



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:21 PM UTC

PDB ID : 1GLA / pdb_00001gla
Title : STRUCTURE OF THE REGULATORY COMPLEX OF ESCHERICHIA COLI IIIGLC WITH GLYCEROL KINASE
Authors : Hurley, J.H.; Worthylake, D.; Faber, H.R.; Meadow, N.D.; Roseman, S.; Pettigrew, D.W.; Remington, S.J.
Deposited on : 1992-10-28
Resolution : 2.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

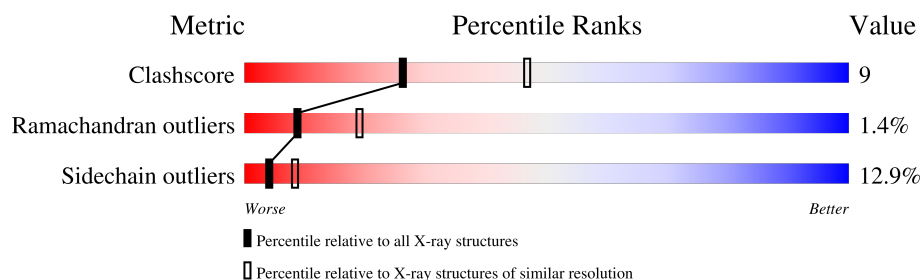
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	F	168	
2	G	501	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4985 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 GLUCOSE-SPECIFIC PROTEIN IIIGlc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	161	Total	C	N	O	S	0	0	0
			1201	769	190	240	2			

- Molecule 2 is a protein called GLYCEROL KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	489	Total	C	N	O	S	0	0	0
			3778	2385	654	720	19			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			6	3	3		

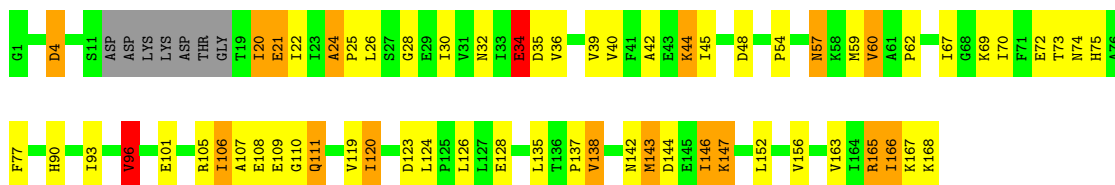
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

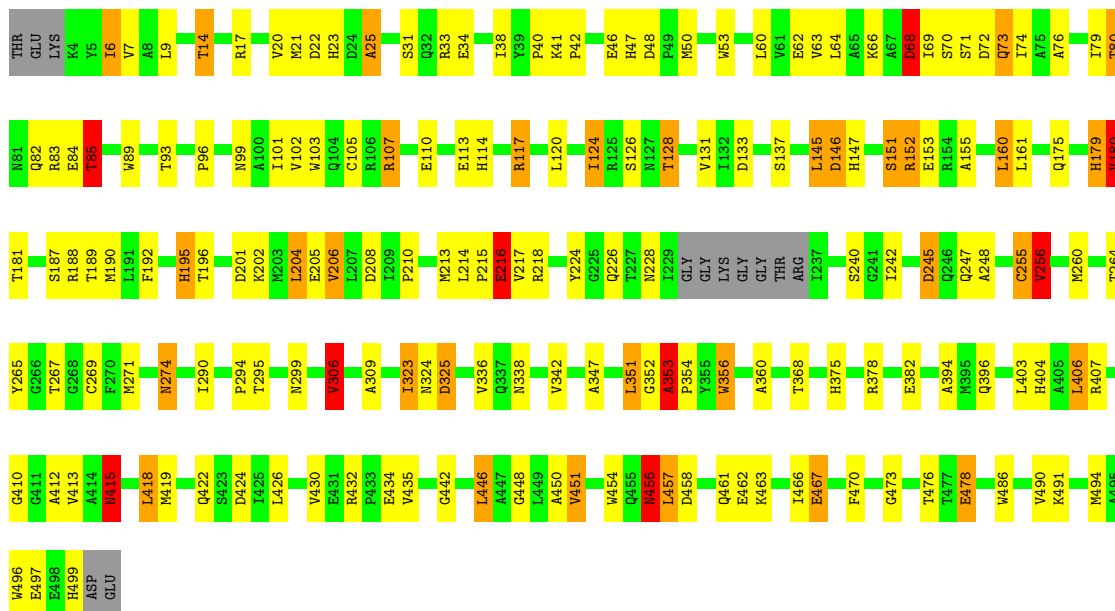
• Molecule 1: GLUCOSE-SPECIFIC PROTEIN IIIGlc

