



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:04 am GMT

PDB ID : 2V5H
Title : Controlling the storage of nitrogen as arginine: the complex of PII and acetylglutamate kinase from *Synechococcus elongatus* PCC 7942
Authors : Llacer, J.L.; Marco-Marin, C.; Gil-Ortiz, F.; Fita, I.; Rubio, V.
Deposited on : 2007-07-04
Resolution : 2.75 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

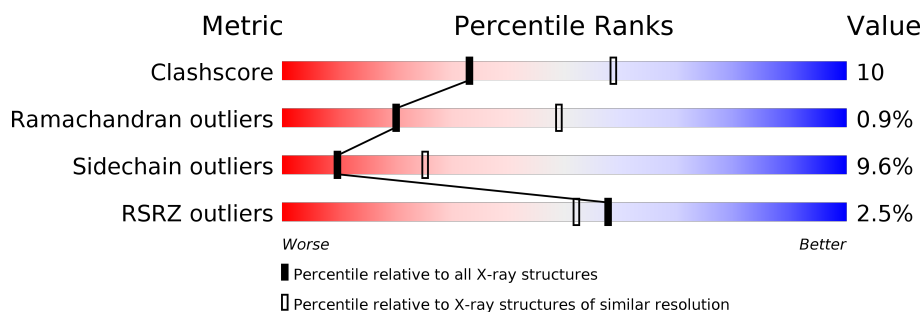
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.






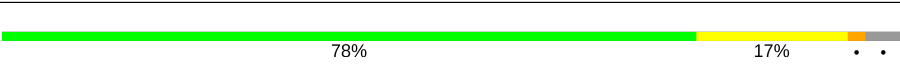
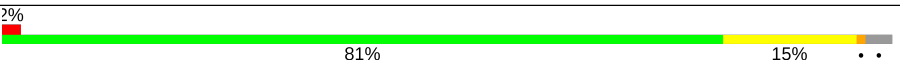
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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>2%</div> <div>71% 13% • 12%</div> </div>
1	B	321	<div> <div>%</div> <div>73% 14% • 10%</div> </div>
1	C	321	<div> <div>%</div> <div>72% 13% • 12%</div> </div>
1	D	321	<div> <div>2%</div> <div>73% 12% • • 11%</div> </div>
1	E	321	<div> <div>3%</div> <div>72% 13% • 11%</div> </div>
1	F	321	<div> <div>2%</div> <div>71% 13% • 11%</div> </div>
2	G	112	<div> <div>7%</div> <div>77% 20% • •</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	112	
2	I	112	
2	J	112	
2	K	112	
2	L	112	

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
5	GOL	E	1295	-	-	-	X
6	CL	K	1109	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18185 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.

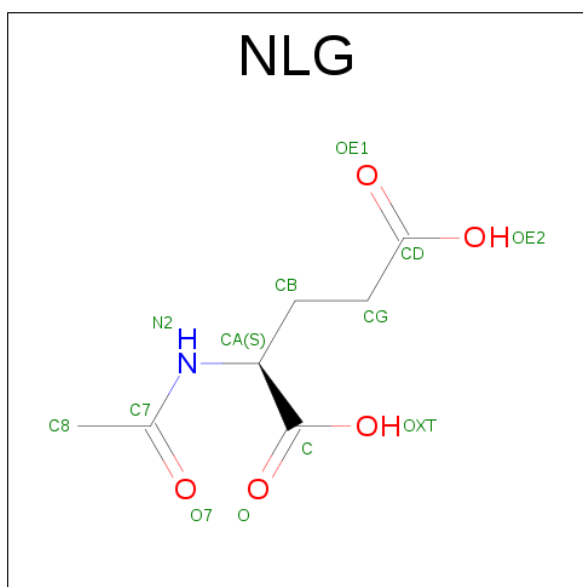
- Molecule 1 is a protein called ACETYLGLUTAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	1	0
			2126	1333	386	396	11			
1	B	289	Total	C	N	O	S	0	2	0
			2165	1357	390	407	11			
1	C	284	Total	C	N	O	S	0	1	0
			2128	1334	383	400	11			
1	D	286	Total	C	N	O	S	0	1	0
			2137	1339	385	402	11			
1	E	286	Total	C	N	O	S	0	2	0
			2142	1341	385	405	11			
1	F	287	Total	C	N	O	S	0	1	0
			2142	1342	386	403	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	111	Total	C	N	O	S	0	0	0
			853	540	149	162	2			
2	H	108	Total	C	N	O	S	0	0	0
			840	531	148	159	2			
2	I	109	Total	C	N	O	S	0	0	0
			838	531	147	158	2			
2	J	110	Total	C	N	O	S	0	0	0
			850	537	150	161	2			
2	K	108	Total	C	N	O	S	0	0	0
			840	531	148	159	2			
2	L	109	Total	C	N	O	S	0	0	0
			841	532	148	159	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	C	1	Total	C	N	O	0	0
			13	7	1	5		
3	D	1	Total	C	N	O	0	0
			13	7	1	5		
3	E	1	Total	C	N	O	0	0
			13	7	1	5		
3	F	1	Total	C	N	O	0	0
			13	7	1	5		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	2	Total	Cl	0	0
			2	2		
6	G	1	Total	Cl	0	0
			1	1		
6	J	2	Total	Cl	0	0
			2	2		
6	K	1	Total	Cl	0	0
			1	1		

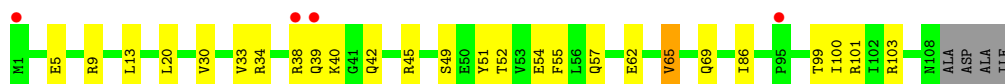
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	29	Total	O	0	0
			29	29		
7	B	22	Total	O	0	0
			22	22		
7	C	16	Total	O	0	0
			16	16		
7	D	16	Total	O	0	0
			16	16		

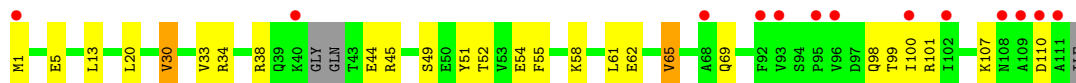
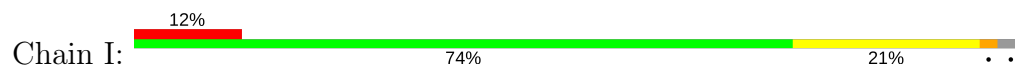
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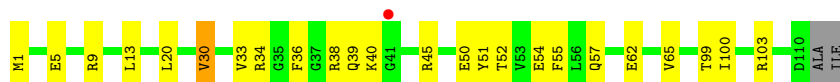
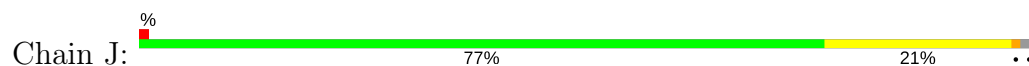
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	22	Total 22	O 22	0	0
7	F	23	Total 23	O 23	0	0
7	G	9	Total 9	O 9	0	0
7	H	11	Total 11	O 11	0	0
7	I	8	Total 8	O 8	0	0
7	J	10	Total 10	O 10	0	0
7	K	7	Total 7	O 7	0	0
7	L	14	Total 14	O 14	0	0



