Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 09:40 am BST

PDB ID	:	7AHU
Title	:	Anti-FX Fab of mim8 in complex with human FXa
Authors	:	Johansson, E.
Deposited on	:	2020-09-25
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 following versions of software and data (see references ⓘ) were used in the production of this report:

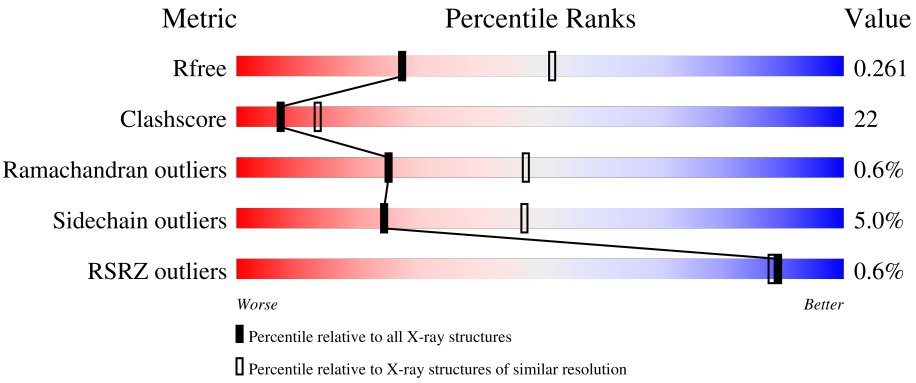
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	216	58% 38%
1	L	216	65% 33%
2	B	222	68% 29%
2	H	222	69% 29%
3	C	241	53% 41%

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Mol	Chain	Length	Quality of chain
3	E	241	
4	D	58	
4	F	58	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11641 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 Anti-FX Fab of mim8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1669	1042	284	338	5			
1	A	216	Total	C	N	O	S	0	0	0
			1669	1042	284	338	5			

- Molecule 2 is a protein called Anti-FX Fab of mim8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1689	1068	275	337	9			
2	B	222	Total	C	N	O	S	0	0	0
			1689	1068	275	337	9			

- Molecule 3 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	234	Total	C	N	O	S	0	0	0
			1838	1157	322	345	14			
3	E	234	Total	C	N	O	S	0	0	0
			1838	1157	322	345	14			

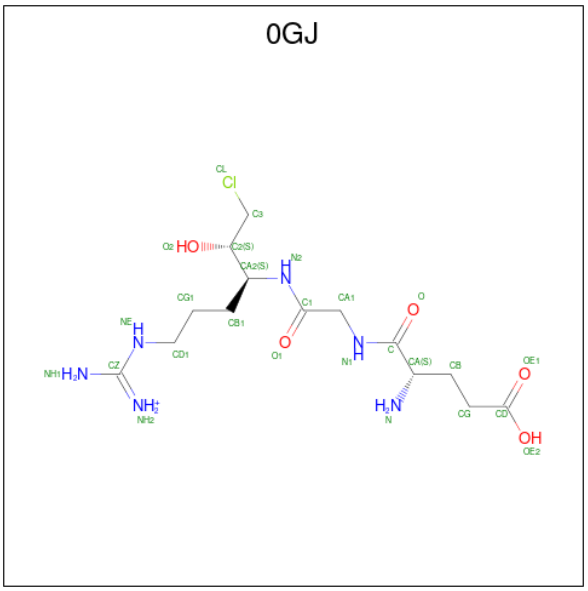
- Molecule 4 is a protein called Coagulation factor X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	52	Total	C	N	O	S	0	0	0
			381	230	65	79	7			
4	F	51	Total	C	N	O	S	0	0	0
			372	224	63	78	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	251	MET	-	initiating methionine	UNP P00742
F	251	MET	-	initiating methionine	UNP P00742

- Molecule 5 is L-alpha-glutamyl-N-{(1S)-4-{[amino(iminio)methyl]amino}-1-[(1S)-2-chloro-1-hydroxyethyl]butyl}glycinamide (three-letter code: 0GJ) (formula: $C_{14}H_{28}ClN_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 25 14 6 5	0	0
5	E	1	Total C N O 25 14 6 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	80	Total O 80 80	0	0
7	H	64	Total O 64 64	0	0