Chain F: 



• Molecule 2: GLYCEROL KINASE

Chain G: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.40Å 124.30Å 133.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4985	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	F	0.93	5/1216 (0.4%)	1.75	26/1645 (1.6%)
2	G	0.98	13/3856 (0.3%)	1.84	76/5244 (1.4%)
All	All	0.97	18/5072 (0.4%)	1.82	102/6889 (1.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	75	HIS	CD2-NE2	-7.58	1.29	1.37
1	F	138	VAL	CA-CB	6.99	1.62	1.53
1	F	146	ILE	CA-CB	6.82	1.62	1.54
2	G	47	HIS	CD2-NE2	-6.71	1.30	1.37
2	G	195	HIS	CD2-NE2	-6.67	1.30	1.37
2	G	375	HIS	CD2-NE2	-6.54	1.30	1.37
2	G	179	HIS	CD2-NE2	-6.04	1.31	1.37
2	G	499	HIS	CD2-NE2	-6.03	1.31	1.37
2	G	114	HIS	CD2-NE2	-6.01	1.31	1.37
1	F	90	HIS	CD2-NE2	-5.99	1.31	1.37
2	G	147	HIS	CD2-NE2	-5.96	1.31	1.37
2	G	23	HIS	CD2-NE2	-5.90	1.31	1.37
2	G	85	THR	CA-CB	5.70	1.60	1.53
1	F	75	HIS	CG-ND1	-5.66	1.32	1.38
2	G	404	HIS	CD2-NE2	-5.46	1.31	1.37
2	G	306	VAL	CA-CB	5.45	1.60	1.54
2	G	195	HIS	CG-ND1	-5.08	1.32	1.38
2	G	375	HIS	CG-ND1	-5.00	1.32	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	323	ILE	N-CA-C	12.89	125.96	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	68	ASP	CA-CB-CG	10.21	122.81	112.60
2	G	201	ASP	CA-CB-CG	10.12	122.72	112.60
2	G	404	HIS	CA-CB-CG	-9.60	104.20	113.80
2	G	93	THR	N-CA-C	9.51	121.25	111.07
2	G	356	TRP	CA-C-O	-9.49	106.94	120.51
2	G	323	ILE	CB-CA-C	-9.25	101.94	110.63
1	F	143	MET	CA-CB-CG	-9.08	95.95	114.10
1	F	57	ASN	N-CA-C	8.97	129.90	110.80
1	F	143	MET	N-CA-C	8.96	123.76	113.01
1	F	4	ASP	CA-CB-CG	-8.85	103.75	112.60
2	G	63	VAL	N-CA-C	8.79	120.64	110.62
1	F	142	ASN	CA-CB-CG	8.63	121.23	112.60
2	G	245	ASP	CA-CB-CG	8.34	120.94	112.60
2	G	25	ALA	N-CA-C	8.05	127.95	110.80
2	G	22	ASP	CA-CB-CG	8.02	120.62	112.60
2	G	451	VAL	N-CA-CB	-7.79	102.23	112.36
2	G	153	GLU	N-CA-C	-7.71	102.68	112.93
2	G	180	VAL	N-CA-C	7.59	119.77	108.46
2	G	161	LEU	N-CA-C	7.49	121.13	109.07
2	G	255	CYS	CA-C-O	-7.42	109.89	120.51
1	F	123	ASP	CA-CB-CG	7.04	119.64	112.60
2	G	256	VAL	N-CA-C	7.04	123.98	109.34
2	G	456	ASN	N-CA-C	6.82	118.72	107.73
2	G	131	VAL	N-CA-CB	-6.74	100.39	111.44
1	F	106	ILE	CA-C-O	-6.65	112.47	120.78
2	G	216	GLU	N-CA-C	-6.65	99.07	109.25
2	G	457	LEU	N-CA-C	6.50	120.07	111.75
1	F	22	ILE	N-CA-C	-6.44	97.84	107.37
2	G	353	ALA	CA-C-O	-6.43	111.34	120.16
1	F	44	LYS	N-CA-C	6.35	120.34	112.47
2	G	63	VAL	CB-CA-C	-6.29	103.80	112.04
2	G	394	ALA	CA-C-N	6.29	128.61	120.44
2	G	394	ALA	C-N-CA	6.29	128.61	120.44
2	G	72	ASP	CA-CB-CG	6.27	118.87	112.60
2	G	188	ARG	CB-CG-CD	-6.25	96.93	111.30
2	G	325	ASP	CA-CB-CG	6.24	118.84	112.60
2	G	496	TRP	CG-CD2-CE3	6.15	140.05	133.90