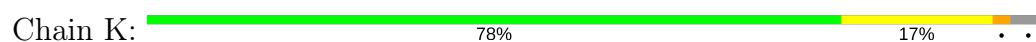
• Molecule 2: NITROGEN REGULATORY PROTEIN P-II



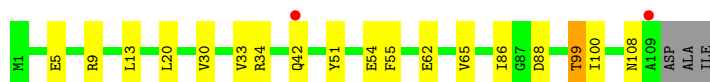
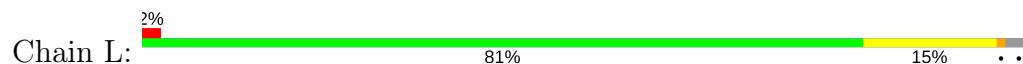
• Molecule 2: NITROGEN REGULATORY PROTEIN P-II



• Molecule 2: NITROGEN REGULATORY PROTEIN P-II



• Molecule 2: NITROGEN REGULATORY PROTEIN P-II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.38Å 161.03Å 91.56Å 90.00° 106.53° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 45.79 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.75) 100.0 (45.79-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.236 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18185	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: GOL, CL, NLG, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/2155	0.71	2/2920 (0.1%)
1	B	0.56	0/2196	0.70	2/2979 (0.1%)
1	C	0.52	0/2157	0.69	2/2923 (0.1%)
1	D	0.53	1/2166 (0.0%)	0.65	0/2935
1	E	0.55	0/2171	0.65	0/2943
1	F	0.50	1/2171 (0.0%)	0.61	0/2943
2	G	0.50	0/860	0.66	0/1155
2	H	0.52	0/847	0.71	0/1137
2	I	0.51	0/844	0.67	0/1133
2	J	0.52	0/857	0.70	0/1151
2	K	0.55	0/847	0.72	0/1137
2	L	0.57	0/848	0.71	1/1139 (0.1%)
All	All	0.54	2/18119 (0.0%)	0.68	7/24495 (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	D	0	2
1	E	0	1
1	F	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	218	LYS	CD-CE	6.18	1.66	1.51
1	F	251	CYS	CB-SG	-5.38	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	HIS	CB-CA-C	9.76	129.91	110.40
1	C	11	ALA	CB-CA-C	-8.28	97.68	110.10
1	C	10	ALA	N-CA-C	6.89	129.59	111.00
1	B	10	ALA	CB-CA-C	-6.07	100.99	110.10
1	B	10	ALA	N-CA-C	5.95	127.06	111.00
2	L	9	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	88	HIS	N-CA-C	-5.17	97.04	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	12	ASP	Peptide
1	D	9	GLY	Peptide
1	E	9	GLY	Peptide
1	F	11	ALA	Peptide
1	F	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	2126	0	2176	54	0
1	B	2165	0	2190	53	0
1	C	2128	0	2173	50	0
1	D	2137	0	2178	58	0
1	E	2142	0	2172	54	0
1	F	2142	0	2181	48	1
2	G	853	0	892	12	0
2	H	840	0	880	16	0
2	I	838	0	874	16	0
2	J	850	0	887	14	0
2	K	840	0	880	15	1
2	L	841	0	879	8	0
3	A	13	0	9	1	0
3	B	13	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	13	0	9	1	0
3	D	13	0	9	2	0
3	E	13	0	9	0	0
3	F	13	0	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	E	6	0	8	1	0
6	G	1	0	0	0	0
6	H	2	0	0	1	0
6	J	2	0	0	1	0
6	K	1	0	0	4	0
7	A	29	0	0	3	0
7	B	22	0	0	0	0
7	C	16	0	0	2	0
7	D	16	0	0	1	0
7	E	22	0	0	5	0
7	F	23	0	0	1	0
7	G	9	0	0	2	0
7	H	11	0	0	2	0
7	I	8	0	0	0	0
7	J	10	0	0	3	0
7	K	7	0	0	1	0
7	L	14	0	0	1	0
All	All	18185	0	18424	357	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 10.

