
1:B:32:GLY:HA3	1:B:46:ARG:HG2	1.96	0.48
1:C:241:ASP:O	1:C:242:ALA:C	2.55	0.48
1:C:436:GLY:O	1:C:571:ILE:HD13	2.12	0.48
1:A:37:ASP:OD1	1:A:37:ASP:C	2.57	0.48
1:A:485:LYS:HA	1:A:485:LYS:HD3	1.66	0.48
1:C:7:ILE:HD13	1:C:215:THR:HA	1.94	0.48
1:A:481:GLU:OE2	1:A:485:LYS:NZ	2.47	0.48
1:C:271:ILE:HG21	1:C:438:GLN:NE2	2.29	0.48
1:C:192:ASP:OD1	1:C:194:LEU:HB2	2.14	0.48
1:C:255:GLU:HG2	1:C:403:LYS:HE2	1.96	0.47
1:C:371:LEU:HD23	1:C:387:LEU:HB2	1.97	0.47
1:C:591:LYS:NZ	3:C:2205:HOH:O	2.12	0.47
1:A:240:TYR:CE2	1:C:236:SER:O	2.67	0.47
1:B:329:GLU:O	1:B:333:ARG:HG2	2.13	0.47
1:B:267:LEU:CD2	1:B:414:MET:CE	2.87	0.47
1:C:266:THR:O	1:C:270:ARG:HD2	2.14	0.47
1:C:389:LEU:HD23	1:C:411:VAL:HG13	1.96	0.47
1:A:254:LYS:O	1:A:258:GLU:HG3	2.14	0.47
1:A:498:ALA:O	1:A:501:GLU:HG2	2.15	0.47
1:B:466:HIS:HE1	3:B:2025:HOH:O	1.97	0.47
1:A:234:ILE:HD12	1:A:234:ILE:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:SER:O	1:A:374:CYS:HA	2.15	0.47
1:A:435:HIS:HB3	3:A:2325:HOH:O	2.15	0.47
1:B:338:ARG:O	1:B:341:SER:HB2	2.16	0.46
1:A:104:HIS:HE1	1:A:108:ARG:CD	2.26	0.46
1:C:486:LEU:HD13	1:C:584:ALA:HA	1.97	0.46
1:C:505:GLY:N	1:C:506:PRO:CD	2.78	0.46
1:A:146:LEU:HD23	1:A:211:ILE:HD12	1.97	0.46
1:A:487:LYS:HG2	1:A:488:GLU:N	2.30	0.46
1:B:47:ARG:CB	1:B:54:LEU:HD22	2.46	0.46
1:C:464:LYS:HE3	3:C:2192:HOH:O	2.16	0.46
1:B:564:MET:HG3	1:B:576:TYR:CE2	2.51	0.46
1:C:74:TRP:CE3	1:C:602:ALA:HB3	2.51	0.46
1:A:549:GLN:HG3	1:A:564:MET:O	2.15	0.45
1:A:311:ARG:NH1	3:A:2242:HOH:O	2.14	0.45
1:B:7:ILE:HD13	1:B:214:ILE:O	2.17	0.45
1:B:7:ILE:CD1	1:B:214:ILE:HG22	2.46	0.45
1:B:309:VAL:CG2	1:B:477:PRO:HB2	2.46	0.45
1:A:145:VAL:O	1:A:149:ILE:HG12	2.17	0.45
1:B:533:ILE:HG23	1:B:543:LEU:HD22	1.99	0.45
1:C:447:MET:O	1:C:450:GLN:HB2	2.17	0.45
1:C:521:PRO:O	1:C:526:LEU:HD13	2.16	0.45
1:B:351:GLU:HG3	1:B:606:THR:HG21	1.96	0.45
1:B:485:LYS:HA	1:B:485:LYS:HD3	1.59	0.45
1:C:197:LEU:N	1:C:198:PRO:CD	2.79	0.45
1:A:103:ASN:H	1:A:103:ASN:ND2	2.08	0.45
1:A:76:THR:CG2	1:A:77:HIS:N	2.81	0.44
1:A:457:LEU:HD21	1:A:562:ILE:HD11	1.99	0.44
1:A:88:HIS:NE2	1:A:122:THR:HG21	2.32	0.44
1:A:313:TRP:CD2	1:A:413:LEU:HD13	2.52	0.44
1:B:315:GLU:O	1:B:319:GLY:HA2	2.17	0.44
1:B:326:ILE:HD13	1:C:501:GLU:HB3	1.99	0.44
1:C:453:ARG:NH1	1:C:453:ARG:CG	2.81	0.44
1:C:590:ILE:HD12	1:C:590:ILE:HA	1.87	0.44
1:A:310:SER:HB3	1:A:412:LEU:HD13	2.00	0.44
1:C:62:PRO:HB3	3:C:2069:HOH:O	2.17	0.44
1:C:167:ASP:HB3	3:C:2132:HOH:O	2.17	0.44
