



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:25 pm GMT

PDB ID : 2JJ4
Title : THE COMPLEX OF PII AND ACETYLGLUTAMATE KINASE FROM
SYNECHOCOCCUS ELONGATUS PCC7942
Authors : Llacer, J.L.; Marco-Marin, C.; Gil-Ortiz, F.; Fita, I.; Rubio, V.
Deposited on : 2007-07-04
Resolution : 3.46 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

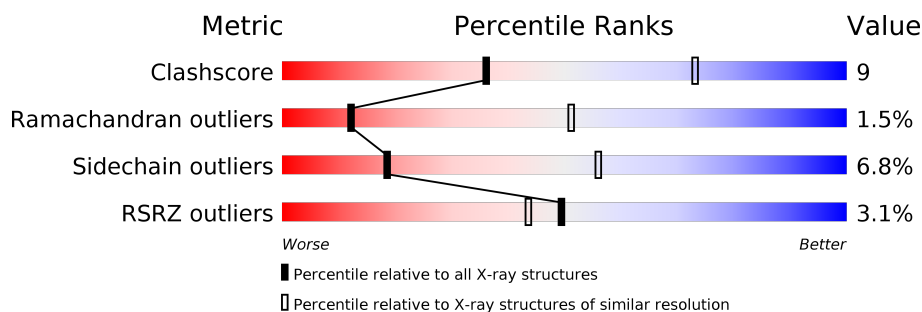
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)

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.

Mol	Chain	Length	Quality of chain
1	A	321	<div> <div></div> <div>72% 13% • 12%</div> </div>
1	B	321	<div> <div></div> <div>72% 14% • 12%</div> </div>
1	C	321	<div> <div>7%</div> <div>76% 11% • 11%</div> </div>
2	D	112	<div> <div>4%</div> <div>71% 25% • •</div> </div>
2	E	112	<div> <div></div> <div>67% 27% • •</div> </div>
2	F	112	<div> <div>4%</div> <div>68% 29% • •</div> </div>

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
3	NLG	A	1292	-	-	-	X
3	NLG	B	1292	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8557 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.

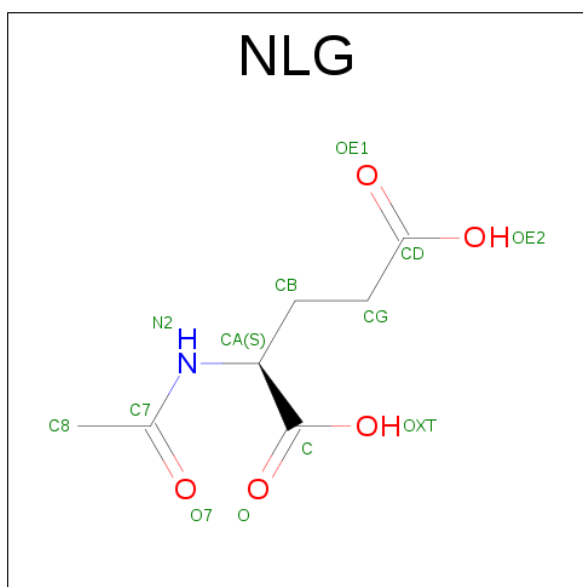
- Molecule 1 is a protein called ACETYLGLUTAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2028	1268	359	390	11			
1	B	284	Total	C	N	O	S	0	1	0
			2059	1291	368	389	11			
1	C	285	Total	C	N	O	S	0	0	0
			1972	1223	355	384	10			

- Molecule 2 is a protein called NITROGEN REGULATORY PROTEIN P-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	111	Total	C	N	O	S	0	0	0
			819	517	139	161	2			
2	E	108	Total	C	N	O	S	0	0	0
			828	523	145	158	2			
2	F	109	Total	C	N	O	S	0	0	0
			825	522	143	158	2			

- Molecule 3 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: C₇H₁₁NO₅).