All (357) 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:J:38:ARG:HD2	2:J:52:THR:O	1.69	0.93
1:C:12:ASP:N	1:C:13:ARG:HB2	1.85	0.91
1:A:211:ARG:HG2	7:A:2020:HOH:O	1.71	0.90
1:D:211:ARG:HH11	1:D:211:ARG:HG3	1.35	0.88
1:B:11:ALA:HA	1:B:13:ARG:HG3	1.65	0.79
1:D:211:ARG:HH11	1:D:211:ARG:CG	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:42:GLN:HB3	2:L:86:ILE:HD13	1.66	0.78
2:I:38:ARG:HG3	2:I:52:THR:O	1.85	0.76
1:A:276:LEU:HD13	1:C:14:VAL:HG21	1.68	0.75
2:G:1:MET:N	7:G:2001:HOH:O	2.20	0.74
2:H:39:GLN:HB3	2:H:40:LYS:HA	1.69	0.74
1:E:226:ARG:HH21	1:E:293:TYR:HA	1.53	0.73
1:C:156:ASN:C	1:C:156:ASN:HD22	1.92	0.72
1:A:75:ASN:OD1	1:A:92:ARG:NH2	2.23	0.71
1:D:284:ILE:H	1:D:284:ILE:HD13	1.53	0.71
1:F:156:ASN:HD22	1:F:156:ASN:C	1.94	0.71
1:B:9:GLY:CA	1:B:10:ALA:HB3	2.20	0.71
1:D:75:ASN:OD1	1:D:92:ARG:NH2	2.23	0.71
1:E:15:ARG:NH1	1:E:16:ILE:HD11	2.05	0.71
1:C:75:ASN:OD1	1:C:92:ARG:NH2	2.23	0.70
1:E:15:ARG:NH1	1:E:16:ILE:CD1	2.54	0.70
1:D:156:ASN:C	1:D:156:ASN:HD22	1.95	0.70
1:E:75:ASN:OD1	1:E:92:ARG:NH2	2.25	0.70
1:B:156:ASN:C	1:B:156:ASN:HD22	1.94	0.70
2:J:9:ARG:HG3	7:J:2010:HOH:O	1.92	0.70
2:K:103:ARG:HG2	6:K:1109:CL:CL	2.30	0.69
2:K:103:ARG:HD3	6:K:1109:CL:CL	2.29	0.69
1:E:190:THR:HG21	7:E:2011:HOH:O	1.92	0.69
1:D:14:VAL:HG21	1:F:276:LEU:HD13	1.75	0.68
1:A:60:VAL:HG22	1:C:60:VAL:HG22	1.76	0.68
1:A:284:ILE:HD13	1:A:284:ILE:H	1.59	0.67
1:D:190:THR:HG21	7:D:2009:HOH:O	1.95	0.67
1:B:75:ASN:OD1	1:B:92:ARG:NH2	2.27	0.67
1:C:92:ARG:O	1:C:94:THR:HG22	1.95	0.67
1:F:75:ASN:OD1	1:F:92:ARG:NH2	2.28	0.67
1:C:129:CYS:SG	1:C:131:THR:HG23	2.35	0.66
1:E:15:ARG:HH12	1:E:16:ILE:HD11	1.59	0.66
1:B:293:TYR:O	1:B:293:TYR:CG	2.49	0.66
1:F:208:THR:HG23	1:F:210:THR:H	1.60	0.66
1:D:208:THR:HG23	1:D:210:THR:H	1.60	0.66
1:C:12:ASP:CA	1:C:13:ARG:HB2	2.26	0.65
1:B:14:VAL:HG21	1:E:276:LEU:HD13	1.79	0.65
2:J:34:ARG:HB3	2:J:55:PHE:HB3	1.79	0.65
1:E:156:ASN:HD22	1:E:156:ASN:C	2.00	0.65
2:G:34:ARG:HB3	2:G:55:PHE:HB3	1.77	0.65
1:B:92:ARG:HD2	3:B:1297:NLG:O	1.96	0.64
1:A:208:THR:HG23	1:A:210:THR:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:ILE:HD13	1:F:284:ILE:H	1.62	0.64
1:F:211:ARG:HH12	1:F:221:GLU:HB3	1.63	0.64
1:A:156:ASN:HD22	1:A:156:ASN:C	2.01	0.64
1:B:161[A]:GLU:HB2	1:B:162:PRO:HD3	1.79	0.64
1:B:208:THR:HG23	1:B:210:THR:H	1.63	0.63
2:I:34:ARG:HB3	2:I:55:PHE:HB3	1.80	0.63
1:A:280:THR:HG22	1:A:282:ALA:H	1.62	0.63
1:B:129:CYS:SG	1:B:131:THR:HG23	2.38	0.63
1:B:9:GLY:HA3	1:B:11:ALA:H	1.64	0.63
1:B:284:ILE:HD13	1:B:284:ILE:H	1.62	0.63
1:B:9:GLY:HA2	1:B:10:ALA:HB3	1.80	0.63
1:C:284:ILE:H	1:C:284:ILE:HD13	1.64	0.62
2:H:34:ARG:HB3	2:H:55:PHE:HB3	1.81	0.62
2:H:39:GLN:HB3	2:H:40:LYS:CA	2.29	0.62
2:J:9:ARG:NH2	7:J:2001:HOH:O	2.32	0.62
2:K:34:ARG:HB3	2:K:55:PHE:HB3	1.81	0.62
1:E:280:THR:HG22	1:E:281:ASP:N	2.15	0.62
1:D:16:ILE:N	1:D:16:ILE:HD12	2.13	0.62
1:A:129:CYS:SG	1:A:131:THR:HG23	2.40	0.62
2:H:39:GLN:CB	2:H:40:LYS:HA	2.28	0.61
1:D:211:ARG:NH1	1:D:211:ARG:HG3	2.11	0.61
1:B:156:ASN:HD21	1:B:158:GLU:HB2	1.65	0.61
1:E:129:CYS:SG	1:E:131:THR:HG23	2.40	0.61
1:A:280:THR:HG22	1:A:281:ASP:N	2.16	0.60
1:A:20:ALA:HB2	1:C:13:ARG:HH12	1.66	0.60
1:E:284:ILE:H	1:E:284:ILE:HD13	1.65	0.60
1:D:276:LEU:HD13	1:F:14:VAL:HG21	1.83	0.60
1:A:156:ASN:ND2	1:A:158:GLU:H	2.00	0.60
1:C:261:ARG:NH1	7:C:2013:HOH:O	2.35	0.59
1:C:208:THR:HG23	1:C:210:THR:H	1.66	0.59
1:D:16:ILE:HG21	1:F:13:ARG:HA	1.84	0.59
1:E:60:VAL:HG13	1:E:60:VAL:O	2.02	0.59
2:I:1:MET:HE2	2:I:110:ASP:H	1.68	0.59
1:D:156:ASN:ND2	1:D:158:GLU:H	2.01	0.59
1:D:104:MET:HB3	1:E:104:MET:HB3	1.85	0.58
1:E:28:ALA:HA	7:E:2005:HOH:O	2.02	0.58
2:L:42:GLN:HB3	2:L:86:ILE:CD1	2.33	0.58
1:A:156:ASN:HD22	1:A:158:GLU:H	1.51	0.58
1:C:280:THR:HG22	1:C:281:ASP:N	2.19	0.58
1:A:233:ARG:HH11	1:A:233:ARG:HG3	1.67	0.58
2:L:34:ARG:HB3	2:L:55:PHE:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HG23	1:F:13:ARG:HB3	1.86	0.58
1:D:156:ASN:HD22	1:D:158:GLU:H	1.52	0.57
1:E:9:GLY:CA	1:E:10:ALA:HB3	2.34	0.57
2:G:57:GLN:HG3	7:G:2008:HOH:O	2.04	0.57
1:C:13:ARG:HD2	1:C:13:ARG:O	2.04	0.57
1:F:129:CYS:SG	1:F:131:THR:HG23	2.44	0.57
1:E:30:ARG:HD2	7:E:2018:HOH:O	2.04	0.57
1:F:156:ASN:HD21	1:F:158:GLU:HB2	1.69	0.57
1:C:156:ASN:ND2	1:C:158:GLU:H	2.02	0.57
1:D:280:THR:HG22	1:D:281:ASP:N	2.19	0.57
1:B:208:THR:CG2	1:B:210:THR:H	2.17	0.56
1:D:156:ASN:HD21	1:D:158:GLU:HB2	1.70	0.56
1:D:60:VAL:HG22	1:F:60:VAL:HG22	1.87	0.56
1:A:92:ARG:O	1:A:94:THR:HG22	2.05	0.56
1:C:156:ASN:HD21	1:C:158:GLU:HB2	1.70	0.56
1:B:280:THR:HG22	1:B:282:ALA:H	1.70	0.56
1:B:14:VAL:HG11	1:E:272:HIS:HB3	1.86	0.56
1:B:60:VAL:HG13	1:B:60:VAL:O	2.05	0.56
1:E:156:ASN:HD21	1:E:158:GLU:HB2	1.70	0.56
1:C:11:ALA:C	1:C:13:ARG:HB2	2.25	0.56
1:E:156:ASN:HD22	1:E:158:GLU:H	1.53	0.56
1:B:156:ASN:ND2	1:B:158:GLU:H	2.03	0.56
1:D:284:ILE:H	1:D:284:ILE:CD1	2.19	0.56
1:F:12:ASP:C	1:F:14:VAL:H	2.09	0.56
2:H:9:ARG:HG3	7:H:2010:HOH:O	2.06	0.55
1:D:208:THR:CG2	1:D:210:THR:H	2.19	0.55
1:A:80:ARG:NH2	7:A:2009:HOH:O	2.23	0.55
1:B:9:GLY:HA3	1:B:11:ALA:N	2.21	0.55
1:B:280:THR:HG22	1:B:281:ASP:N	2.22	0.55
2:I:101:ARG:NH1	2:I:101:ARG:HB3	2.22	0.55
2:L:51:TYR:CD2	2:L:54:GLU:HG3	2.42	0.54