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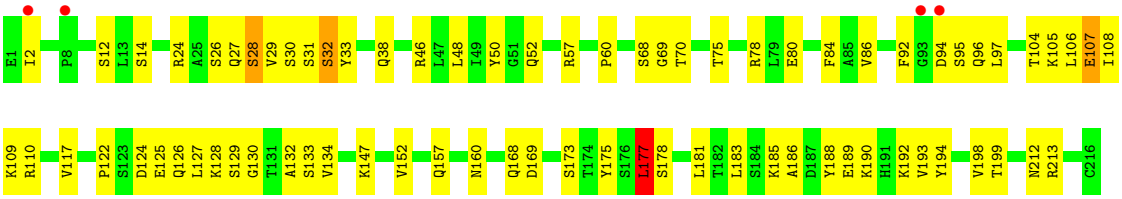
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	59	Total O 59 59	0	0
7	B	66	Total O 66 66	0	0
7	C	79	Total O 79 79	0	0
7	D	18	Total O 18 18	0	0
7	E	65	Total O 65 65	0	0
7	F	13	Total O 13 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

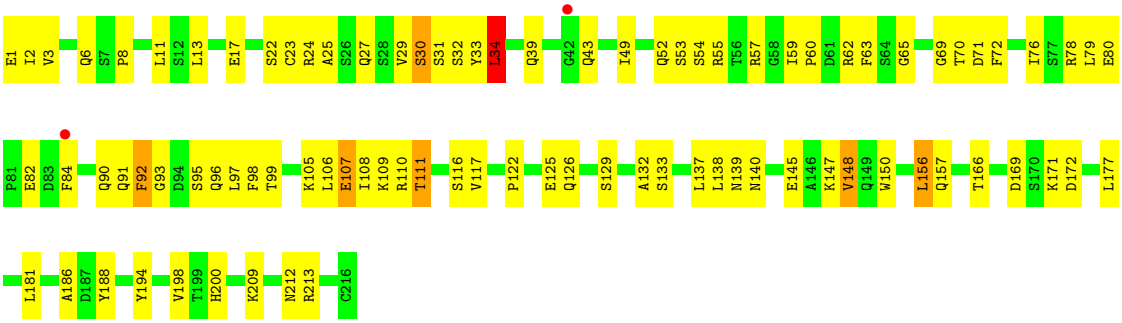
• Molecule 1: Anti-FX Fab of mim8 light chain

Chain L:



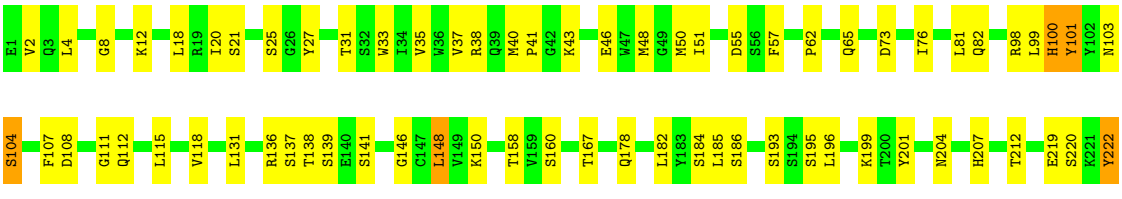
• Molecule 1: Anti-FX Fab of mim8 light chain

Chain A:



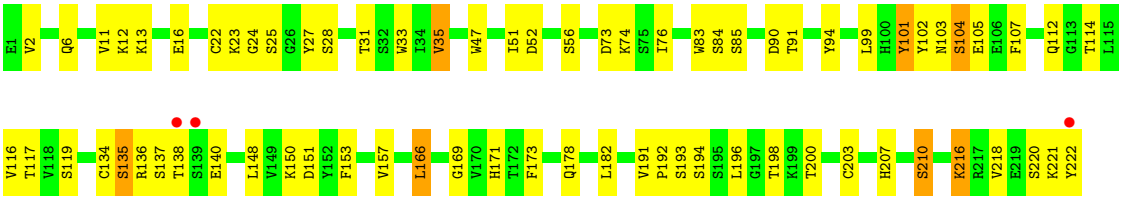
• Molecule 2: Anti-FX Fab of mim8 heavy chain

Chain H:



• Molecule 2: Anti-FX Fab of mim8 heavy chain

Chain B:

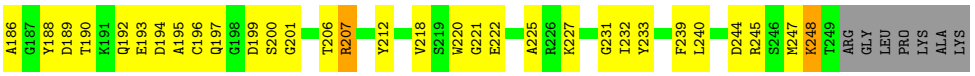


• Molecule 3: Coagulation factor X

Chain C:

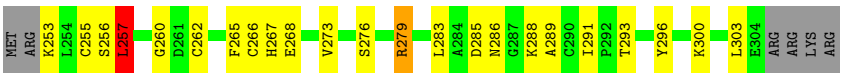
• Molecule 3: Coagulation factor X

Chain E:



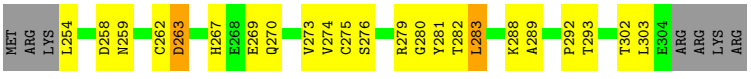
• Molecule 4: Coagulation factor X

Chain D:



• Molecule 4: Coagulation factor X

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.13Å 105.25Å 145.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.60 48.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.59-2.60) 99.2 (48.59-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18_3845, PHENIX 1.18_3845	Depositor
R, R_{free}	0.203 , 0.263 0.196 , 0.261	Depositor DCC
R_{free} test set	1984 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11641	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9207e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0GJ, CA

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	0.53	0/1704	0.91	1/2308 (0.0%)
1	L	0.52	0/1704	0.87	1/2308 (0.0%)
2	B	0.58	1/1734 (0.1%)	0.87	2/2360 (0.1%)
2	H	0.57	0/1734	0.92	3/2360 (0.1%)
3	C	0.62	1/1876 (0.1%)	0.96	2/2528 (0.1%)
3	E	0.61	3/1876 (0.2%)	0.89	1/2528 (0.0%)
4	D	0.71	0/387	0.99	2/523 (0.4%)
4	F	0.57	0/378	0.96	1/512 (0.2%)
All	All	0.58	5/11393 (0.0%)	0.91	13/15427 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	27	CYS	CB-SG	5.94	1.92	1.82
3	E	200	SER	CB-OG	-5.69	1.34	1.42
3	C	200	SER	CB-OG	-5.22	1.35	1.42
2	B	22	CYS	CB-SG	-5.15	1.73	1.81
3	E	58	CYS	CB-SG	-5.10	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	LEU	CA-CB-CG	6.08	129.28	115.30
3	C	113	ILE	CG1-CB-CG2	-6.04	98.12	111.40
2	B	105	GLU	N-CA-CB	6.00	121.41	110.60
2	B	166	LEU	CA-CB-CG	5.75	128.52	115.30
3	C	33	LEU	CA-CB-CG	5.57	128.10	115.30
4	F	283	LEU	CA-CB-CG	5.52	127.99	115.30
1	L	177	LEU	CA-CB-CG	5.29	127.47	115.30
2	H	185	LEU	CA-CB-CG	5.20	127.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	21	SER	N-CA-CB	5.19	118.29	110.50
3	E	108	ARG	NE-CZ-NH2	-5.16	117.72	120.30
4	D	257	LEU	CB-CG-CD2	5.05	119.58	111.00
4	D	257	LEU	CA-CB-CG	5.04	126.89	115.30
2	H	222	TYR	N-CA-CB	5.03	119.65	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1669	0	1619	82	0
1	L	1669	0	1619	68	0
2	B	1689	0	1635	58	0
2	H	1689	0	1635	57	0
3	C	1838	0	1786	101	0
3	E	1838	0	1786	105	0
4	D	381	0	345	25	0
4	F	372	0	332	21	0
5	C	25	0	22	4	0
5	E	25	0	21	7	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	A	59	0	0	17	0
7	B	66	0	0	20	2
7	C	79	0	0	24	2
7	D	18	0	0	6	0
7	E	65	0	0	24	2
7	F	13	0	0	4	0
7	H	64	0	0	15	2
7	L	80	0	0	17	0
All	All	11641	0	10800	495	4

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 22.