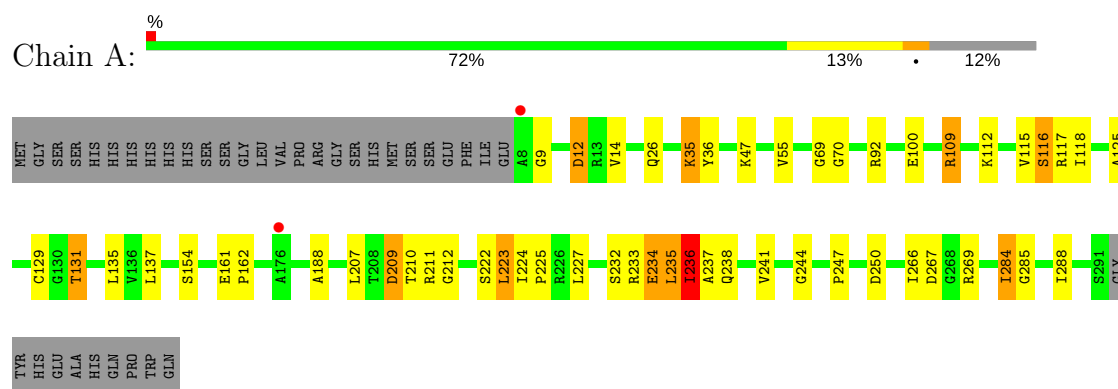


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	7	1	5		
3	B	1	Total	C	N	O	0	0
			13	7	1	5		

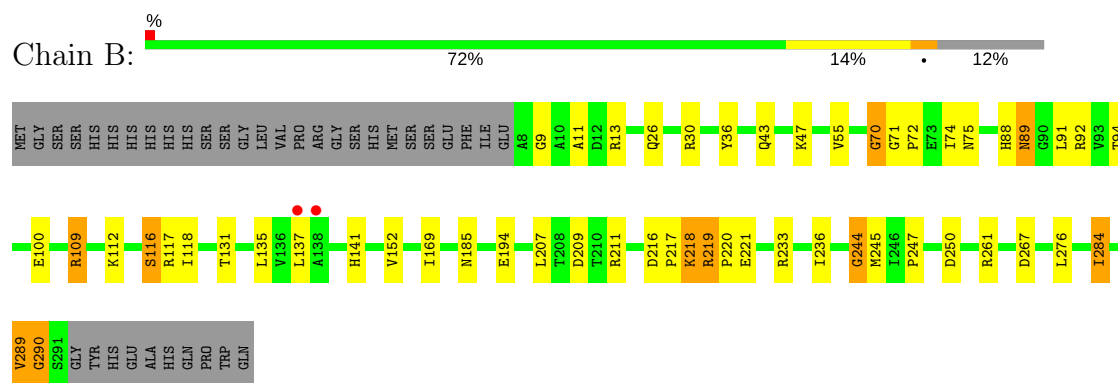
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

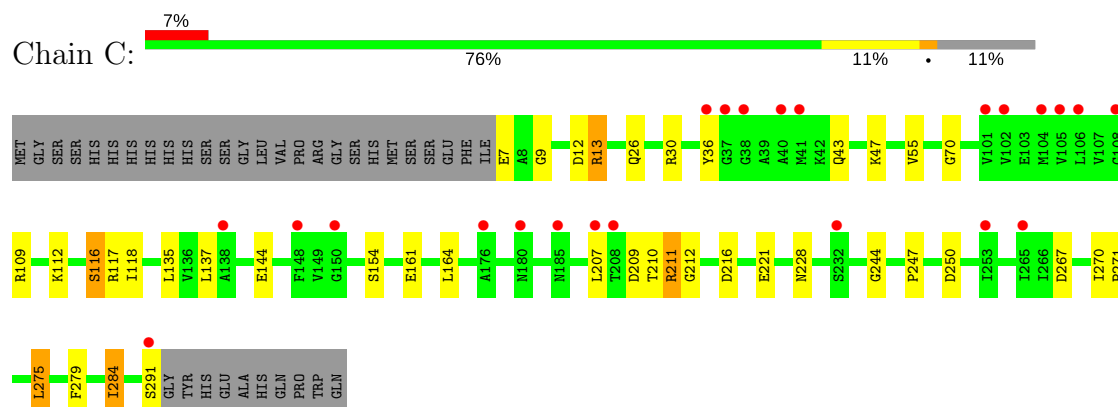
• Molecule 1: ACETYLGLUTAMATE KINASE



• Molecule 1: ACETYLGLUTAMATE KINASE



• Molecule 1: ACETYLGLUTAMATE KINASE



● Molecule 2: NITROGEN REGULATORY PROTEIN P-II

Chain D: 