1:C:467:ALA:O	1:C:494:ALA:HA	2.18	0.44
1:C:490:SER:C	3:C:2194:HOH:O	2.59	0.44
1:A:477:PRO:HA	1:A:480:LEU:HD12	1.99	0.43
1:A:88:HIS:CD2	1:A:122:THR:HG21	2.53	0.43
1:A:371:LEU:HD23	1:A:387:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:NH1	1:B:85:ALA:O	2.46	0.43
1:A:240:TYR:CE2	1:C:236:SER:HB3	2.54	0.43
1:A:240:TYR:CD2	1:C:235:GLU:CG	3.00	0.43
1:B:47:ARG:HB2	1:B:54:LEU:HD22	2.00	0.43
1:C:469:PHE:O	1:C:496:ALA:HA	2.18	0.43
1:C:553:PHE:HB3	1:C:561:ILE:HD12	2.01	0.43
1:C:405:PHE:CE2	1:C:409:LEU:HD11	2.53	0.43
1:A:240:TYR:CG	1:C:235:GLU:CG	3.01	0.42
1:C:487:LYS:HG2	1:C:488:GLU:N	2.33	0.42
1:A:433:ILE:HG12	1:A:570:VAL:HG21	2.01	0.42
1:B:528:LYS:HD2	1:B:528:LYS:HA	1.76	0.42
1:A:104:HIS:HD2	1:A:123:ASP:OD1	2.01	0.42
1:B:493:HIS:CD2	1:C:466:HIS:ND1	2.85	0.42
1:B:237:ASN:O	1:B:238:LEU:CB	2.66	0.42
1:A:453:ARG:HH12	1:A:457:LEU:CD1	2.32	0.42
1:C:533:ILE:HG23	1:C:543:LEU:HD22	2.01	0.42
1:B:201:ARG:O	1:B:236:SER:HB2	2.20	0.42
1:B:599:ARG:O	1:B:600:ASN:HB2	2.19	0.42
1:C:104:HIS:CD2	1:C:104:HIS:C	2.97	0.42
1:B:493:HIS:CE1	1:C:495:GLU:OE1	2.59	0.41
1:A:453:ARG:HG3	1:A:453:ARG:NH1	2.28	0.41
1:B:237:ASN:O	1:B:238:LEU:HB3	2.20	0.41
1:A:245:LYS:CE	3:A:2179:HOH:O	2.68	0.41
1:A:254:LYS:NZ	1:A:258:GLU:OE2	2.37	0.41
1:B:26:ARG:O	1:B:602:ALA:HB1	2.20	0.41
1:C:77:HIS:O	1:C:78:GLY:O	2.39	0.41
1:B:187:ASN:ND2	1:B:219:VAL:HG23	2.36	0.41
1:B:309:VAL:HG22	1:B:477:PRO:HB2	2.02	0.41
1:B:608:GLU:C	1:C:503:LYS:HZ1	2.28	0.41
1:A:201:ARG:NH1	1:A:240:TYR:CE1	2.87	0.41
1:C:62:PRO:HA	3:C:2069:HOH:O	2.19	0.41
1:B:326:ILE:HG12	1:B:328:SER:OG	2.21	0.41
1:A:71:HIS:HB3	1:A:86:HIS:HB2	2.03	0.41
1:A:457:LEU:HD21	1:A:562:ILE:CG1	2.51	0.41
1:B:23:LEU:HD21	1:B:192:ASP:HB3	2.03	0.41
1:B:433:ILE:HG12	1:B:570:VAL:HG21	2.03	0.41
1:B:443:ARG:HH12	1:B:568:GLU:CD	2.28	0.41
1:B:516:VAL:HG21	1:B:536:VAL:HG11	2.03	0.41
1:C:587:VAL:HG11	3:C:2196:HOH:O	2.20	0.41
1:B:11:ASP:HA	1:B:65:GLY:O	2.21	0.41
1:B:528:LYS:HE2	1:C:608:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:O	1:A:489:ILE:HG12	2.21	0.40
1:C:276:VAL:HG23	1:C:434:VAL:HG23	2.03	0.40
1:B:177:PRO:HB2	1:B:191:SER:O	2.22	0.40
1:A:20:LEU:HD11	1:A:70:ALA:HB1	2.04	0.40
1:A:88:HIS:CD2	1:A:124:THR:HB	2.57	0.40
1:A:524:GLU:H	1:A:524:GLU:CD	2.29	0.40
1:A:24:GLU:HG2	1:A:28:TYR:HB3	2.02	0.40
1:B:51:VAL:C	1:B:53:MET:H	2.29	0.40
1:C:549:GLN:NE2	1:C:565:PRO:HA	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:O	1:C:82:GLU:OE1[2_656]	1.92	0.28