2	G	415	ASN	CA-CB-CG	6.08	118.67	112.60
1	F	34	GLU	CA-CB-CG	6.07	126.23	114.10
2	G	245	ASP	N-CA-C	6.02	118.64	111.71
2	G	336	VAL	N-CA-C	6.01	118.94	113.10
2	G	47	HIS	CB-CG-CD2	-6.00	123.41	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	84	GLU	N-CA-C	5.99	123.56	110.80
1	F	107	ALA	N-CA-C	5.96	118.02	110.33
2	G	338	ASN	CA-CB-CG	5.91	118.51	112.60
2	G	151	SER	N-CA-C	5.88	123.31	110.80
1	F	147	LYS	N-CA-C	5.87	117.76	111.36
2	G	131	VAL	CB-CA-C	5.84	119.49	110.50
2	G	146	ASP	CA-CB-CG	5.82	118.42	112.60
1	F	4	ASP	N-CA-C	5.78	119.51	112.23
1	F	111	GLN	N-CA-C	5.74	119.61	109.96
1	F	90	HIS	CB-CG-CD2	-5.73	123.76	131.20
2	G	23	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	F	142	ASN	N-CA-CB	-5.71	102.67	110.56
2	G	14	THR	N-CA-CB	-5.71	102.99	110.88
1	F	96	VAL	CB-CA-C	-5.71	98.80	111.77
2	G	180	VAL	N-CA-CB	-5.70	102.09	111.44
1	F	60	VAL	N-CA-CB	-5.70	102.89	112.47
2	G	228	ASN	OD1-CG-ND2	-5.70	116.90	122.60
2	G	435	VAL	N-CA-C	-5.69	99.03	107.51
1	F	24	ALA	CA-C-N	5.68	125.35	119.56
1	F	24	ALA	C-N-CA	5.68	125.35	119.56
2	G	356	TRP	O-C-N	-5.65	115.08	122.59
2	G	147	HIS	CA-CB-CG	-5.64	108.16	113.80
2	G	202	LYS	N-CA-C	-5.64	104.75	111.69
2	G	206	VAL	N-CA-CB	-5.62	103.45	110.47
2	G	356	TRP	CG-CD2-CE3	5.59	139.49	133.90
2	G	48	ASP	CA-C-N	5.57	125.93	119.47
2	G	48	ASP	C-N-CA	5.57	125.93	119.47
2	G	117	ARG	CA-CB-CG	5.54	125.19	114.10
2	G	70	SER	CB-CA-C	-5.53	103.86	110.94
1	F	57	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	F	39	VAL	N-CA-C	5.51	119.76	112.76
2	G	356	TRP	CA-CB-CG	-5.51	103.14	113.60
2	G	496	TRP	CB-CG-CD1	-5.47	118.69	126.90
2	G	188	ARG	CD-NE-CZ	-5.44	116.79	124.40
2	G	267	THR	CA-CB-OG1	-5.43	101.45	109.60
1	F	20	ILE	N-CA-C	5.43	116.01	108.84
2	G	342	VAL	N-CA-C	5.39	116.04	109.30
1	F	144	ASP	CA-CB-CG	5.35	117.95	112.60
2	G	179	HIS	CB-CG-CD2	-5.34	124.26	131.20
2	G	451	VAL	CB-CA-C	5.32	116.78	110.93
1	F	124	LEU	N-CA-C	5.24	121.38	109.81
2	G	496	TRP	CE2-CD2-CG	-5.23	100.92	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	188	ARG	CG-CD-NE	5.23	123.50	112.00
2	G	323	ILE	CA-C-O	-5.21	113.61	119.35
2	G	463	LYS	N-CA-C	5.21	117.71	111.71
2	G	424	ASP	CA-CB-CG	5.20	117.80	112.60
1	F	144	ASP	N-CA-C	-5.19	105.54	111.14
2	G	73	GLN	N-CA-C	5.18	119.45	113.18
2	G	160	LEU	N-CA-C	5.16	117.81	109.40
2	G	53	TRP	CG-CD2-CE3	5.10	139.00	133.90
2	G	228	ASN	CB-CG-ND2	5.07	124.01	116.40
2	G	152	ARG	CB-CG-CD	-5.07	99.65	111.30
2	G	274	ASN	CA-CB-CG	5.03	117.63	112.60
2	G	133	ASP	CA-C-N	5.02	124.68	119.56
2	G	133	ASP	C-N-CA	5.02	124.68	119.56
2	G	486	TRP	CE2-CD2-CG	-5.01	101.19	107.20
2	G	146	ASP	N-CA-C	5.01	118.85	112.34
2	G	432	ARG	CA-C-N	5.00	125.47	120.52
2	G	432	ARG	C-N-CA	5.00	125.47	120.52