● Molecule 2: NITROGEN REGULATORY PROTEIN P-II

Chain E: 



● Molecule 2: NITROGEN REGULATORY PROTEIN P-II

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.90Å 149.54Å 162.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.46 53.45 – 3.46	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.46) 99.9 (53.45-3.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.294 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	89.6	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 86.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8557	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: NLG

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	0.34	0/2057	0.51	0/2802
1	B	0.34	0/2088	0.56	1/2842 (0.0%)
1	C	0.42	1/1999 (0.1%)	0.52	1/2728 (0.0%)
2	D	0.32	0/826	0.49	0/1116
2	E	0.36	0/835	0.57	0/1124
2	F	0.36	0/832	0.52	0/1120
All	All	0.36	1/8637 (0.0%)	0.53	2/11732 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	2
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	GLN	CD-OE1	12.61	1.51	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	GLY	N-CA-C	-5.19	100.12	113.10
1	C	43	GLN	CG-CD-OE1	-5.04	111.52	121.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	GLU	Peptide
1	A	236	ILE	Peptide
1	A	9	GLY	Peptide
1	B	218	LYS	Peptide
1	B	244	GLY	Peptide
1	B	289	VAL	Peptide
1	B	9	GLY	Peptide
1	C	7	GLU	Peptide
1	C	9	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2028	0	1970	52	0
1	B	2059	0	2038	41	0
1	C	1972	0	1847	19	0
2	D	819	0	813	19	0
2	E	828	0	852	19	0
2	F	825	0	844	15	0
3	A	13	0	9	2	0
3	B	13	0	9	3	0
All	All	8557	0	8382	154	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 (154) 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:C:12:ASP:HA	1:C:13:ARG:CB	1.55	1.25
1:A:235:LEU:HA	1:A:236:ILE:C	1.71	1.10
1:C:12:ASP:CA	1:C:13:ARG:CB	2.30	1.07
1:A:235:LEU:HD12	1:A:235:LEU:O	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:H	1:B:220:PRO:CD	1.71	1.03
1:A:236:ILE:HG22	1:A:237:ALA:N	1.80	0.96
1:B:218:LYS:CB	1:B:219:ARG:CB	2.45	0.94
1:B:289:VAL:HB	1:B:290:GLY:HA3	1.49	0.94
2:F:10:PRO:HA	2:F:59:LEU:HD12	1.53	0.90