1:B:275:LEU:HB3	1:E:14:VAL:HG22	1.89	0.54
1:D:16:ILE:H	1:D:16:ILE:HD12	1.70	0.54
1:B:14:VAL:HG11	1:E:272:HIS:CB	2.37	0.54
1:E:92:ARG:O	1:E:94:THR:HG22	2.07	0.54
1:D:208:THR:HG23	1:D:210:THR:N	2.22	0.54
1:A:284:ILE:H	1:A:284:ILE:CD1	2.19	0.54
2:J:51:TYR:CD2	2:J:54:GLU:HG3	2.43	0.54
1:A:104:MET:HB3	1:B:104:MET:HB3	1.89	0.54
1:D:129:CYS:SG	1:D:131:THR:HG23	2.48	0.54
1:B:156:ASN:HD22	1:B:158:GLU:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:ASN:ND2	1:F:158:GLU:H	2.06	0.54
2:H:51:TYR:CD2	2:H:54:GLU:HG3	2.43	0.54
1:F:156:ASN:HD22	1:F:158:GLU:H	1.56	0.54
2:K:51:TYR:CD2	2:K:54:GLU:HG3	2.43	0.54
2:J:36:PHE:HB2	2:J:38:ARG:CZ	2.38	0.53
1:D:12:ASP:O	1:D:16:ILE:HD13	2.08	0.53
1:E:156:ASN:ND2	1:E:158:GLU:H	2.06	0.53
1:F:60:VAL:O	1:F:60:VAL:HG13	2.08	0.53
1:E:15:ARG:NH1	1:E:16:ILE:HD12	2.23	0.53
1:E:233:ARG:HH11	1:E:233:ARG:HG3	1.74	0.53
1:E:60:VAL:CG1	1:E:60:VAL:O	2.55	0.53
1:F:280:THR:HG22	1:F:281:ASP:N	2.23	0.53
1:B:92:ARG:O	1:B:94:THR:HG22	2.09	0.53
1:A:13:ARG:HB3	1:C:16:ILE:HG23	1.92	0.53
1:D:280:THR:HG22	1:D:282:ALA:H	1.74	0.53
1:D:284:ILE:N	1:D:284:ILE:HD13	2.24	0.53
1:B:208:THR:HG23	1:B:210:THR:N	2.24	0.52
1:F:280:THR:HG22	1:F:282:ALA:H	1.74	0.52
2:K:30:VAL:HG13	2:K:61:LEU:HD13	1.91	0.52
1:C:156:ASN:HD22	1:C:158:GLU:H	1.55	0.52
1:B:60:VAL:CG1	1:B:60:VAL:O	2.58	0.52
2:G:42:GLN:HB3	2:G:86:ILE:HD13	1.92	0.52
1:C:104:MET:HB3	1:F:104:MET:HB3	1.91	0.52
1:D:270:ILE:HD11	1:D:276:LEU:HD23	1.92	0.51
1:B:21:LEU:HB3	1:B:22:PRO:HD3	1.93	0.51
1:D:13:ARG:HB3	1:F:16:ILE:HG23	1.92	0.51
1:D:60:VAL:HG13	1:D:60:VAL:O	2.10	0.51
1:A:215:GLU:HG3	1:A:215:GLU:O	2.10	0.51
1:A:208:THR:CG2	1:A:210:THR:H	2.23	0.51
1:A:92:ARG:HG2	1:A:94:THR:HG22	1.92	0.51
1:F:233:ARG:HG3	1:F:233:ARG:HH11	1.75	0.51
1:A:272:HIS:HB3	1:C:14:VAL:HG11	1.92	0.51
1:B:293:TYR:CD2	1:B:293:TYR:O	2.64	0.51
1:F:12:ASP:C	1:F:14:VAL:N	2.64	0.51
1:A:208:THR:HG23	1:A:210:THR:N	2.25	0.51
1:C:211:ARG:NH2	1:C:220:PRO:O	2.45	0.50
1:B:215:GLU:HB3	1:B:222:SER:HB2	1.93	0.50
2:I:51:TYR:CD2	2:I:54:GLU:HG3	2.46	0.50
2:H:38:ARG:NE	2:H:52:THR:O	2.44	0.50
1:A:211:ARG:NH1	1:A:267:ASP:OD2	2.45	0.50
1:E:280:THR:HG22	1:E:282:ALA:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:38:ARG:HG3	2:K:42:GLN:HB2	1.94	0.50
1:D:233:ARG:HH11	1:D:233:ARG:HG3	1.75	0.50
2:H:39:GLN:O	2:H:42:GLN:HB3	2.10	0.50
1:F:92:ARG:O	1:F:94:THR:HG22	2.11	0.50
1:C:69:GLY:HA3	3:C:1292:NLG:HGC1	1.94	0.50
1:E:13:ARG:O	1:E:17:LEU:HB2	2.12	0.50
2:K:103:ARG:HB3	2:L:88:ASP:HB2	1.93	0.50
1:B:284:ILE:H	1:B:284:ILE:CD1	2.25	0.49
1:B:92:ARG:HH11	3:B:1297:NLG:C	2.25	0.49
2:J:57:GLN:HG3	7:J:2008:HOH:O	2.11	0.49
1:C:12:ASP:CA	1:C:13:ARG:CB	2.90	0.49
1:E:154:SER:HA	2:K:49:SER:HA	1.94	0.49
1:C:60:VAL:HG13	1:C:60:VAL:O	2.12	0.49
1:F:14:VAL:HG12	1:F:15:ARG:N	2.27	0.49
1:B:276:LEU:O	1:B:280:THR:HB	2.12	0.49
1:D:254:ARG:HD3	2:I:45:ARG:HD3	1.94	0.49
1:A:166:ARG:CZ	1:B:162:PRO:HG2	2.43	0.49
1:E:92:ARG:HG2	1:E:94:THR:HG22	1.95	0.49
2:K:103:ARG:CD	6:K:1109:CL:CL	2.97	0.49
1:C:270:ILE:HD11	1:C:276:LEU:HD23	1.94	0.48
1:A:88:HIS:CD2	1:A:93:VAL:HG21	2.48	0.48
1:A:280:THR:HG22	1:A:281:ASP:H	1.78	0.48
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.77	0.48
2:J:30:VAL:HG23	2:K:34:ARG:HB2	1.94	0.48
2:K:57:GLN:HG3	7:K:2006:HOH:O	2.13	0.48
1:A:284:ILE:HD13	1:A:284:ILE:N	2.27	0.48
1:C:280:THR:HG22	1:C:282:ALA:H	1.76	0.48
1:A:276:LEU:O	1:A:280:THR:HB	2.13	0.48
1:C:280:THR:HG22	1:C:281:ASP:H	1.79	0.48
1:D:21:LEU:HB3	1:D:22:PRO:HD3	1.96	0.48
1:D:276:LEU:O	1:D:280:THR:HB	2.13	0.48
1:A:280:THR:HG22	1:A:282:ALA:N	2.28	0.48
1:F:60:VAL:CG1	1:F:60:VAL:O	2.62	0.48
2:K:39:GLN:HB2	2:K:42:GLN:HG3	1.95	0.48
1:B:60:VAL:HG22	1:E:60:VAL:HG22	1.94	0.48
2:G:51:TYR:CD2	2:G:54:GLU:HG3	2.49	0.48
1:C:21:LEU:HB3	1:C:22:PRO:HD3	1.96	0.47
1:D:69:GLY:HA3	3:D:1294:NLG:HGC2	1.95	0.47
1:D:16:ILE:CG2	1:F:13:ARG:HA	2.44	0.47
1:D:60:VAL:CG1	1:D:60:VAL:O	2.63	0.47
2:J:103:ARG:HD3	6:J:1111:CL:CL	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:THR:HG22	1:E:281:ASP:H	1.79	0.47
1:B:156:ASN:ND2	1:B:158:GLU:HB2	2.28	0.47
1:F:21:LEU:HB3	1:F:22:PRO:HD3	1.97	0.47
2:L:42:GLN:OE1	2:L:86:ILE:HD11	2.15	0.47
7:A:2009:HOH:O	1:B:81:VAL:HG12	2.14	0.47
1:A:14:VAL:HG22	1:C:275:LEU:HB3	1.96	0.47
1:A:92:ARG:HD2	3:A:1292:NLG:O	2.15	0.47
1:C:284:ILE:H	1:C:284:ILE:CD1	2.28	0.47
1:C:233:ARG:HH11	1:C:233:ARG:HG3	1.80	0.47
1:D:156:ASN:ND2	1:D:156:ASN:C	2.67	0.47
1:E:136:VAL:HG13	1:E:152:VAL:HG13	1.97	0.46
1:E:276:LEU:O	1:E:280:THR:HB	2.15	0.46
1:C:156:ASN:C	1:C:156:ASN:ND2	2.65	0.46
1:C:208:THR:HG23	1:C:210:THR:N	2.30	0.46
2:I:38:ARG:CG	2:I:52:THR:O	2.60	0.46
1:B:41:MET:O	1:B:47:LYS:HE3	2.16	0.46
1:C:208:THR:CG2	1:C:210:THR:H	2.27	0.46
1:B:254:ARG:HD3	2:H:45:ARG:HD3	1.98	0.46
1:E:284:ILE:CD1	1:E:284:ILE:H	2.27	0.46
1:E:254:ARG:HD3	2:K:45:ARG:HD3	1.98	0.46
1:F:208:THR:HG22	1:F:266:ILE:O	2.16	0.46
1:A:166:ARG:NH2	1:B:162:PRO:HG2	2.31	0.46
1:D:211:ARG:HH11	1:D:211:ARG:CB	2.29	0.46
1:D:17:LEU:HD12	1:D:17:LEU:HA	1.78	0.45
1:F:208:THR:HG23	1:F:210:THR:N	2.29	0.45
1:B:92:ARG:HG2	1:B:94:THR:HG22	1.98	0.45
1:C:60:VAL:CG1	1:C:60:VAL:O	2.64	0.45
1:F:270:ILE:HD11	1:F:276:LEU:HD23	1.99	0.45