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	F	1201	0	1217	26	0
2	G	3778	0	3633	67	0
3	G	6	0	8	1	0
All	All	4985	0	4858	92	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 9.

All (92) 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)
2:G:155:ALA:HB1	2:G:210:PRO:HG3	1.45	0.96
1:F:25:PRO:HG3	1:F:62:PRO:HB3	1.56	0.88
1:F:48:ASP:HB3	1:F:143:MET:SD	2.18	0.83
2:G:145:LEU:HB3	2:G:152:ARG:NH1	2.03	0.74
2:G:274:ASN:HD21	2:G:299:ASN:HD22	1.36	0.71
1:F:143:MET:HE3	1:F:146:ILE:HD11	1.74	0.69
2:G:105:CYS:SG	2:G:107:ARG:HD2	2.32	0.69
2:G:82:GLN:OE1	2:G:85:THR:HG21	1.94	0.67
2:G:17:ARG:HA	2:G:31:SER:O	1.95	0.66
2:G:407:ARG:HH21	2:G:466:ILE:HD11	1.61	0.65
2:G:128:THR:HG21	2:G:190:MET:HA	1.80	0.63
2:G:347:ALA:HB2	2:G:351:LEU:HD13	1.81	0.62
2:G:415:ASN:HD22	2:G:418:LEU:H	1.45	0.62
2:G:269:CYS:HB2	2:G:306:VAL:HG22	1.82	0.61
2:G:187:SER:HB3	2:G:290:ILE:HD12	1.84	0.60
2:G:415:ASN:ND2	2:G:418:LEU:H	1.99	0.59
2:G:448:GLY:HA3	2:G:454:TRP:CE3	2.38	0.59
1:F:74:ASN:ND2	1:F:105:ARG:HE	2.01	0.58
2:G:218:ARG:HG2	2:G:218:ARG:HH11	1.68	0.58
2:G:152:ARG:HH21	2:G:208:ASP:HB3	1.71	0.56
2:G:89:TRP:HA	2:G:96:PRO:HA	1.86	0.56
1:F:20:ILE:HB	1:F:166:ILE:HG13	1.87	0.55
2:G:396:GLN:HE21	2:G:403:LEU:H	1.55	0.55
2:G:85:THR:HB	2:G:102:VAL:HA	1.88	0.54
2:G:473:GLY:O	2:G:476:THR:HG22	2.07	0.53
2:G:38:ILE:HG22	2:G:40:PRO:HD3	1.89	0.53
2:G:180:VAL:HG23	2:G:216:GLU:HB3	1.89	0.52
2:G:9:LEU:HD11	2:G:60:LEU:HD13	1.92	0.52
2:G:248:ALA:O	2:G:442:GLY:HA3	2.09	0.52
2:G:255:CYS:O	2:G:260:MET:SD	2.68	0.51
1:F:101:GLU:HG2	1:F:126:LEU:HD21	1.92	0.50
2:G:271:MET:HE2	2:G:406:LEU:HD21	1.93	0.50
1:F:32:ASN:HB2	1:F:35:ASP:OD2	2.12	0.49
2:G:256:VAL:HG13	2:G:294:PRO:HG3	1.94	0.49
2:G:353:ALA:HB1	2:G:354:PRO:HD2	1.95	0.49
2:G:204:LEU:HD21	2:G:214:LEU:HD11	1.95	0.49
1:F:135:LEU:O	1:F:137:PRO:HD3	2.12	0.49
1:F:21:GLU:HG3	1:F:165:ARG:HG3	1.94	0.48
1:F:28:GLY:O	1:F:156:VAL:HG22	2.12	0.48
1:F:30:ILE:HD11	1:F:163:VAL:HG12	1.95	0.48
2:G:265:TYR:HB3	2:G:412:ALA:HB3	1.95	0.48
2:G:458:ASP:HA	2:G:461:GLN:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:126:SER:O	2:G:195:HIS:HE1	1.96	0.48
2:G:264:THR:O	2:G:269:CYS:HA	2.14	0.48
2:G:240:SER:HB2	2:G:450:ALA:HB3	1.96	0.48
2:G:46:GLU:HG2	2:G:99:ASN:HB3	1.95	0.47
1:F:40:VAL:HA	1:F:45:ILE:HD12	1.96	0.47
1:F:108:GLU:HB3	1:F:111:GLN:OE1	2.15	0.47
2:G:7:VAL:HG22	2:G:20:VAL:HG22	1.97	0.47