All (495) 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:A:1:GLU:HA	1:A:96:GLN:HG2	1.36	1.06
3:C:64:ARG:HH22	3:C:86:VAL:HB	1.27	0.96
3:C:17:VAL:HG21	3:C:225:ALA:HB2	1.47	0.96
2:H:48:MET:SD	7:H:330:HOH:O	2.24	0.94
3:C:84:HIS:HD2	3:C:113:ILE:HG22	1.30	0.93
2:B:12:LYS:NZ	7:B:302:HOH:O	2.01	0.92
3:E:180:THR:HG22	3:E:182:ASN:H	1.37	0.90
2:B:207:HIS:HD1	2:B:210:SER:HG	1.18	0.87
2:B:136:ARG:HH21	2:B:220:SER:HB2	1.40	0.86
2:B:114:THR:O	7:B:301:HOH:O	1.94	0.84
3:C:24:ASP:OD2	3:C:118:ASN:ND2	2.10	0.84
4:D:253:LYS:HB2	4:D:256:SER:HB2	1.57	0.84
3:C:51:TYR:O	7:C:401:HOH:O	1.95	0.84
2:H:38:ARG:NE	2:H:46:GLU:OE1	2.11	0.84
1:L:27:GLN:H	1:L:70:THR:HG22	1.43	0.84
2:B:207:HIS:ND1	2:B:210:SER:OG	2.12	0.82
3:C:84:HIS:CD2	3:C:113:ILE:HG22	2.13	0.82
3:C:22:CYS:O	3:C:72:ARG:NH1	2.12	0.82
3:E:80:GLY:O	3:E:116:ARG:NH2	2.13	0.82
3:E:72:ARG:O	7:E:401:HOH:O	1.96	0.82
3:E:207:ARG:HB2	3:E:212:TYR:CE2	2.14	0.82
1:A:96:GLN:NE2	7:A:305:HOH:O	2.13	0.81
3:C:108:ARG:NH2	7:C:409:HOH:O	2.14	0.81
3:C:116:ARG:HG2	3:C:119:VAL:HG22	1.63	0.80
3:E:71:ASP:HA	3:E:81:GLU:HG2	1.63	0.79
1:L:48:LEU:HB2	7:L:335:HOH:O	1.83	0.79
4:D:255:CYS:SG	7:D:413:HOH:O	2.41	0.78
2:B:73:ASP:OD2	2:B:76:ILE:HG12	1.82	0.78
3:C:168:ARG:NH1	3:C:181:GLN:OE1	2.17	0.78
1:L:125:GLU:O	7:L:301:HOH:O	2.03	0.77
3:C:227:LYS:O	7:C:402:HOH:O	2.03	0.76
3:E:69:VAL:O	3:E:81:GLU:HA	1.86	0.76
1:L:122:PRO:HD3	1:L:134:VAL:HG22	1.67	0.75
1:L:130:GLY:HA2	1:L:185:LYS:HD3	1.67	0.75
1:L:80:GLU:OE1	7:L:302:HOH:O	2.04	0.74
2:H:182:LEU:N	7:H:304:HOH:O	2.21	0.74
1:A:148:VAL:HG12	1:A:198:VAL:HG12	1.69	0.74
1:A:23:CYS:SG	7:A:342:HOH:O	2.45	0.73
3:E:245:ARG:NH1	7:E:406:HOH:O	2.20	0.73
1:A:54:SER:OG	7:A:301:HOH:O	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:OE2	7:A:302:HOH:O	2.05	0.73
1:L:32:SER:OG	1:L:33:TYR:N	2.16	0.73
3:C:220:TRP:HA	5:C:301:0GJ:HG21	1.69	0.72
1:L:117:VAL:HG21	1:L:198:VAL:HG21	1.69	0.72
2:B:76:ILE:O	7:B:303:HOH:O	2.09	0.71
3:E:153:ARG:HE	3:E:154:GLN:H	1.35	0.71
4:D:293:THR:O	7:D:401:HOH:O	2.08	0.71
3:C:161:LEU:O	7:C:406:HOH:O	2.08	0.71
3:E:172:LYS:HA	3:E:179:ILE:HD13	1.72	0.70
3:C:111:THR:OG1	7:C:403:HOH:O	2.04	0.70
3:E:93:ASN:ND2	7:E:409:HOH:O	2.23	0.70
3:C:170:SER:O	7:C:405:HOH:O	2.08	0.70
3:E:126:GLU:OE2	4:F:267:HIS:NE2	2.22	0.70
3:E:116:ARG:NH1	7:E:411:HOH:O	2.25	0.69
2:H:38:ARG:NH2	2:H:46:GLU:OE2	2.20	0.69
3:E:70:GLY:O	7:E:402:HOH:O	2.11	0.69