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	606/609 (100%)	591 (98%)	11 (2%)	4 (1%)	18	10
1	B	606/609 (100%)	557 (92%)	33 (5%)	16 (3%)	4	0
1	C	606/609 (100%)	580 (96%)	25 (4%)	1 (0%)	43	37
All	All	1818/1827 (100%)	1728 (95%)	69 (4%)	21 (1%)	10	4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	106	PRO
1	B	235	GLU
1	B	238	LEU

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Mol	Chain	Res	Type
1	B	240	TYR
1	B	284	ASN
1	B	423	LYS
1	A	225	THR
1	B	105	GLU
1	C	78	GLY
1	A	78	GLY
1	A	224	LYS
1	A	242	ALA
1	B	91	GLU
1	B	163	SER
1	B	41	HIS
1	B	51	VAL
1	B	114	ARG
1	B	218	SER
1	B	283	PRO
1	B	239	GLN
1	B	242	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	497/501 (99%)	466 (94%)	31 (6%)	16	9
1	B	388/501 (77%)	349 (90%)	39 (10%)	7	3
1	C	479/501 (96%)	444 (93%)	35 (7%)	13	7
All	All	1364/1503 (91%)	1259 (92%)	105 (8%)	12	6

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	76	THR
1	A	77	HIS
1	A	83	VAL

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Mol	Chain	Res	Type
1	A	100	ILE
1	A	103	ASN
1	A	112	LYS
1	A	121	GLU
1	A	137	GLN
1	A	208	GLU
1	A	225	THR
1	A	229	VAL
1	A	276	VAL
1	A	368	LEU
1	A	371	LEU
1	A	389	LEU
1	A	406	THR
1	A	438	GLN
1	A	453	ARG
1	A	457	LEU
1	A	468	LEU
1	A	485	LYS
1	A	487	LYS
1	A	491	TYR
1	A	502	LEU
1	A	524	GLU
1	A	528	LYS
1	A	531	SER
1	A	543	LEU
1	A	559	MET
1	A	590	ILE
1	B	7	ILE
1	B	33	LEU
1	B	45	LEU
1	B	54	LEU
1	B	89	VAL
1	B	97	HIS
1	B	100	ILE
1	B	119	VAL
1	B	124	THR
1	B	158	THR
1	B	194	LEU
1	B	233	ASP
1	B	234	ILE
1	B	238	LEU
1	B	276	VAL

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Mol	Chain	Res	Type
1	B	328	SER
1	B	333	ARG
1	B	335	SER
1	B	351	GLU
1	B	371	LEU
1	B	380	SER
1	B	383	ARG
1	B	389	LEU
1	B	406	THR
1	B	413	LEU
1	B	449	SER
1	B	453	ARG
1	B	457	LEU
1	B	468	LEU
1	B	485	LYS
1	B	501	GLU
1	B	502	LEU
1	B	517	ILE
1	B	528	LYS
1	B	531	SER
1	B	543	LEU
1	B	554	VAL
1	B	563	GLU
1	B	590	ILE
1	C	1	CYS
1	C	39	GLU
1	C	52	GLN
1	C	97	HIS
1	C	103	ASN
1	C	108	ARG
1	C	112	LYS
1	C	121	GLU
1	C	135	LEU
1	C	194	LEU
1	C	208	GLU
1	C	224	LYS
1	C	225	THR
1	C	232	GLN
1	C	276	VAL
1	C	302	THR
1	C	324	VAL
1	C	351	GLU

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Mol	Chain	Res	Type
1	C	368	LEU
1	C	406	THR
1	C	413	LEU
1	C	434	VAL
1	C	438	GLN
1	C	453	ARG
1	C	464	LYS
1	C	501	GLU
1	C	502	LEU
1	C	519	VAL
1	C	523	ASN
1	C	528	LYS
1	C	531	SER
1	C	556	SER
1	C	559	MET
1	C	590	ILE
1	C	600	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	84	ASN
1	A	103	ASN
1	A	104	HIS
1	A	237	ASN
1	A	250	HIS
1	A	265	ASN
1	A	446	GLN
1	A	542	GLN
1	B	86	HIS
1	B	97	HIS
1	B	250	HIS
1	B	265	ASN
1	B	296	GLN
1	B	466	HIS
1	B	493	HIS
1	B	542	GLN
1	B	600	ASN
1	C	9	GLN
1	C	56	GLN
1	C	71	HIS

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Mol	Chain	Res	Type
1	C	84	ASN
1	C	86	HIS
1	C	103	ASN
1	C	250	HIS
1	C	265	ASN
1	C	431	HIS
1	C	438	GLN
1	C	450	GLN
1	C	493	HIS
1	C	522	ASN
1	C	523	ASN
1	C	542	GLN
1	C	549	GLN
1	C	566	HIS
1	C	600	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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	F6R	A	1609	-	15,15,15	2.51	6 (40%)	16,21,21	2.94	8 (50%)
2	F6R	C	1609	-	15,15,15	1.30	1 (6%)	16,21,21	2.86	8 (50%)
2	F6R	B	1609	-	15,15,15	0.95	0	16,21,21	2.60	8 (50%)