1:B:112:LYS:O	1:B:116:SER:HB2	2.16	0.45
1:F:254:ARG:HD3	2:J:45:ARG:HD3	1.98	0.45
1:F:41:MET:O	1:F:47:LYS:HE3	2.17	0.45
1:A:270:ILE:HD11	1:A:276:LEU:HD23	1.97	0.45
1:F:17:LEU:HD12	1:F:17:LEU:HA	1.80	0.45
1:A:21:LEU:HB3	1:A:22:PRO:HD3	1.98	0.45
1:B:156:ASN:HD21	1:B:158:GLU:CB	2.30	0.45
2:H:57:GLN:HG3	7:H:2009:HOH:O	2.16	0.45
1:A:291:SER:HA	7:L:2002:HOH:O	2.17	0.45
1:B:280:THR:HG22	1:B:282:ALA:N	2.32	0.45
1:F:156:ASN:ND2	1:F:156:ASN:C	2.66	0.45
1:F:211:ARG:NH1	1:F:221:GLU:HB3	2.32	0.45
1:A:156:ASN:HD21	1:A:158:GLU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:THR:CG2	1:F:210:THR:H	2.28	0.45
1:A:60:VAL:O	1:A:60:VAL:HG13	2.16	0.44
1:B:156:ASN:C	1:B:156:ASN:ND2	2.66	0.44
1:D:154:SER:HA	2:I:49:SER:HA	2.00	0.44
2:G:100:ILE:HG23	2:G:107:LYS:HG2	1.99	0.44
1:A:121:THR:HG22	1:A:121:THR:O	2.17	0.44
2:H:5:GLU:HG2	2:H:62:GLU:HG2	1.99	0.44
1:E:261:ARG:NH1	7:E:2018:HOH:O	2.50	0.44
1:A:233:ARG:NH1	1:A:233:ARG:HG3	2.32	0.44
1:E:156:ASN:ND2	1:E:158:GLU:HB2	2.32	0.44
2:K:103:ARG:CG	6:K:1109:CL:CL	3.00	0.44
1:D:13:ARG:HB3	1:D:13:ARG:HH11	1.83	0.44
1:E:12:ASP:C	1:E:14:VAL:H	2.19	0.44
1:E:94:THR:HG21	1:E:185:ASN:HD22	1.83	0.44
1:E:84:GLU:HA	1:E:85:PRO:HD3	1.81	0.44
1:F:276:LEU:O	1:F:280:THR:HB	2.17	0.44
1:B:151:GLU:CD	1:B:254:ARG:HH22	2.21	0.44
1:D:70:GLY:H	3:D:1294:NLG:HGC2	1.83	0.44
2:L:99:THR:HB	2:L:108:ASN:HB2	2.00	0.44
1:A:156:ASN:HD22	1:A:157:SER:N	2.16	0.43
1:E:30:ARG:CD	7:E:2018:HOH:O	2.62	0.43
1:F:261:ARG:NH1	7:F:2020:HOH:O	2.51	0.43
2:J:51:TYR:HD2	2:J:54:GLU:HG3	1.82	0.43
1:F:156:ASN:ND2	1:F:158:GLU:HB2	2.32	0.43
2:I:101:ARG:HH11	2:I:101:ARG:HB3	1.82	0.43
1:A:136:VAL:HG13	1:A:152:VAL:HG13	2.00	0.43
1:E:270:ILE:HD11	1:E:276:LEU:HD23	2.01	0.43
1:F:13:ARG:HB3	1:F:13:ARG:HH11	1.84	0.43
2:J:5:GLU:HG2	2:J:62:GLU:HG2	2.00	0.43
1:A:12:ASP:C	1:A:14:VAL:H	2.22	0.43
1:B:121:THR:O	1:B:121:THR:HG22	2.19	0.43
1:B:156:ASN:HD22	1:B:157:SER:N	2.14	0.43
1:B:161[A]:GLU:CB	1:B:162:PRO:HD3	2.48	0.43
1:E:41:MET:HE3	1:E:110:VAL:CG1	2.49	0.43
1:D:12:ASP:C	1:D:14:VAL:N	2.72	0.43
1:F:277:GLU:HA	1:F:284:ILE:HD11	1.99	0.43
2:L:5:GLU:HG2	2:L:62:GLU:HG2	2.00	0.43
1:D:156:ASN:HD21	1:D:158:GLU:CB	2.32	0.43
1:F:139:ARG:NH2	2:J:50:GLU:OE2	2.45	0.43
1:F:267:ASP:OD1	1:F:269:ARG:HB2	2.19	0.43
1:A:60:VAL:CG1	1:A:60:VAL:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:GLY:CA	1:E:10:ALA:CB	2.96	0.42
1:C:109:ARG:HH12	1:F:100:GLU:HG2	1.83	0.42
1:D:16:ILE:N	1:D:16:ILE:CD1	2.82	0.42
2:G:5:GLU:HG2	2:G:62:GLU:HG2	2.01	0.42
2:G:63:ILE:HD11	2:G:73:VAL:HG11	2.02	0.42
2:I:5:GLU:HG2	2:I:62:GLU:HG2	2.00	0.42
1:A:88:HIS:O	1:A:89:ASN:C	2.57	0.42
2:G:65:VAL:HG13	2:G:69:GLN:HB2	2.01	0.42
1:A:277:GLU:HA	1:A:284:ILE:HD11	2.02	0.42
1:C:100:GLU:HG2	1:F:109:ARG:HH12	1.84	0.42
1:E:277:GLU:HA	1:E:284:ILE:HD11	2.02	0.42
1:E:280:THR:CG2	1:E:281:ASP:N	2.83	0.42
1:D:121:THR:HG22	1:D:121:THR:O	2.19	0.42
1:A:156:ASN:ND2	1:A:156:ASN:C	2.72	0.42
1:C:121:THR:HG22	1:C:121:THR:O	2.19	0.42
1:C:136:VAL:HG13	1:C:152:VAL:HG13	2.02	0.42
1:C:156:ASN:HD22	1:C:157:SER:N	2.17	0.42
1:D:156:ASN:ND2	1:D:158:GLU:HB2	2.33	0.42
1:D:14:VAL:HG12	1:D:15:ARG:N	2.35	0.42
1:B:275:LEU:CB	1:E:14:VAL:HG22	2.49	0.41
2:G:34:ARG:HB2	2:I:30:VAL:HG23	2.01	0.41
1:D:228:ASN:HD22	1:D:292:GLY:C	2.24	0.41
1:E:121:THR:HG22	1:E:121:THR:O	2.18	0.41
1:E:21:LEU:HB3	1:E:22:PRO:HD3	2.02	0.41
1:C:154:SER:HA	2:G:49:SER:HA	2.02	0.41
2:K:28:MET:HB2	2:K:28:MET:HE3	1.97	0.41
1:A:63:ARG:HH22	1:A:165:GLU:CD	2.23	0.41
1:C:276:LEU:O	1:C:280:THR:HB	2.20	0.41
1:D:12:ASP:C	1:D:14:VAL:H	2.23	0.41
1:A:73:GLU:OE1	1:A:73:GLU:HA	2.20	0.41
1:B:154:SER:HA	2:H:49:SER:HA	2.02	0.41
1:D:280:THR:HG22	1:D:282:ALA:N	2.35	0.41
1:D:14:VAL:HG22	1:F:275:LEU:HB3	2.01	0.41
2:I:44:GLU:OE1	2:I:58:LYS:NZ	2.52	0.41
1:D:16:ILE:H	1:D:16:ILE:CD1	2.33	0.41
1:E:41:MET:HE3	1:E:110:VAL:HG11	2.01	0.41
1:E:233:ARG:NH1	1:E:233:ARG:HG3	2.35	0.41
2:I:65:VAL:HG13	2:I:69:GLN:HB2	2.03	0.41
2:I:38:ARG:HD2	2:I:52:THR:O	2.21	0.41
1:D:181:GLY:O	5:E:1295:GOL:H31	2.20	0.41
2:H:103:ARG:HD3	6:H:1110:CL:CL	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLU:HA	1:C:284:ILE:HD11	2.03	0.41
1:F:112:LYS:O	1:F:116:SER:HB2	2.21	0.41
2:H:42:GLN:HG3	2:H:86:ILE:HD13	2.03	0.41
1:C:156:ASN:ND2	1:C:158:GLU:HB2	2.35	0.41
1:C:280:THR:HG22	1:C:282:ALA:N	2.36	0.41
1:D:112:LYS:O	1:D:116:SER:HB2	2.21	0.41
1:D:211:ARG:NH1	1:D:211:ARG:HB2	2.36	0.41
1:A:14:VAL:HG22	1:C:275:LEU:CB	2.51	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.93	0.41
1:D:156:ASN:HD22	1:D:157:SER:N	2.18	0.41
1:A:280:THR:CG2	1:A:281:ASP:N	2.83	0.40
1:C:41:MET:O	1:C:47:LYS:HE3	2.21	0.40
1:E:284:ILE:HD13	1:E:284:ILE:N	2.34	0.40
2:I:30:VAL:HG13	2:I:61:LEU:HD13	2.03	0.40
1:A:112:LYS:O	1:A:116:SER:HB2	2.21	0.40
1:F:139:ARG:HE	2:J:50:GLU:CD	2.25	0.40
2:H:65:VAL:HG13	2:H:69:GLN:HB2	2.02	0.40
1:C:156:ASN:HD21	1:C:158:GLU:CB	2.33	0.40
1:C:30:ARG:HD2	7:C:2013:HOH:O	2.21	0.40
2:G:99:THR:O	2:G:107:LYS:HA	2.21	0.40
2:I:98:GLN:HE21	2:I:107:LYS:HD3	1.84	0.40
1:E:280:THR:HG22	1:E:282:ALA:N	2.36	0.40
2:H:42:GLN:HG3	2:H:86:ILE:CD1	2.52	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:F:80:ARG:NH2	2:K:22:ASN:O[1_455]	2.02	0.18