1:B:244:GLY:HA2	1:B:247:PRO:HD2	1.52	0.89
2:D:38:ARG:NH2	2:D:54:GLU:O	2.05	0.89
2:E:10:PRO:HA	2:E:59:LEU:HD12	1.56	0.88
2:D:10:PRO:HA	2:D:59:LEU:HD12	1.58	0.85
1:B:218:LYS:N	1:B:219:ARG:CB	2.40	0.84
1:B:219:ARG:H	1:B:220:PRO:HD2	1.41	0.84
1:C:284:ILE:HD13	1:C:284:ILE:H	1.43	0.83
1:B:284:ILE:HD13	1:B:284:ILE:H	1.43	0.81
1:A:284:ILE:HD13	1:A:284:ILE:H	1.44	0.81
1:B:218:LYS:CA	1:B:219:ARG:CB	2.58	0.81
1:B:218:LYS:H	1:B:219:ARG:CB	1.93	0.81
1:A:235:LEU:CA	1:A:236:ILE:C	2.51	0.77
1:A:235:LEU:HA	1:A:237:ALA:N	1.99	0.77
1:B:219:ARG:N	1:B:220:PRO:CD	2.48	0.76
2:D:110:ASP:CB	2:D:111:ALA:HA	2.16	0.75
1:A:234:GLU:O	1:A:237:ALA:HB3	1.87	0.73
1:A:233:ARG:O	1:A:236:ILE:HB	1.90	0.71
1:B:70:GLY:O	1:B:74:ILE:HG13	1.90	0.71
1:B:219:ARG:H	1:B:220:PRO:HD3	1.57	0.70
1:A:236:ILE:N	1:A:236:ILE:HD12	2.07	0.69
2:D:40:LYS:HE3	2:D:41:GLY:HA2	1.74	0.68
2:D:34:ARG:HB3	2:D:55:PHE:HB3	1.77	0.67
1:A:236:ILE:H	1:A:241:VAL:HB	1.60	0.66
1:A:222:SER:O	1:A:223:LEU:C	2.33	0.66
2:E:34:ARG:HB3	2:E:55:PHE:HB3	1.78	0.66
2:F:34:ARG:HB3	2:F:55:PHE:HB3	1.77	0.65
1:B:219:ARG:N	1:B:220:PRO:HD2	2.12	0.64
1:C:112:LYS:O	1:C:116:SER:HB2	1.97	0.64
1:A:36:TYR:HA	1:A:207:LEU:HD12	1.79	0.64
1:B:112:LYS:O	1:B:116:SER:HB2	1.98	0.63
1:C:36:TYR:HA	1:C:207:LEU:HD12	1.79	0.63
2:D:36:PHE:HB2	2:D:38:ARG:NH1	2.14	0.63
2:E:65:VAL:HG13	2:E:69:GLN:HB2	1.80	0.62
1:B:36:TYR:HA	1:B:207:LEU:HD12	1.81	0.61
2:D:65:VAL:HG13	2:D:69:GLN:HB2	1.82	0.60
1:B:284:ILE:HD13	1:B:284:ILE:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:TYR:HB2	2:D:56:LEU:HD13	1.84	0.60
1:B:47:LYS:HD3	1:B:117:ARG:CZ	2.32	0.59
1:A:112:LYS:O	1:A:116:SER:HB2	2.03	0.58
1:A:161:GLU:HB2	1:A:162:PRO:HD3	1.85	0.58
2:F:46:TYR:HB2	2:F:56:LEU:HD13	1.85	0.57
1:A:235:LEU:CD1	1:A:235:LEU:O	2.44	0.57
1:A:129:CYS:SG	1:A:131:THR:HG23	2.45	0.57
1:C:284:ILE:N	1:C:284:ILE:HD13	2.16	0.57
1:A:109:ARG:HD2	1:B:100:GLU:HG2	1.87	0.56
1:A:47:LYS:HD3	1:A:117:ARG:CZ	2.35	0.56
1:C:47:LYS:HD3	1:C:117:ARG:CZ	2.34	0.56
1:A:236:ILE:CG2	1:A:237:ALA:N	2.52	0.56
1:B:152:VAL:O	2:E:45:ARG:NH2	2.38	0.56
1:A:236:ILE:CD1	1:A:236:ILE:N	2.69	0.55
2:F:18:ILE:HG22	2:F:19:ALA:N	2.22	0.55
2:E:46:TYR:HB2	2:E:56:LEU:HD13	1.90	0.54