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	F6R	A	1609	-	-	4/20/20/20	-
2	F6R	C	1609	-	2/2/5/5	10/20/20/20	-
2	F6R	B	1609	-	2/2/5/5	8/20/20/20	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1609	F6R	C6-C5	-5.72	1.44	1.51
2	A	1609	F6R	C5-C4	-4.64	1.45	1.53
2	A	1609	F6R	O4-C4	-3.34	1.34	1.43
2	C	1609	F6R	C6-C5	-3.25	1.47	1.51
2	A	1609	F6R	O2-C2	3.19	1.26	1.21
2	A	1609	F6R	C4-C3	-2.38	1.48	1.53
2	A	1609	F6R	O5-C5	-2.01	1.39	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1609	F6R	O4-C4-C3	5.91	119.89	109.29
2	A	1609	F6R	O4-C4-C3	5.81	119.72	109.29
2	C	1609	F6R	O4-C4-C3	5.80	119.69	109.29
2	C	1609	F6R	O5-C5-C4	5.10	121.18	109.25
2	A	1609	F6R	O5-C5-C6	4.81	120.60	109.99
2	A	1609	F6R	C5-C4-C3	4.31	119.13	112.05
2	B	1609	F6R	O3-C3-C4	-4.21	101.23	110.38
2	A	1609	F6R	O3-C3-C4	-4.19	101.29	110.38
2	C	1609	F6R	O3-C3-C4	-3.89	101.93	110.38
2	C	1609	F6R	O6-C6-C5	-3.86	99.07	109.36
2	C	1609	F6R	O4-C4-C5	3.73	117.40	108.93
2	B	1609	F6R	O4-C4-C5	3.55	117.00	108.93
2	A	1609	F6R	O4-C4-C5	3.53	116.96	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1609	F6R	O5-C5-C4	3.29	116.95	109.25
2	A	1609	F6R	C6-C5-C4	3.05	117.96	112.22
2	C	1609	F6R	O5-C5-C6	3.00	116.61	109.99
2	B	1609	F6R	O5-C5-C4	2.94	116.14	109.25
2	A	1609	F6R	O6-C6-C5	-2.87	101.71	109.36
2	C	1609	F6R	C6-C5-C4	2.78	117.46	112.22
2	B	1609	F6R	O6-C6-C5	-2.71	102.11	109.36
2	B	1609	F6R	C5-C4-C3	2.35	115.91	112.05
2	B	1609	F6R	O6-P-O3P	-2.26	100.33	106.44
2	B	1609	F6R	O5-C5-C6	2.17	114.77	109.99
2	C	1609	F6R	C5-C4-C3	2.04	115.41	112.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1609	F6R	C5
2	B	1609	F6R	C4
2	C	1609	F6R	C5
2	C	1609	F6R	C4

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1609	F6R	O4-C4-C5-C6
2	A	1609	F6R	C4-C5-C6-O6
2	B	1609	F6R	C2-C3-C4-O4
2	B	1609	F6R	O3-C3-C4-C5
2	B	1609	F6R	O3-C3-C4-O4
2	B	1609	F6R	C4-C5-C6-O6
2	B	1609	F6R	O5-C5-C6-O6
2	C	1609	F6R	O1-C1-C2-O2
2	C	1609	F6R	C2-C3-C4-C5
2	C	1609	F6R	C2-C3-C4-O4
2	C	1609	F6R	O3-C3-C4-C5
2	C	1609	F6R	O3-C3-C4-O4
2	C	1609	F6R	C3-C4-C5-O5
2	C	1609	F6R	C4-C5-C6-O6
2	A	1609	F6R	C3-C4-C5-O5
2	B	1609	F6R	C2-C3-C4-C5
2	B	1609	F6R	C3-C4-C5-O5
2	A	1609	F6R	O1-C1-C2-O2
2	C	1609	F6R	O5-C5-C6-O6