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	283/321 (88%)	274 (97%)	5 (2%)	4 (1%)	13	35
1	B	289/321 (90%)	277 (96%)	8 (3%)	4 (1%)	13	35
1	C	283/321 (88%)	274 (97%)	7 (2%)	2 (1%)	25	56
1	D	285/321 (89%)	280 (98%)	2 (1%)	3 (1%)	17	43
1	E	286/321 (89%)	280 (98%)	4 (1%)	2 (1%)	25	56
1	F	286/321 (89%)	273 (96%)	9 (3%)	4 (1%)	13	35
2	G	109/112 (97%)	103 (94%)	5 (5%)	1 (1%)	20	49
2	H	106/112 (95%)	102 (96%)	4 (4%)	0	100	100
2	I	105/112 (94%)	101 (96%)	4 (4%)	0	100	100
2	J	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	20	49
2	K	106/112 (95%)	101 (95%)	4 (4%)	1 (1%)	20	49
2	L	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
All	All	2353/2598 (91%)	2270 (96%)	61 (3%)	22 (1%)	20	49

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	ASP
1	F	178	ASP
1	A	10	ALA
1	A	70	GLY
1	A	89	ASN
1	A	178	ASP
1	B	70	GLY
1	C	70	GLY
1	D	13	ARG
1	D	70	GLY
1	D	178	ASP
1	E	70	GLY
1	E	178	ASP
1	F	13	ARG
1	F	70	GLY
2	G	110	ASP
2	J	40	LYS
1	C	178	ASP
2	K	38	ARG
1	B	10	ALA
1	B	219	ARG
1	F	220	PRO