2:G:192:PHE:HE1	2:G:217:VAL:HG11	1.79	0.47
1:F:36:VAL:O	1:F:42:ALA:HB2	2.14	0.46
2:G:210:PRO:HG2	2:G:213:MET:HG3	1.98	0.46
2:G:224:TYR:CE2	2:G:242:ILE:HG13	2.51	0.46
2:G:410:GLY:O	2:G:413:VAL:HG22	2.16	0.46
2:G:85:THR:HG22	2:G:103:TRP:H	1.81	0.46
1:F:152:LEU:HD11	1:F:165:ARG:NH1	2.32	0.45
2:G:419:MET:O	2:G:422:GLN:HB3	2.17	0.45
1:F:70:ILE:HD12	1:F:109:GLU:HA	1.99	0.45
2:G:378:ARG:O	2:G:382:GLU:HG3	2.16	0.45
2:G:76:ALA:HB1	2:G:240:SER:OG	2.16	0.45
1:F:34:GLU:HA	1:F:42:ALA:HA	1.99	0.45
1:F:96:VAL:HG21	2:G:478:GLU:HB3	1.98	0.45
1:F:167:LYS:HD3	1:F:168:LYS:N	2.31	0.45
2:G:62:GLU:HB3	2:G:66:LYS:HZ3	1.83	0.44
2:G:218:ARG:HG2	2:G:218:ARG:NH1	2.32	0.44
2:G:64:LEU:HB3	2:G:69:ILE:O	2.19	0.43
2:G:80:THR:HG22	2:G:245:ASP:HA	2.00	0.43
2:G:442:GLY:O	2:G:446:LEU:HD22	2.17	0.43
2:G:62:GLU:HB3	2:G:66:LYS:NZ	2.33	0.43
1:F:106:ILE:HD13	1:F:106:ILE:HA	1.75	0.43
2:G:430:VAL:HB	2:G:470:PHE:HB2	2.00	0.43
2:G:189:THR:O	2:G:190:MET:HB3	2.18	0.43
2:G:360:ALA:HB2	2:G:494:MET:HA	2.01	0.43
1:F:101:GLU:CG	1:F:126:LEU:HD21	2.49	0.42
2:G:83:ARG:HB2	3:G:600:GOL:H12	2.00	0.42
2:G:323:ILE:HD12	2:G:325:ASP:O	2.19	0.42
1:F:24:ALA:HA	1:F:25:PRO:HD3	1.80	0.42
1:F:59:MET:HG2	1:F:77:PHE:HE1	1.84	0.42
1:F:67:ILE:O	1:F:110:GLY:HA2	2.20	0.42
2:G:396:GLN:NE2	2:G:403:LEU:H	2.16	0.42
2:G:120:LEU:O	2:G:124:ILE:HG22	2.19	0.42
2:G:179:HIS:CE1	2:G:215:PRO:HG3	2.55	0.41
2:G:434:GLU:HB3	2:G:467:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:323:ILE:O	2:G:324:ASN:HB2	2.20	0.41
2:G:101:ILE:HD13	2:G:107:ARG:HD3	2.03	0.41
2:G:456:ASN:ND2	2:G:457:LEU:H	2.17	0.41
2:G:478:GLU:H	2:G:478:GLU:HG2	1.73	0.41
2:G:6:ILE:HD12	2:G:21:MET:O	2.21	0.41
1:F:44:LYS:N	1:F:44:LYS:HD3	2.35	0.41
1:F:119:VAL:O	1:F:120:ILE:HG13	2.21	0.40
2:G:274:ASN:ND2	2:G:299:ASN:HD22	2.13	0.40
2:G:352:GLY:HA2	2:G:356:TRP:HA	2.04	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	F	157/168 (94%)	142 (90%)	14 (9%)	1 (1%)	21	42
2	G	485/501 (97%)	438 (90%)	39 (8%)	8 (2%)	7	16
All	All	642/669 (96%)	580 (90%)	53 (8%)	9 (1%)	9	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	57	ASN
2	G	25	ALA
2	G	256	VAL
2	G	353	ALA
2	G	68	ASP
2	G	151	SER
2	G	175	GLN
2	G	146	ASP
2	G	309	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	F	133/145 (92%)	116 (87%)	17 (13%)	4	8
2	G	385/412 (93%)	335 (87%)	50 (13%)	4	8
All	All	518/557 (93%)	451 (87%)	67 (13%)	4	8