1:L:92:PHE:O	7:L:303:HOH:O	2.09	0.69
2:B:218:VAL:O	7:B:304:HOH:O	2.10	0.69
3:E:166:VAL:HB	3:E:185:CYS:HB3	1.74	0.69
2:B:116:VAL:HG23	7:B:301:HOH:O	1.92	0.69
2:H:8:GLY:O	7:H:301:HOH:O	2.10	0.69
3:C:189:ASP:OD2	3:C:228:GLY:HA2	1.93	0.69
4:F:259:ASN:OD1	7:F:401:HOH:O	2.11	0.69
2:H:167:THR:O	7:H:303:HOH:O	2.11	0.69
1:A:55:ARG:NH1	7:A:303:HOH:O	2.11	0.68
2:H:137:SER:O	2:H:138:THR:OG1	2.11	0.68
1:A:117:VAL:HG21	1:A:198:VAL:HG21	1.75	0.68
3:C:64:ARG:NH1	7:C:407:HOH:O	2.09	0.68
3:E:64:ARG:HD2	3:E:65:PHE:H	1.59	0.68
1:A:49:ILE:HG22	1:A:55:ARG:HG2	1.76	0.67
3:E:77:GLU:N	3:E:77:GLU:OE1	2.25	0.67
1:A:53:SER:OG	7:A:304:HOH:O	2.12	0.67
1:A:57:ARG:HD2	4:F:282:THR:HB	1.77	0.67
3:C:131:GLU:OE1	3:C:235:LYS:NZ	2.28	0.67
2:H:182:LEU:O	7:H:304:HOH:O	2.12	0.67
3:C:163:VAL:HG22	7:C:406:HOH:O	1.93	0.67
2:B:52:ASP:OD1	7:B:305:HOH:O	2.13	0.66
3:E:46:ILE:O	7:E:403:HOH:O	2.14	0.66
1:L:108:ILE:O	1:L:168:GLN:NE2	2.29	0.66
1:A:39:GLN:NE2	1:A:43:GLN:O	2.28	0.66
2:B:136:ARG:NH2	2:B:220:SER:HB2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:85:GLU:HB2	3:E:110:LYS:NZ	2.10	0.66
1:L:122:PRO:HG3	1:L:132:ALA:HB1	1.78	0.66
3:C:54:THR:HG22	3:C:55:ALA:H	1.61	0.66
3:E:47:LEU:HD23	7:E:403:HOH:O	1.95	0.66
1:A:25:ALA:O	7:A:307:HOH:O	2.14	0.65
1:A:84:PHE:CD2	1:A:106:LEU:HG	2.30	0.65
3:E:175:SER:HB3	3:E:179:ILE:HD11	1.76	0.65
1:A:27:GLN:HG2	1:A:70:THR:HG22	1.77	0.65
1:A:126:GLN:O	1:A:129:SER:OG	2.11	0.65
2:H:98:ARG:O	7:H:306:HOH:O	2.14	0.65
1:L:57:ARG:NH1	4:D:285:ASP:OD2	2.28	0.65
2:H:104:SER:OG	7:H:307:HOH:O	2.14	0.65
1:A:29:VAL:O	1:A:30:SER:OG	2.12	0.65
2:B:138:THR:HG21	2:B:193:SER:HB3	1.79	0.65
1:A:157:GLN:O	7:A:309:HOH:O	2.15	0.64
1:A:213:ARG:NH1	7:A:318:HOH:O	2.31	0.64
1:A:59:ILE:O	7:A:308:HOH:O	2.14	0.64
3:C:48:SER:O	7:C:401:HOH:O	2.13	0.64
2:H:98:ARG:NH2	2:H:108:ASP:OD2	2.27	0.64
1:A:110:ARG:NH1	1:A:111:THR:HG23	2.13	0.64
7:C:419:HOH:O	4:D:300:LYS:HE2	1.97	0.64
1:A:82:GLU:H	1:A:82:GLU:CD	2.01	0.64
5:E:301:0GJ:HG2	5:E:301:0GJ:H1	1.63	0.64
3:C:16:ILE:N	3:C:199:ASP:OD2	2.31	0.63
2:B:35:VAL:HG22	2:B:47:TRP:HE1	1.63	0.63
1:A:60:PRO:HG2	1:A:63:PHE:CD2	2.32	0.63
1:L:94:ASP:OD2	3:C:51:TYR:OH	2.15	0.63
1:A:91:GLN:HG2	1:A:92:PHE:H	1.65	0.62
3:C:207:ARG:HB2	3:C:212:TYR:CE2	2.34	0.62
2:H:195:SER:HB2	2:H:199:LYS:HE3	1.81	0.62
1:A:34:LEU:HD12	1:A:91:GLN:HG3	1.82	0.62
3:C:143:SER:OG	7:C:408:HOH:O	2.11	0.62
3:C:210:ASP:OD1	3:C:210:ASP:N	2.33	0.62