2:E:5:GLU:HG2	2:E:62:GLU:HG2	1.89	0.54
1:A:284:ILE:HD13	1:A:284:ILE:N	2.17	0.54
2:D:5:GLU:HG2	2:D:62:GLU:HG2	1.89	0.54
1:A:100:GLU:HG2	1:B:109:ARG:HD2	1.90	0.53
1:A:92:ARG:NH1	3:A:1292:NLG:OXT	2.42	0.53
2:D:36:PHE:HB2	2:D:38:ARG:CZ	2.39	0.52
1:A:236:ILE:HD12	1:A:236:ILE:H	1.75	0.52
2:F:5:GLU:HG2	2:F:62:GLU:HG2	1.93	0.51
1:B:92:ARG:H	3:B:1292:NLG:H8C2	1.75	0.51
1:A:236:ILE:HG22	1:A:237:ALA:CA	2.40	0.51
1:B:194:GLU:OE1	2:E:48:GLY:HA2	2.11	0.51
1:A:232:SER:O	1:A:236:ILE:HD13	2.12	0.50
1:C:12:ASP:N	1:C:13:ARG:CB	2.75	0.50
1:A:235:LEU:N	1:A:236:ILE:HB	2.27	0.50
1:A:235:LEU:CA	1:A:237:ALA:N	2.71	0.50
2:E:100:ILE:HD12	2:E:107:LYS:HG2	1.94	0.50
1:A:235:LEU:H	1:A:236:ILE:HB	1.77	0.50
1:B:284:ILE:N	1:B:284:ILE:CD1	2.76	0.48
1:C:161:GLU:HA	1:C:164:LEU:HB2	1.95	0.48
1:B:55:VAL:HG22	1:B:118:ILE:HG23	1.96	0.48
1:C:154:SER:HA	2:D:49:SER:HA	1.95	0.48
1:C:211:ARG:HA	1:C:267:ASP:HB2	1.96	0.47
1:C:244:GLY:HA2	1:C:247:PRO:HD2	1.97	0.47
1:A:211:ARG:HA	1:A:267:ASP:HB2	1.96	0.47
1:C:284:ILE:N	1:C:284:ILE:CD1	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:O	1:A:235:LEU:N	2.48	0.47
1:A:154:SER:HA	2:F:49:SER:HA	1.97	0.47
1:A:35:LYS:HE2	1:A:188:ALA:HB3	1.97	0.46
1:B:88:HIS:O	1:B:89:ASN:C	2.53	0.46
1:A:236:ILE:HG22	1:A:237:ALA:H	1.73	0.46
1:A:284:ILE:N	1:A:284:ILE:CD1	2.78	0.46
1:A:244:GLY:HA2	1:A:247:PRO:HD2	1.98	0.46
2:D:30:VAL:HG23	2:E:34:ARG:HB2	1.98	0.46
1:B:244:GLY:CA	1:B:247:PRO:HD2	2.34	0.45
1:A:235:LEU:N	1:A:237:ALA:H	2.14	0.45
2:E:39:GLN:CB	2:E:40:LYS:CA	2.95	0.45
1:A:236:ILE:N	1:A:241:VAL:HB	2.30	0.45
1:B:220:PRO:HA	1:B:221:GLU:HA	1.73	0.45
1:B:11:ALA:HB1	1:B:13:ARG:HE	1.81	0.45
1:A:55:VAL:HG22	1:A:118:ILE:HG23	1.98	0.45
1:A:235:LEU:HA	1:A:236:ILE:O	2.12	0.44
1:A:223:LEU:HD23	1:A:224:ILE:O	2.17	0.44
1:A:227:LEU:O	1:A:288:ILE:HA	2.18	0.44
1:A:233:ARG:C	1:A:235:LEU:H	2.21	0.44
1:C:55:VAL:HG22	1:C:118:ILE:HG23	1.99	0.44
1:B:211:ARG:HA	1:B:267:ASP:HB2	1.98	0.44
2:D:38:ARG:NH1	2:D:44:GLU:OE2	2.51	0.44
1:B:91:LEU:HD11	1:B:141:HIS:CE1	2.53	0.43
1:B:289:VAL:HB	1:B:290:GLY:CA	2.35	0.43
1:B:30:ARG:NH1	1:B:261:ARG:HH22	2.17	0.43
1:B:71:GLY:HA2	1:B:74:ILE:HD12	1.99	0.43