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	224/256 (88%)	203 (91%)	21 (9%)	10	26
1	B	226/256 (88%)	205 (91%)	21 (9%)	10	27
1	C	225/256 (88%)	203 (90%)	22 (10%)	9	24
1	D	225/256 (88%)	201 (89%)	24 (11%)	8	20
1	E	225/256 (88%)	204 (91%)	21 (9%)	10	27
1	F	225/256 (88%)	200 (89%)	25 (11%)	7	19
2	G	90/93 (97%)	81 (90%)	9 (10%)	9	23
2	H	90/93 (97%)	82 (91%)	8 (9%)	11	29
2	I	88/93 (95%)	81 (92%)	7 (8%)	14	35
2	J	90/93 (97%)	81 (90%)	9 (10%)	9	23
2	K	90/93 (97%)	83 (92%)	7 (8%)	15	36
2	L	89/93 (96%)	82 (92%)	7 (8%)	14	35
All	All	1887/2094 (90%)	1706 (90%)	181 (10%)	10	25

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	VAL
1	A	21	LEU
1	A	35	LYS
1	A	45	GLU
1	A	48	GLU
1	A	73	GLU
1	A	94	THR
1	A	131	THR
1	A	135	LEU
1	A	137	LEU
1	A	156	ASN
1	A	159	VAL
1	A	190	THR

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Mol	Chain	Res	Type
1	A	208	THR
1	A	215	GLU
1	A	251	CYS
1	A	254	ARG
1	A	270	ILE
1	A	276	LEU
1	A	284	ILE
1	B	21	LEU
1	B	35	LYS
1	B	45	GLU
1	B	48	GLU
1	B	60	VAL
1	B	94	THR
1	B	131	THR
1	B	134	ARG
1	B	135	LEU
1	B	137	LEU
1	B	156	ASN
1	B	159	VAL
1	B	190	THR
1	B	208	THR
1	B	211	ARG
1	B	254	ARG
1	B	261	ARG
1	B	269	ARG
1	B	270	ILE
1	B	276	LEU
1	B	284	ILE
1	C	12	ASP
1	C	13	ARG
1	C	21	LEU
1	C	35	LYS
1	C	48	GLU
1	C	94	THR
1	C	131	THR
1	C	134	ARG
1	C	135	LEU
1	C	137	LEU
1	C	156	ASN
1	C	159	VAL
1	C	190	THR
1	C	208	THR

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Mol	Chain	Res	Type
1	C	211	ARG
1	C	221	GLU
1	C	234	GLU
1	C	254	ARG
1	C	261	ARG
1	C	270	ILE
1	C	276	LEU
1	C	284	ILE
1	D	12	ASP
1	D	13	ARG
1	D	15	ARG
1	D	21	LEU
1	D	35	LYS
1	D	48	GLU
1	D	73	GLU
1	D	94	THR
1	D	131	THR
1	D	135	LEU
1	D	137	LEU
1	D	156	ASN
1	D	159	VAL
1	D	179	GLU
1	D	190	THR
1	D	208	THR
1	D	211	ARG
1	D	221	GLU
1	D	251	CYS
1	D	254	ARG
1	D	261	ARG
1	D	270	ILE
1	D	276	LEU
1	D	284	ILE
1	E	14	VAL
1	E	21	LEU
1	E	35	LYS
1	E	45	GLU
1	E	84	GLU
1	E	94	THR
1	E	131	THR
1	E	134	ARG
1	E	135	LEU
1	E	137	LEU

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Mol	Chain	Res	Type
1	E	156	ASN
1	E	159	VAL
1	E	190	THR
1	E	211	ARG
1	E	221	GLU
1	E	251	CYS
1	E	254	ARG
1	E	261	ARG
1	E	270	ILE
1	E	276	LEU
1	E	284	ILE
1	F	12	ASP
1	F	13	ARG
1	F	14	VAL
1	F	21	LEU
1	F	35	LYS
1	F	45	GLU
1	F	48	GLU
1	F	84[A]	GLU
1	F	84[B]	GLU
1	F	94	THR
1	F	131	THR
1	F	135	LEU
1	F	137	LEU
1	F	156	ASN
1	F	159	VAL
1	F	190	THR
1	F	208	THR
1	F	221	GLU
1	F	223	LEU
1	F	251	CYS
1	F	254	ARG
1	F	261	ARG
1	F	270	ILE
1	F	276	LEU
1	F	284	ILE
2	G	13	LEU
2	G	20	LEU
2	G	30	VAL
2	G	33	VAL
2	G	39	GLN
2	G	40	LYS

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Mol	Chain	Res	Type
2	G	65	VAL
2	G	99	THR
2	G	100	ILE
2	H	13	LEU
2	H	20	LEU
2	H	30	VAL
2	H	33	VAL
2	H	65	VAL
2	H	99	THR
2	H	100	ILE
2	H	101	ARG
2	I	13	LEU
2	I	20	LEU
2	I	30	VAL
2	I	33	VAL
2	I	65	VAL
2	I	99	THR
2	I	100	ILE
2	J	1	MET
2	J	13	LEU
2	J	20	LEU
2	J	30	VAL
2	J	33	VAL
2	J	39	GLN
2	J	65	VAL
2	J	99	THR
2	J	100	ILE
2	K	13	LEU
2	K	20	LEU
2	K	30	VAL
2	K	58	LYS
2	K	65	VAL
2	K	99	THR
2	K	100	ILE
2	L	13	LEU
2	L	20	LEU
2	L	30	VAL
2	L	33	VAL
2	L	65	VAL
2	L	99	THR
2	L	100	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	88	HIS
1	A	156	ASN
1	A	182	GLN
1	B	26	GLN
1	B	88	HIS
1	B	89	ASN
1	B	156	ASN
1	C	156	ASN
1	C	200	ASN
1	D	26	GLN
1	D	156	ASN
1	D	200	ASN
1	E	88	HIS
1	E	156	ASN
1	E	200	ASN
1	F	156	ASN
1	F	200	ASN
2	I	108	ASN
2	J	98	GLN

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](#)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NLG	A	1292	-	6,12,12	2.17	1 (16%)	6,15,15	1.63	2 (33%)
3	NLG	B	1297	-	6,12,12	2.26	1 (16%)	6,15,15	1.72	2 (33%)
3	NLG	C	1292	-	6,12,12	2.22	1 (16%)	6,15,15	1.76	2 (33%)
3	NLG	D	1294	-	6,12,12	2.24	1 (16%)	6,15,15	1.30	0
3	NLG	E	1294	-	6,12,12	2.21	1 (16%)	6,15,15	1.52	2 (33%)
5	GOL	E	1295	-	5,5,5	0.40	0	5,5,5	0.31	0
3	NLG	F	1293	-	6,12,12	2.26	1 (16%)	6,15,15	1.28	1 (16%)