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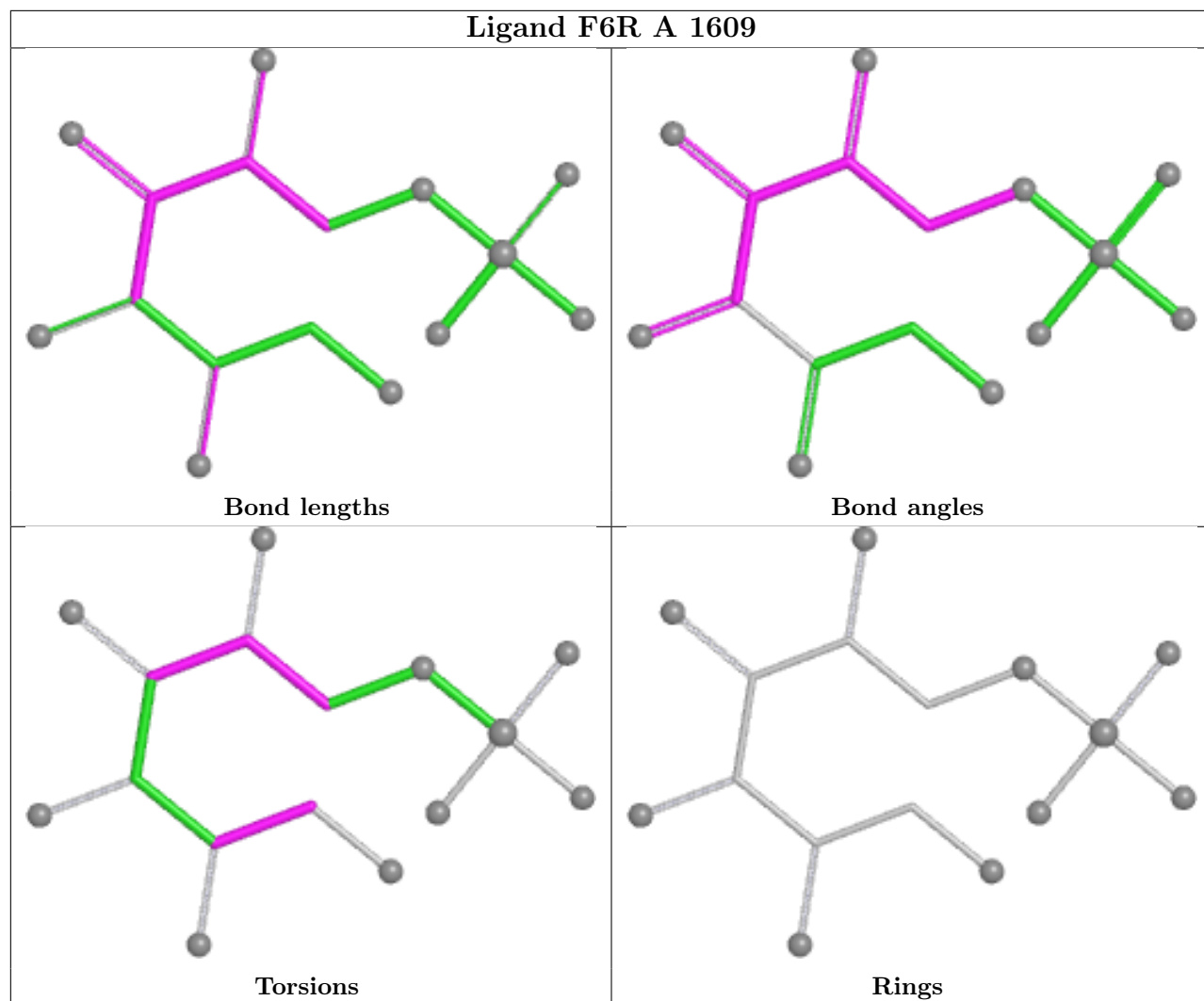
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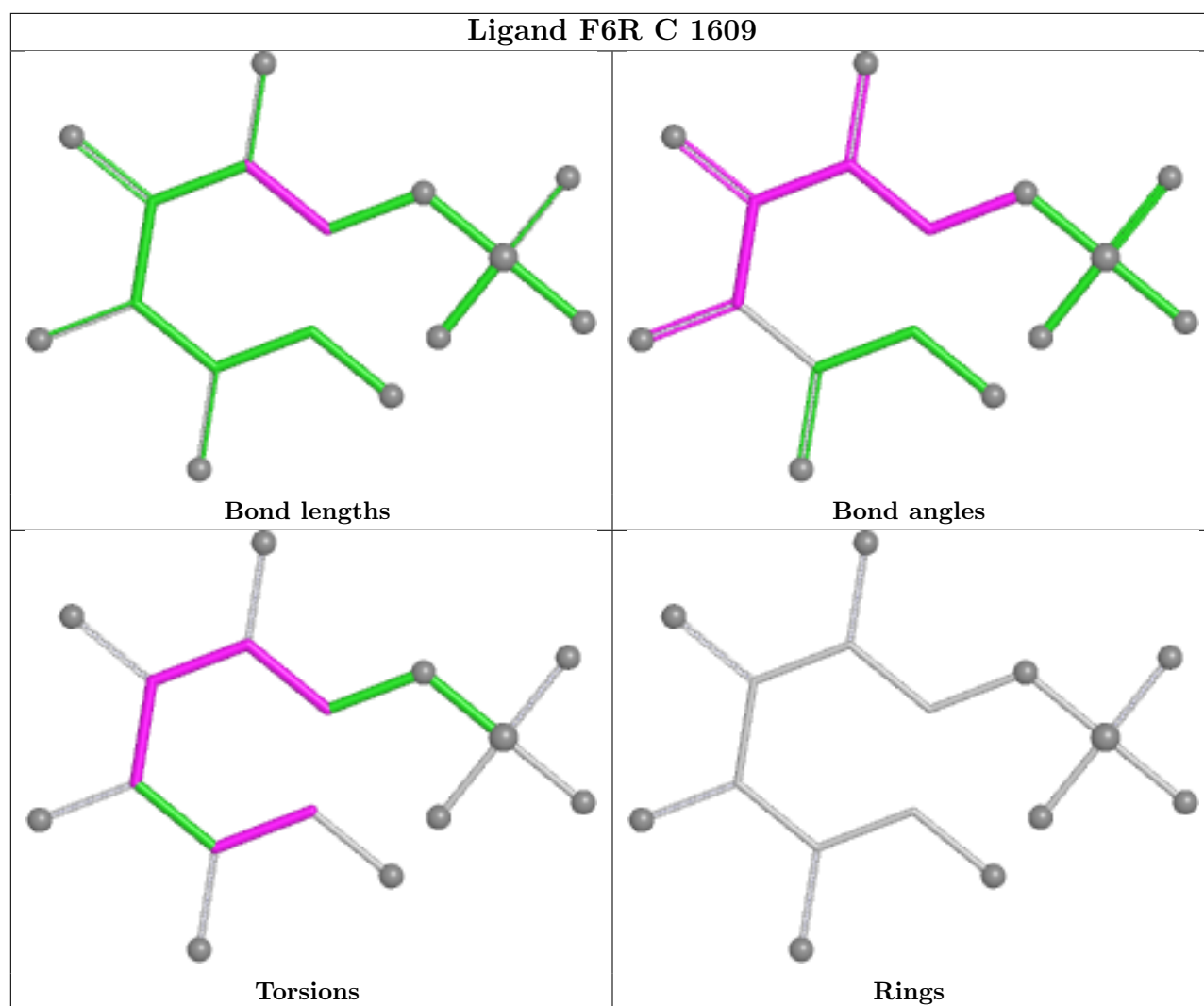
Mol	Chain	Res	Type	Atoms
2	B	1609	F6R	O4-C4-C5-C6
2	C	1609	F6R	O1-C1-C2-C3
2	C	1609	F6R	O4-C4-C5-C6