2:D:43:THR:HG22	2:D:52:THR:HG22	2.00	0.43
1:B:185:ASN:ND2	3:B:1292:NLG:H2	2.17	0.43
2:F:43:THR:HG22	2:F:52:THR:HG22	2.00	0.43
1:B:233:ARG:HA	1:B:236:ILE:HD12	2.01	0.43
2:F:13:LEU:HD11	2:F:30:VAL:HG11	2.00	0.43
1:B:233:ARG:HH22	2:E:85:GLU:HG2	1.83	0.42
1:B:185:ASN:HD21	3:B:1292:NLG:H2	1.68	0.42
1:A:12:ASP:C	1:A:14:VAL:H	2.21	0.42
1:C:275:LEU:HD13	1:C:279:PHE:CD1	2.53	0.42
2:E:13:LEU:HD11	2:E:30:VAL:HG11	2.00	0.42
2:F:3:LYS:HB2	2:F:96:VAL:CG2	2.49	0.42
2:D:3:LYS:HB2	2:D:96:VAL:CG2	2.50	0.42
2:E:52:THR:OG1	2:E:53:VAL:N	2.53	0.42
1:A:115:VAL:HG13	1:A:125:ALA:HB3	2.02	0.42
2:F:28:MET:HG3	2:F:63:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASP:HA	1:B:217:PRO:HD3	1.78	0.42
1:A:69:GLY:HA3	3:A:1292:NLG:OE2	2.20	0.41
1:A:266:ILE:HA	1:A:285:GLY:HA3	2.02	0.41
1:B:152:VAL:HB	2:E:45:ARG:NH2	2.35	0.41
1:A:210:THR:C	1:A:212:GLY:H	2.23	0.41
2:E:99:THR:O	2:E:107:LYS:HA	2.20	0.41
2:E:39:GLN:CB	2:E:40:LYS:C	2.88	0.41
2:F:39:GLN:O	2:F:42:GLN:HB2	2.20	0.41
2:F:4:ILE:HB	2:F:63:ILE:HG13	2.03	0.41
2:D:40:LYS:HA	2:D:41:GLY:HA2	1.73	0.41
1:B:72:PRO:HA	1:B:75:ASN:HD22	1.85	0.41
2:F:30:VAL:CG1	2:F:61:LEU:HD13	2.51	0.41
2:D:30:VAL:CG1	2:D:61:LEU:HD13	2.51	0.41
1:A:233:ARG:HH22	2:F:85:GLU:HG2	1.86	0.41
1:C:30:ARG:HE	1:C:30:ARG:HA	1.85	0.41
1:A:236:ILE:O	1:A:238:GLN:N	2.54	0.41
2:D:38:ARG:NE	2:D:52:THR:O	2.52	0.41
2:E:36:PHE:HB2	2:E:38:ARG:CZ	2.50	0.41
1:A:209:ASP:OD1	1:A:209:ASP:N	2.54	0.40
1:C:210:THR:C	1:C:212:GLY:H	2.24	0.40
2:E:100:ILE:CD1	2:E:107:LYS:HG2	2.51	0.40
2:F:52:THR:OG1	2:F:53:VAL:N	2.54	0.40
1:A:209:ASP:HA	1:A:269:ARG:HG3	2.04	0.40
1:B:118:ILE:HG21	1:B:169:ILE:HD12	2.02	0.40
1:C:228:ASN:CB	1:C:291:SER:HB2	2.52	0.40
1:C:270:ILE:HA	1:C:271:PRO:HD3	2.00	0.40
2:D:103:ARG:O	2:E:82:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	282/321 (88%)	261 (93%)	16 (6%)	5 (2%)	10	47
1	B	283/321 (88%)	262 (93%)	17 (6%)	4 (1%)	13	52
1	C	283/321 (88%)	262 (93%)	18 (6%)	3 (1%)	17	58
2	D	109/112 (97%)	97 (89%)	11 (10%)	1 (1%)	20	63
2	E	106/112 (95%)	95 (90%)	9 (8%)	2 (2%)	9	46
2	F	107/112 (96%)	95 (89%)	10 (9%)	2 (2%)	9	46
All	All	1170/1299 (90%)	1072 (92%)	81 (7%)	17 (2%)	12	51