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	4	ASP
1	F	21	GLU
1	F	26	LEU
1	F	34	GLU
1	F	54	PRO
1	F	60	VAL
1	F	69	LYS
1	F	72	GLU
1	F	73	THR
1	F	93	ILE
1	F	96	VAL
1	F	120	ILE
1	F	128	GLU
1	F	138	VAL
1	F	147	LYS
1	F	165	ARG
1	F	166	ILE
2	G	6	ILE
2	G	14	THR
2	G	33	ARG
2	G	34	GLU
2	G	41	LYS
2	G	42	PRO
2	G	50	MET
2	G	68	ASP
2	G	71	SER
2	G	73	GLN

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Mol	Chain	Res	Type
2	G	74	ILE
2	G	79	ILE
2	G	80	THR
2	G	85	THR
2	G	107	ARG
2	G	110	GLU
2	G	113	GLU
2	G	117	ARG
2	G	124	ILE
2	G	128	THR
2	G	137	SER
2	G	145	LEU
2	G	160	LEU
2	G	180	VAL
2	G	181	THR
2	G	196	THR
2	G	204	LEU
2	G	205	GLU
2	G	206	VAL
2	G	216	GLU
2	G	226	GLN
2	G	247	GLN
2	G	256	VAL
2	G	295	THR
2	G	306	VAL
2	G	351	LEU
2	G	368	THR
2	G	406	LEU
2	G	415	ASN
2	G	418	LEU
2	G	426	LEU
2	G	446	LEU
2	G	451	VAL
2	G	456	ASN
2	G	462	GLU
2	G	467	GLU
2	G	478	GLU
2	G	490	VAL
2	G	491	LYS
2	G	497	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	74	ASN
2	G	37	GLN
2	G	47	HIS
2	G	81	ASN
2	G	104	GLN
2	G	185	ASN
2	G	195	HIS
2	G	226	GLN
2	G	263	ASN
2	G	284	ASN
2	G	299	ASN
2	G	340	ASN
2	G	387	GLN
2	G	396	GLN
2	G	415	ASN
2	G	461	GLN
2	G	480	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](#)

1 ligand is 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
3	GOL	G	600	-	5,5,5	0.83	0	5,5,5	0.99	0

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
3	GOL	G	600	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	600	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	600	GOL	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.