



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:38 PM GMT

PDB ID : 1GLA
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

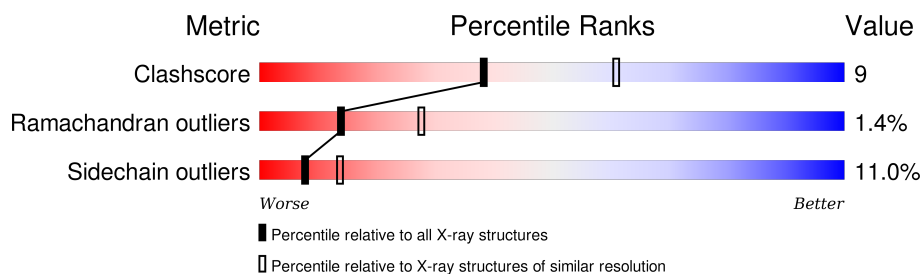
1 Overall quality at a glance

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	F	168	 64% 27% . . .
2	G	501	 64% 27% 6% . .

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.

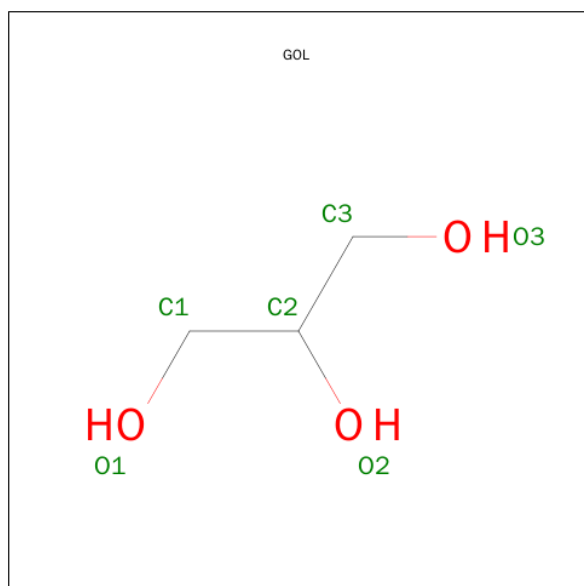
- Molecule 1 is a protein called GLUCOSE-SPECIFIC PROTEIN III Glc.

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 (three-letter code: GOL) (formula: C₃H₈O₃).



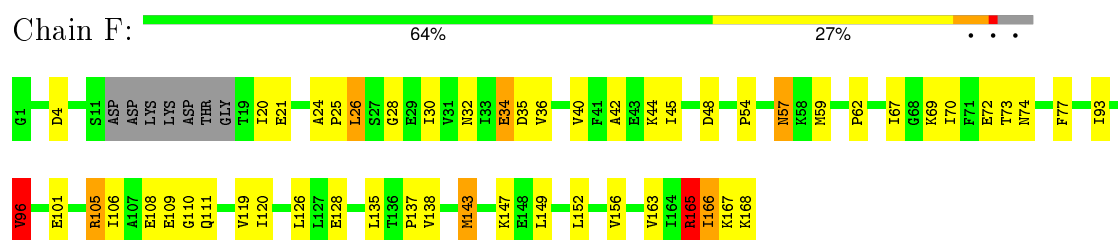
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

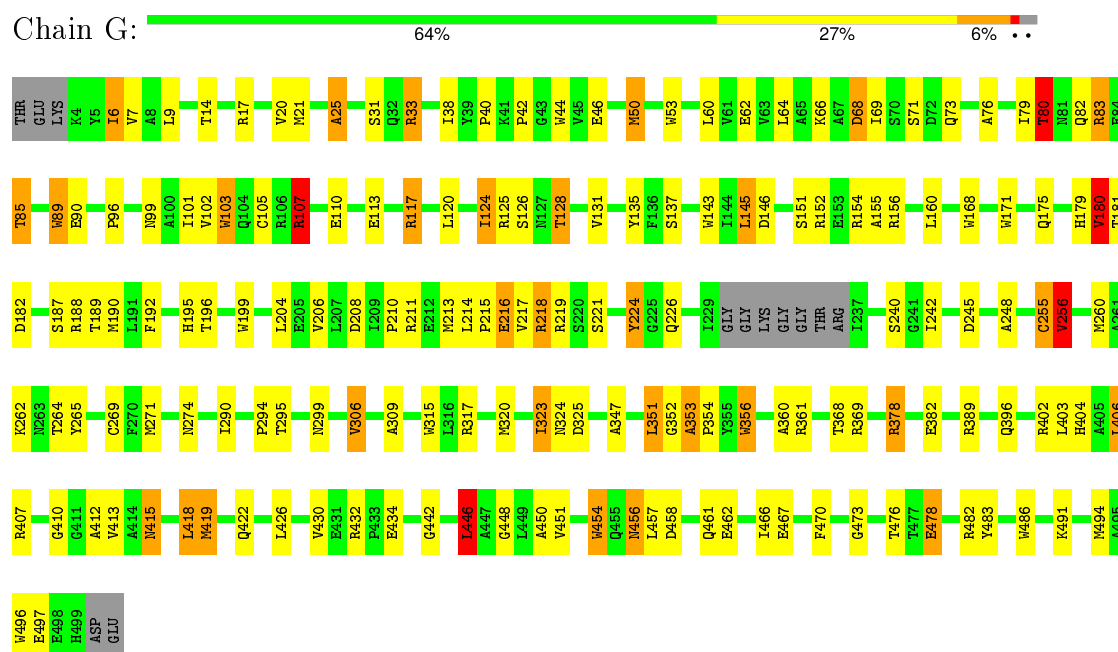
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: GLUCOSE-SPECIFIC PROTEIN IIIGlc