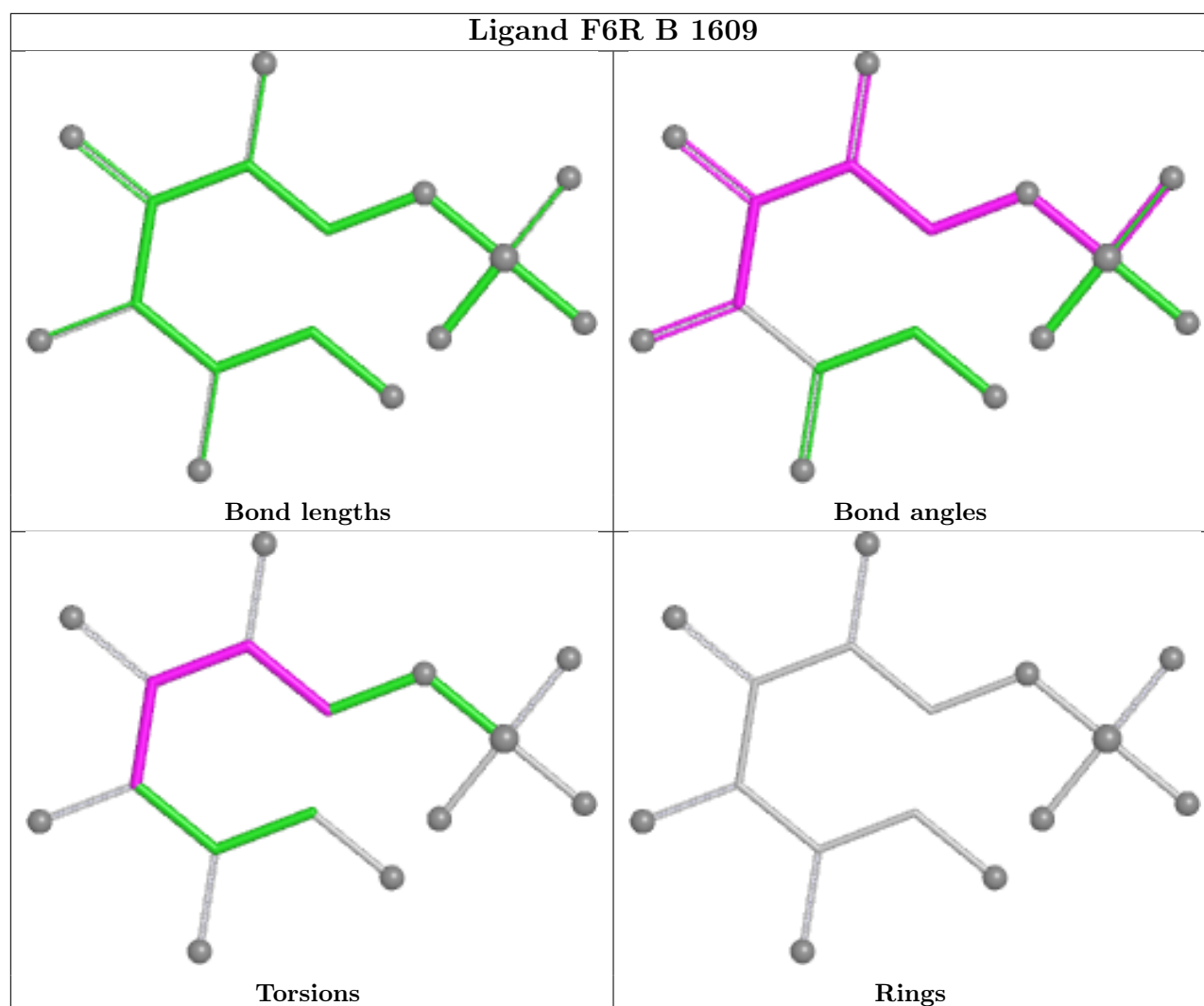
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	39:GLU	C	40:GLY	N	1.11