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	B	219	ARG
1	B	245	MET
1	A	223	LEU
1	C	13	ARG
1	B	89	ASN
2	F	38	ARG
1	A	236	ILE
2	D	106	GLU
1	A	70	GLY
1	A	225	PRO
1	B	70	GLY
1	C	70	GLY
1	C	211	ARG
2	F	106	GLU
2	E	70	VAL
2	E	41	GLY

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	202/256 (79%)	191 (95%)	11 (5%)	26	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	208/256 (81%)	196 (94%)	12 (6%)	23	60
1	C	185/256 (72%)	173 (94%)	12 (6%)	20	58
2	D	82/93 (88%)	75 (92%)	7 (8%)	12	44
2	E	87/93 (94%)	78 (90%)	9 (10%)	8	35
2	F	85/93 (91%)	78 (92%)	7 (8%)	13	47
All	All	849/1047 (81%)	791 (93%)	58 (7%)	18	56

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	26	GLN
1	A	35	LYS
1	A	109	ARG
1	A	116	SER
1	A	131	THR
1	A	135	LEU
1	A	137	LEU
1	A	209	ASP
1	A	250	ASP
1	A	284	ILE
1	B	26	GLN
1	B	43	GLN
1	B	94	THR
1	B	109	ARG
1	B	116	SER
1	B	131	THR
1	B	135	LEU
1	B	137	LEU
1	B	209	ASP
1	B	250	ASP
1	B	276	LEU
1	B	284	ILE
1	C	26	GLN
1	C	109	ARG
1	C	116	SER
1	C	135	LEU
1	C	137	LEU
1	C	144	GLU
1	C	209	ASP

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Mol	Chain	Res	Type
1	C	216	ASP
1	C	221	GLU
1	C	250	ASP
1	C	275	LEU
1	C	284	ILE
2	D	1	MET
2	D	14	ASP
2	D	29	THR
2	D	40	LYS
2	D	54	GLU
2	D	65	VAL
2	D	100	ILE
2	E	1	MET
2	E	14	ASP
2	E	29	THR
2	E	38	ARG
2	E	42	GLN
2	E	54	GLU
2	E	65	VAL
2	E	100	ILE
2	E	108	ASN
2	F	1	MET
2	F	14	ASP
2	F	18	ILE
2	F	29	THR
2	F	54	GLU
2	F	65	VAL
2	F	100	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	143	GLN
1	B	88	HIS
1	B	143	GLN
1	C	43	GLN
1	C	89	ASN
1	C	143	GLN
2	E	22	ASN
2	E	108	ASN
2	F	22	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](#)

2 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$
3	NLG	A	1292	-	6,12,12	2.13	1 (16%)	6,15,15	1.32	2 (33%)
3	NLG	B	1292	-	6,12,12	2.12	1 (16%)	6,15,15	1.11	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	NLG	A	1292	-	-	0/7/13/13	0/0/0/0
3	NLG	B	1292	-	-	0/7/13/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1292	NLG	C8-C7	-5.19	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1292	NLG	C8-C7	-5.16	1.39	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1292	NLG	CB-CA-C	-2.09	109.25	112.28
3	A	1292	NLG	O7-C7-C8	-2.00	118.41	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1292	NLG	2	0
3	B	1292	NLG	3	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

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	284/321 (88%)	0.19	2 (0%) 87 83	58, 72, 86, 88	1 (0%)
1	B	284/321 (88%)	0.20	2 (0%) 87 83	58, 72, 86, 89	0
1	C	285/321 (88%)	0.43	23 (8%) 13 14	58, 72, 86, 89	1 (0%)
2	D	111/112 (99%)	0.40	5 (4%) 34 29	65, 75, 85, 87	1 (0%)
2	E	108/112 (96%)	0.29	1 (0%) 84 78	65, 75, 84, 86	0
2	F	109/112 (97%)	0.11	4 (3%) 42 37	65, 75, 84, 86	0
All	All	1181/1299 (90%)	0.27	37 (3%) 49 43	58, 74, 85, 89	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	MET	3.3
1	C	291	SER	3.2
1	C	265	ILE	3.1
1	C	108	GLY	3.1
1	C	176	ALA	3.0
1	C	208	THR	2.8
1	C	150	GLY	2.8
2	D	65	VAL	2.8
1	C	38	GLY	2.7
1	C	37	GLY	2.6
1	C	138	ALA	2.4
1	C	106	LEU	2.4
1	B	138	ALA	2.4
2	E	79	ALA	2.4
2	D	103	ARG	2.3
2	F	27	GLY	2.3
1	C	207	LEU	2.3
1	C	253	ILE	2.3
1	A	8	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	102	ILE	2.3
1	C	105	VAL	2.2
2	D	104	THR	2.2
1	A	176	ALA	2.2
2	D	38	ARG	2.2
2	D	68	ALA	2.2
2	F	26	VAL	2.2
1	C	185	ASN	2.1
2	F	109	ALA	2.1
1	C	102	VAL	2.1
1	C	148	PHE	2.1
1	C	180	ASN	2.1
1	C	101	VAL	2.1
1	C	36	TYR	2.1
1	B	137	LEU	2.1
1	C	104	MET	2.0
1	C	232	SER	2.0
1	C	40	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NLG	A	1292	13/13	0.88	0.41	1.67	72,72,74,75	0
3	NLG	B	1292	13/13	0.88	0.44	1.39	72,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.