• Molecule 2: GLYCEROL KINASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.69	0/1216	1.40	8/1645 (0.5%)
2	G	0.79	0/3856	1.62	88/5244 (1.7%)
All	All	0.76	0/5072	1.57	96/6889 (1.4%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	MET	CA-CB-CG	-10.21	95.95	113.30
2	G	496	TRP	CD1-CG-CD2	9.62	114.00	106.30
2	G	356	TRP	CA-C-N	9.42	137.93	117.20
2	G	482	ARG	NE-CZ-NH1	9.20	124.90	120.30
2	G	432	ARG	NE-CZ-NH1	8.37	124.49	120.30
2	G	143	TRP	CD1-CG-CD2	8.22	112.88	106.30
2	G	107	ARG	NE-CZ-NH1	8.17	124.39	120.30
2	G	496	TRP	CE2-CD2-CG	-7.97	100.92	107.30
2	G	89	TRP	CD1-CG-CD2	7.90	112.62	106.30
2	G	315	TRP	CD1-CG-CD2	7.79	112.53	106.30
2	G	454	TRP	CD1-CG-CD2	7.75	112.50	106.30
2	G	211	ARG	NE-CZ-NH2	-7.75	116.42	120.30
2	G	486	TRP	CD1-CG-CD2	7.67	112.44	106.30
2	G	486	TRP	CE2-CD2-CG	-7.64	101.19	107.30
2	G	378	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	G	168	TRP	CE2-CD2-CG	-7.48	101.32	107.30
2	G	199	TRP	CD1-CG-CD2	7.45	112.26	106.30
2	G	482	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	G	361	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	F	105	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	G	83	ARG	NE-CZ-NH1	7.17	123.89	120.30
2	G	143	TRP	CE2-CD2-CG	-7.17	101.56	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	44	TRP	CD1-CG-CD2	7.16	112.03	106.30
2	G	89	TRP	CE2-CD2-CG	-7.12	101.60	107.30
2	G	154	ARG	NE-CZ-NH1	7.11	123.85	120.30
2	G	356	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	F	57	ASN	N-CA-C	7.00	129.90	111.00
2	G	53	TRP	CD1-CG-CD2	6.99	111.89	106.30
2	G	168	TRP	CD1-CG-CD2	6.99	111.89	106.30
2	G	53	TRP	CE2-CD2-CG	-6.98	101.72	107.30
2	G	171	TRP	CD1-CG-CD2	6.93	111.85	106.30
2	G	154	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	G	496	TRP	CG-CD2-CE3	6.84	140.05	133.90
2	G	171	TRP	CE2-CD2-CG	-6.83	101.84	107.30
2	G	483	TYR	CB-CG-CD2	-6.81	116.92	121.00
2	G	369	ARG	NE-CZ-NH2	-6.75	116.92	120.30
2	G	107	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	G	315	TRP	CE2-CD2-CG	-6.70	101.94	107.30
2	G	432	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	F	96	VAL	CB-CA-C	-6.63	98.80	111.40
2	G	103	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	F	26	LEU	CA-CB-CG	6.59	130.46	115.30
2	G	199	TRP	CE2-CD2-CG	-6.56	102.05	107.30
2	G	419	MET	CG-SD-CE	6.54	110.67	100.20
2	G	103	TRP	CD1-CG-CD2	6.52	111.52	106.30
2	G	44	TRP	CE2-CD2-CG	-6.47	102.12	107.30
2	G	454	TRP	CE2-CD2-CG	-6.47	102.12	107.30
2	G	496	TRP	CB-CG-CD1	-6.39	118.69	127.00
2	G	356	TRP	CD1-CG-CD2	6.38	111.41	106.30
2	G	83	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	G	320	MET	CG-SD-CE	-6.31	90.11	100.20
2	G	255	CYS	CA-C-N	6.30	131.07	117.20
2	G	25	ALA	N-CA-C	6.28	127.95	111.00
2	G	356	TRP	CA-C-O	-6.27	106.94	120.10
2	G	356	TRP	CG-CD2-CE3	6.21	139.49	133.90
2	G	218	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	G	135	TYR	CB-CG-CD2	-6.09	117.34	121.00
2	G	402	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	G	271	MET	CG-SD-CE	-5.98	90.63	100.20
2	G	496	TRP	CG-CD1-NE1	-5.98	104.12	110.10
2	G	389	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	G	389	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	F	34	GLU	CA-CB-CG	5.83	126.23	113.40
2	G	143	TRP	CG-CD1-NE1	-5.82	104.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	317	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	G	180	VAL	CA-CB-CG2	-5.72	102.32	110.90
2	G	53	TRP	CB-CG-CD1	-5.70	119.59	127.00
2	G	33	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	G	53	TRP	CG-CD2-CE3	5.67	139.00	133.90
2	G	188	ARG	CB-CG-CD	-5.64	96.93	111.60
2	G	219	ARG	NE-CZ-NH2	-5.63	117.49	120.30
2	G	188	ARG	CG-CD-NE	5.57	123.50	111.80
2	G	356	TRP	CA-CB-CG	-5.56	103.14	113.70
2	G	323	ILE	N-CA-C	5.54	125.96	111.00
2	G	171	TRP	CB-CG-CD1	-5.54	119.80	127.00
1	F	165	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	G	404	HIS	CA-CB-CG	-5.53	104.20	113.60
2	G	50	MET	CG-SD-CE	-5.44	91.49	100.20
2	G	80	THR	CA-CB-CG2	-5.39	104.86	112.40
2	G	320	MET	CA-CB-CG	-5.38	104.15	113.30
2	G	117	ARG	CA-CB-CG	5.36	125.19	113.40
2	G	156	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	G	486	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	G	361	ARG	NE-CZ-NH2	-5.19	117.71	120.30
2	G	125	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	G	315	TRP	CG-CD1-NE1	-5.15	104.95	110.10
2	G	402	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	G	224	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	F	165	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	G	90	GLU	CA-C-N	-5.10	105.97	117.20
2	G	451	VAL	CA-CB-CG2	-5.09	103.27	110.90
2	G	446	LEU	CA-CB-CG	5.08	126.98	115.30
2	G	406	LEU	CA-CB-CG	5.06	126.94	115.30
2	G	44	TRP	CG-CD1-NE1	-5.05	105.05	110.10
2	G	131	VAL	N-CA-CB	-5.05	100.39	111.50
2	G	143	TRP	CB-CG-CD1	-5.02	120.47	127.00