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	608/609 (99%)	-0.51	3 (0%) 87 89	24, 37, 65, 89	0
1	B	608/609 (99%)	0.74	94 (15%) 5 4	46, 96, 163, 202	0
1	C	608/609 (99%)	0.18	21 (3%) 47 48	29, 61, 114, 141	0
All	All	1824/1827 (99%)	0.14	118 (6%) 25 24	24, 60, 139, 202	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	HIS	5.4
1	B	127	ILE	4.7
1	C	240	TYR	4.7
1	B	236	SER	4.3
1	B	234	ILE	4.2
1	B	41	HIS	4.0
1	B	31	ALA	3.9
1	B	367	TYR	3.8
1	B	93	ILE	3.7
1	B	126	VAL	3.6
1	B	131	VAL	3.6
1	B	51	VAL	3.6
1	B	43	THR	3.5
1	C	435	HIS	3.5
1	B	63	LEU	3.5
1	B	135	LEU	3.5
1	A	240	TYR	3.5
1	C	429	ILE	3.4
1	B	100	ILE	3.4
1	B	122	THR	3.3
1	B	38	ALA	3.3
1	B	62	PRO	3.3
1	B	32	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	551	ALA	3.1
1	B	107	LEU	3.1
1	C	271	ILE	3.1
1	B	167	ASP	3.1
1	B	237	ASN	3.0
1	B	217	ARG	2.9
1	B	57	ALA	2.9
1	B	80	PRO	2.9
1	B	108	ARG	2.9
1	B	240	TYR	2.9
1	B	67	THR	2.8
1	C	424	GLY	2.8
1	B	133	TRP	2.8
1	B	83	VAL	2.8
1	B	134	GLU	2.8
1	B	70	ALA	2.8
1	B	141	LEU	2.8
1	B	94	VAL	2.8
1	B	155	ALA	2.7
1	B	365	LEU	2.7
1	B	89	VAL	2.7
1	B	81	SER	2.7
1	C	433	ILE	2.6
1	C	239	GLN	2.6
1	B	602	ALA	2.6
1	B	101	ILE	2.6
1	C	561	ILE	2.6
1	B	279	SER	2.6
1	B	140	THR	2.6
1	B	144	ALA	2.6
1	C	316	SER	2.6
1	C	434	VAL	2.5
1	B	116	TYR	2.5
1	B	154	GLY	2.5
1	B	103	ASN	2.5
1	C	512	ALA	2.5
1	C	422	LEU	2.5
1	B	39	GLU	2.5
1	B	156	TYR	2.5
1	B	44	ARG	2.5
1	B	221	ILE	2.5
1	B	75	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	130	LEU	2.5
1	B	66	GLY	2.5
1	B	119	VAL	2.4
1	C	276	VAL	2.4
1	B	368	LEU	2.4
1	B	113	ALA	2.4
1	A	137	GLN	2.4
1	B	138	GLY	2.4
1	C	225	THR	2.4
1	B	106	PRO	2.4
1	B	151	GLN	2.3
1	C	427	ALA	2.3
1	B	40	GLY	2.3
1	B	235	GLU	2.3
1	B	1	CYS	2.3
1	B	6	ALA	2.3
1	B	34	ALA	2.3
1	B	111	LEU	2.3
1	B	162	ASP	2.3
1	B	104	HIS	2.3
1	B	110	GLU	2.3
1	B	274	GLY	2.3
1	B	45	LEU	2.3
1	B	88	HIS	2.2
1	B	30	SER	2.2
1	B	58	ALA	2.2
1	B	238	LEU	2.2
1	B	61	HIS	2.2
1	B	7	ILE	2.2
1	B	84	ASN	2.2
1	B	225	THR	2.2
1	B	95	VAL	2.2
1	B	13	ALA	2.2
1	B	128	ALA	2.2
1	B	148	ALA	2.2
1	C	288	LEU	2.2
1	B	222	PHE	2.1
1	C	425	LEU	2.1
1	B	174	SER	2.1
1	B	37	ASP	2.1
1	A	138	GLY	2.1
1	B	2	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	560	HIS	2.1
1	B	56	GLN	2.1
1	B	117	THR	2.1
1	C	283	PRO	2.1
1	C	566	HIS	2.1
1	B	136	LYS	2.1
1	B	123	ASP	2.1
1	B	29	ASP	2.0
1	B	8	ALA	2.0
1	B	224	LYS	2.0
1	B	139	GLY	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](#)

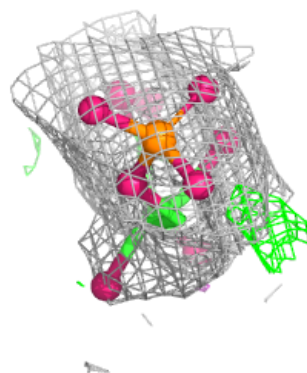
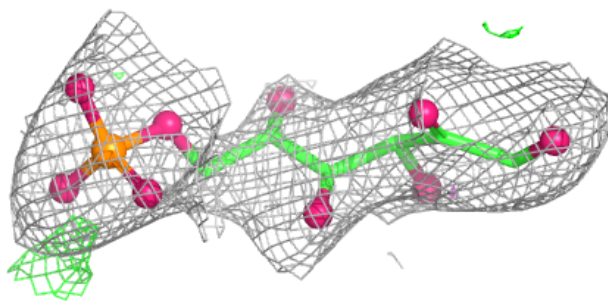
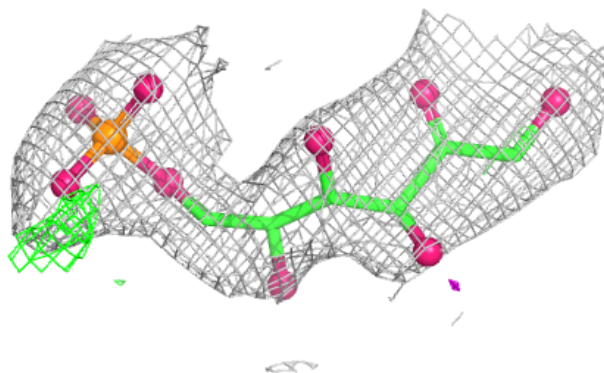
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	F6R	B	1609	16/16	0.93	0.10	67,72,80,82	0
2	F6R	C	1609	16/16	0.95	0.08	52,55,61,62	0
2	F6R	A	1609	16/16	0.99	0.04	25,27,28,29	0