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	1297	-	-	0/7/13/13	0/0/0/0
3	NLG	C	1292	-	-	0/7/13/13	0/0/0/0
3	NLG	D	1294	-	-	0/7/13/13	0/0/0/0
3	NLG	E	1294	-	-	0/7/13/13	0/0/0/0
5	GOL	E	1295	-	-	0/4/4/4	0/0/0/0
3	NLG	F	1293	-	-	0/7/13/13	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1294	NLG	C8-C7	-5.35	1.39	1.50
3	D	1294	NLG	C8-C7	-5.34	1.39	1.50
3	F	1293	NLG	C8-C7	-5.32	1.39	1.50
3	C	1292	NLG	C8-C7	-5.30	1.39	1.50
3	A	1292	NLG	C8-C7	-5.07	1.39	1.50
3	B	1297	NLG	C8-C7	-4.92	1.39	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1297	NLG	CB-CA-C	-3.10	107.78	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1292	NLG	O7-C7-C8	-2.81	116.94	122.06
3	A	1292	NLG	O7-C7-C8	-2.49	117.53	122.06
3	E	1294	NLG	CB-CA-N2	-2.36	106.64	110.22
3	E	1294	NLG	O7-C7-C8	-2.32	117.83	122.06
3	A	1292	NLG	CB-CA-C	-2.26	109.00	112.28
3	C	1292	NLG	CB-CA-C	-2.24	109.03	112.28
3	B	1297	NLG	O7-C7-C8	-2.21	118.04	122.06
3	F	1293	NLG	O7-C7-C8	-2.16	118.13	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1292	NLG	1	0
3	B	1297	NLG	2	0
3	C	1292	NLG	1	0
3	D	1294	NLG	2	0
5	E	1295	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](#)

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%)	0.22	6 (2%) 64 59	31, 37, 46, 50	0
1	B	289/321 (90%)	0.14	3 (1%) 82 80	31, 37, 46, 50	1 (0%)
1	C	284/321 (88%)	0.16	2 (0%) 87 85	31, 37, 45, 50	0
1	D	286/321 (89%)	0.21	5 (1%) 70 67	31, 37, 46, 52	0
1	E	286/321 (89%)	0.22	9 (3%) 49 44	31, 37, 46, 54	1 (0%)
1	F	287/321 (89%)	0.27	6 (2%) 64 59	31, 37, 45, 50	0
2	G	111/112 (99%)	0.49	8 (7%) 16 11	31, 38, 49, 53	0
2	H	108/112 (96%)	0.37	4 (3%) 42 36	31, 37, 46, 56	0
2	I	109/112 (97%)	0.83	13 (11%) 5 3	31, 37, 48, 53	0
2	J	110/112 (98%)	0.32	1 (0%) 84 82	31, 38, 46, 52	0
2	K	108/112 (96%)	0.32	0 100 100	31, 38, 46, 55	0
2	L	109/112 (97%)	0.26	2 (1%) 69 65	31, 38, 45, 48	0
All	All	2371/2598 (91%)	0.27	59 (2%) 58 52	31, 37, 46, 56	2 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	41	GLY	6.2
1	E	293	TYR	6.0
2	I	109	ALA	5.1
1	F	6	ILE	4.8
1	E	12	ASP	4.7
2	I	110	ASP	4.4
1	E	10	ALA	4.2
2	G	110	ASP	4.2
2	G	111	ALA	4.0
2	G	109	ALA	3.7
1	E	84	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	I	111	ALA	3.5
1	D	292	GLY	3.4
2	H	1	MET	3.4
1	E	11	ALA	3.3
1	B	294	HIS	3.1
1	F	220	PRO	3.1
2	I	68	ALA	3.0
1	A	11	ALA	2.9
2	L	109	ALA	2.9
1	F	292	GLY	2.8
2	I	92	PHE	2.7
1	A	15	ARG	2.6
1	A	88	HIS	2.6
1	D	291	SER	2.6
2	G	42	GLN	2.5
2	I	108	ASN	2.5
1	D	237	ALA	2.4
1	B	211	ARG	2.4
2	I	95	PRO	2.3
1	F	281	ASP	2.3
1	F	7	GLU	2.3
2	H	39	GLN	2.3
2	I	100	ILE	2.3
2	H	38	ARG	2.3
1	A	8	ALA	2.2
2	J	41	GLY	2.2
2	I	40	LYS	2.2
1	E	292	GLY	2.2
2	I	1	MET	2.2
2	G	26	VAL	2.1
1	F	282	ALA	2.1
1	E	210	THR	2.1
1	B	224	ILE	2.1
1	C	146	ILE	2.1
2	I	102	ILE	2.1
2	G	81	ALA	2.1
1	E	220	PRO	2.1
1	D	284	ILE	2.1
2	I	96	VAL	2.1
1	A	87	PHE	2.1
2	G	92	PHE	2.1
2	L	42	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	9	GLY	2.0
1	A	85	PRO	2.0
2	I	93	VAL	2.0
1	D	8	ALA	2.0
1	E	38	GLY	2.0
2	H	95	PRO	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
5	GOL	E	1295	6/6	0.84	0.30	2.81	56,56,57,58	0
3	NLG	F	1293	13/13	0.90	0.25	1.48	42,46,47,49	0
3	NLG	D	1294	13/13	0.95	0.20	0.75	41,45,49,49	0
3	NLG	C	1292	13/13	0.92	0.20	0.53	38,39,40,41	0
3	NLG	E	1294	13/13	0.93	0.20	0.52	41,43,44,46	0
3	NLG	B	1297	13/13	0.94	0.19	0.52	42,44,47,48	0
3	NLG	A	1292	13/13	0.91	0.23	0.51	50,53,54,54	0
6	CL	G	1112	1/1	0.94	0.23	0.45	43,43,43,43	0
6	CL	H	1110	1/1	0.90	0.24	0.38	63,63,63,63	0
6	CL	J	1112	1/1	0.90	0.14	-0.69	62,62,62,62	0
6	CL	K	1109	1/1	0.99	0.13	-1.24	39,39,39,39	0
4	NA	E	1296	1/1	0.84	0.14	-1.46	46,46,46,46	0
4	NA	B	1298	1/1	0.91	0.10	-2.21	37,37,37,37	0
6	CL	J	1111	1/1	0.95	0.16	-2.42	30,30,30,30	0
6	CL	H	1109	1/1	0.97	0.12	-2.54	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NA	D	1295	1/1	0.87	0.11	-2.82	50,50,50,50	0
4	NA	A	1293	1/1	0.51	0.18	-	57,57,57,57	0
4	NA	C	1293	1/1	0.86	0.16	-	36,36,36,36	0
4	NA	F	1294	1/1	0.71	0.20	-	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.