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	65	0
3	G	6	0	8	1	0
All	All	4985	0	4858	90	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 (90) 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
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
1:F:32:ASN:HB2	1:F:35:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:265:TYR:HB3	2:G:412:ALA:HB3	1.95	0.48
1:F:30:ILE:HD11	1:F:163:VAL:HG12	1.95	0.48
2:G:458:ASP:HA	2:G:461:GLN:HG2	1.96	0.48
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:410:GLY:O	2:G:413:VAL:HG22	2.16	0.46
2:G:224:TYR:CE2	2:G:242:ILE:HG13	2.51	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:218:ARG:HG2	2:G:218:ARG:NH1	2.32	0.44
2:G:442:GLY:O	2:G:446:LEU:HD22	2.17	0.43
2:G:80:THR:HG22	2:G:245:ASP:HA	2.00	0.43
2:G:64:LEU:HB3	2:G:69:ILE:O	2.19	0.43
2:G:62:GLU:HB3	2:G:66:LYS:NZ	2.33	0.43
2:G:430:VAL:HB	2:G:470:PHE:HB2	2.00	0.43
1:F:106:ILE:HA	1:F:106:ILE:HD13	1.75	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:323:ILE:HD12	2:G:325:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:83:ARG:HB2	3:G:600:GOL:H12	2.00	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:143:MET:HE3	1:F:149:LEU:HD13	2.01	0.42
2:G:396:GLN:NE2	2:G:403:LEU:H	2.16	0.42
1:F:67:ILE:O	1:F:110:GLY:HA2	2.20	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
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%)	30	56
2	G	485/501 (97%)	438 (90%)	39 (8%)	8 (2%)	12	24
All	All	642/669 (96%)	580 (90%)	53 (8%)	9 (1%)	14	28

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%)	120 (90%)	13 (10%)	10	19
2	G	385/412 (93%)	341 (89%)	44 (11%)	7	12
All	All	518/557 (93%)	461 (89%)	57 (11%)	8	14

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	4	ASP
1	F	26	LEU
1	F	54	PRO
1	F	69	LYS
1	F	72	GLU
1	F	73	THR
1	F	93	ILE
1	F	96	VAL
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

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Mol	Chain	Res	Type
2	G	33	ARG
2	G	42	PRO
2	G	50	MET
2	G	68	ASP
2	G	71	SER
2	G	73	GLN
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	182	ASP
2	G	196	THR
2	G	206	VAL
2	G	216	GLU
2	G	221	SER
2	G	226	GLN
2	G	256	VAL
2	G	262	LYS
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	456	ASN
2	G	462	GLU
2	G	478	GLU
2	G	491	LYS
2	G	497	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	74	ASN
2	G	32	GLN
2	G	37	GLN
2	G	47	HIS
2	G	81	ASN
2	G	185	ASN
2	G	195	HIS
2	G	299	ASN
2	G	340	ASN
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 carbohydrates 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	0.89	0	5,5,5	0.87	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	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.