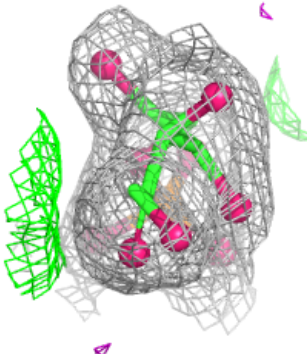
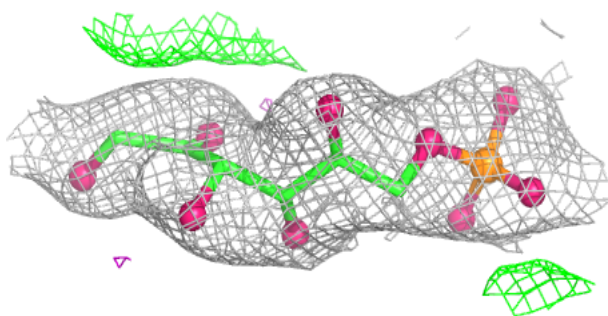
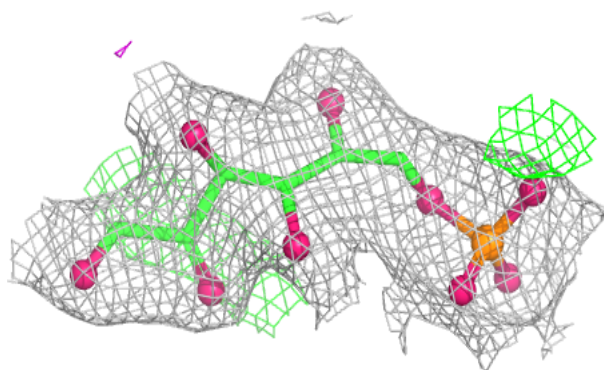
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

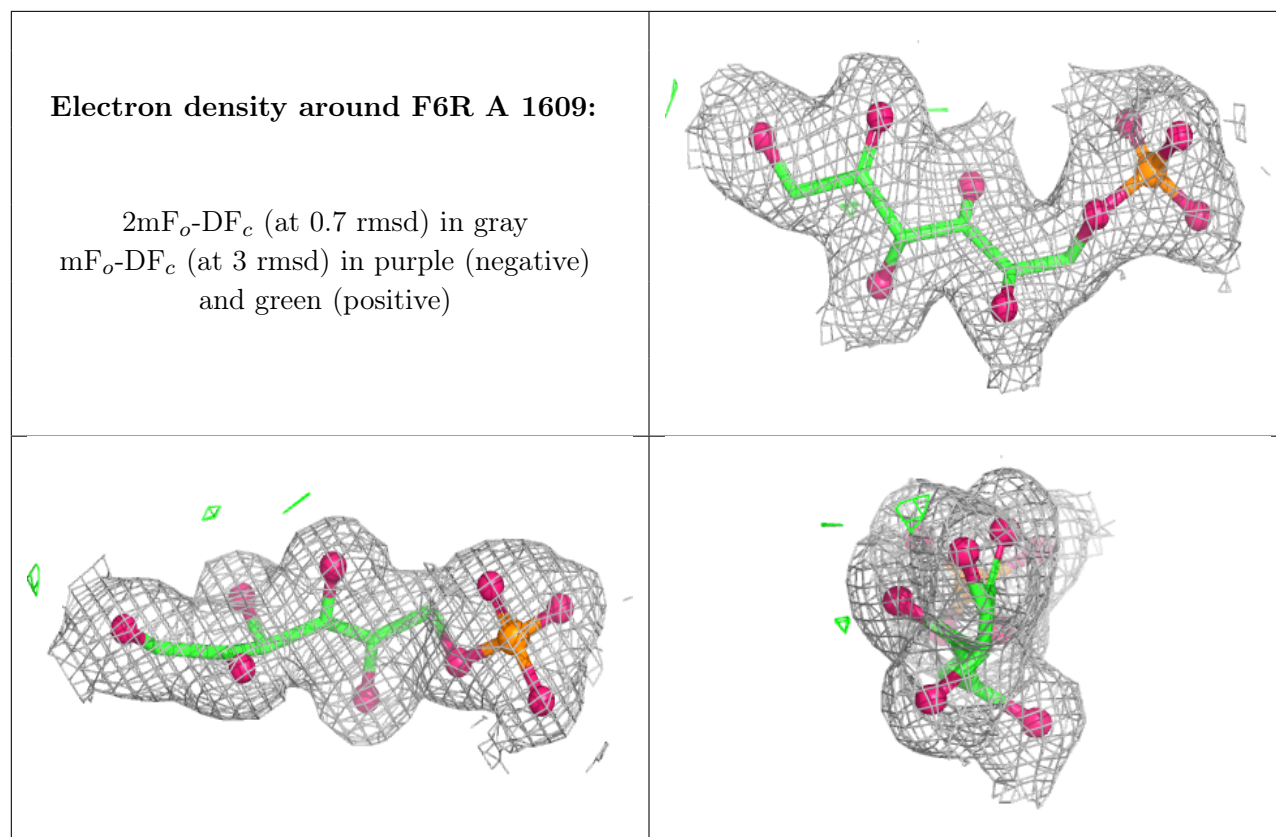
Electron density around F6R B 1609:

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

**Electron density around F6R C 1609:**

$2mF_o-DF_c$ (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.