3:E:166:VAL:HG23	3:E:186:ALA:HA	1.82	0.62
3:E:199:ASP:O	3:E:218:VAL:HG21	2.00	0.62
4:D:279:ARG:NH1	7:D:403:HOH:O	2.33	0.61
1:L:126:GLN:O	1:L:129:SER:OG	2.14	0.61
2:H:219:GLU:O	7:H:308:HOH:O	2.16	0.61
3:E:16:ILE:HD13	3:E:159:LYS:HB2	1.83	0.61
3:E:201:GLY:H	3:E:218:VAL:HG23	1.63	0.61
1:L:124:ASP:O	1:L:128:LYS:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:GLU:HA	3:C:81:GLU:OE2	2.01	0.61
3:E:110:LYS:NZ	7:E:410:HOH:O	2.24	0.61
3:E:201:GLY:N	3:E:218:VAL:HG23	2.16	0.60
3:C:113:ILE:HD11	3:C:115:PHE:CD1	2.36	0.60
3:C:189:ASP:HB3	7:C:453:HOH:O	2.01	0.60
2:H:73:ASP:OD2	2:H:76:ILE:HG12	2.01	0.60
2:H:2:VAL:HA	2:H:25:SER:O	2.02	0.60
1:A:60:PRO:HG3	1:A:62:ARG:HH21	1.67	0.60
3:C:49:GLU:O	3:C:113:ILE:N	2.32	0.60
1:A:122:PRO:HG3	1:A:132:ALA:HB1	1.84	0.59
2:H:40:MET:HB2	2:H:43:LYS:HD2	1.84	0.59
3:E:147:ARG:HH21	3:E:197:GLN:HE21	1.49	0.59
1:A:110:ARG:HG2	1:A:111:THR:N	2.18	0.59
1:A:32:SER:HB2	1:A:69:GLY:H	1.68	0.59
3:C:243:ILE:HB	7:C:421:HOH:O	2.01	0.59
2:B:135:SER:OG	7:B:306:HOH:O	2.15	0.59
1:L:60:PRO:O	7:L:304:HOH:O	2.17	0.58
1:L:147:LYS:HB3	1:L:199:THR:HB	1.84	0.58
1:A:138:LEU:HD12	1:A:177:LEU:HD22	1.84	0.58
3:E:197:GLN:HA	5:E:301:0GJ:HB21	1.84	0.58
3:C:147:ARG:HA	3:C:154:GLN:HA	1.86	0.58
2:B:51:ILE:HD11	2:B:56:SER:HA	1.86	0.57
4:F:281:TYR:HD1	4:F:292:PRO:HA	1.68	0.57
3:C:223:GLY:O	5:C:301:0GJ:NH2	2.38	0.57
5:C:301:0GJ:HG31	7:C:416:HOH:O	2.05	0.57
3:E:91:LYS:NZ	7:E:414:HOH:O	2.32	0.57
1:A:60:PRO:HG2	1:A:63:PHE:HD2	1.69	0.57
3:C:113:ILE:HD11	3:C:115:PHE:CE1	2.40	0.57
1:A:1:GLU:OE1	7:A:310:HOH:O	2.18	0.57
1:A:117:VAL:HG22	1:A:138:LEU:HD23	1.85	0.57
2:B:27:TYR:HA	4:F:274:VAL:HG21	1.87	0.57
3:C:147:ARG:HD3	3:C:152:GLY:O	2.05	0.57
2:B:104:SER:O	3:E:248:LYS:HE2	2.03	0.56
1:L:57:ARG:NH2	7:L:317:HOH:O	2.37	0.56
2:B:136:ARG:HE	2:B:220:SER:HB2	1.71	0.56
2:H:41:PRO:O	2:H:43:LYS:NZ	2.39	0.56
3:E:85:GLU:HB2	3:E:110:LYS:HZ2	1.70	0.56
2:H:112:GLN:OE1	2:H:112:GLN:N	2.36	0.56
3:C:54:THR:HG22	3:C:55:ALA:N	2.21	0.56
3:C:197:GLN:NE2	7:C:416:HOH:O	2.39	0.56
3:E:145:PHE:CZ	3:E:158:LEU:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:301:0GJ:HG2	5:E:301:0GJ:N1	2.21	0.55
4:D:283:LEU:HD12	4:D:289:ALA:O	2.06	0.55
3:C:80:GLY:HA3	3:C:116:ARG:NH1	2.22	0.55
2:H:40:MET:HB2	2:H:43:LYS:HB2	1.87	0.55
3:C:127:ARG:NH2	7:C:417:HOH:O	2.39	0.55
1:A:24:ARG:HA	1:A:70:THR:O	2.06	0.55
3:C:99:THR:HG23	3:C:101:ASP:H	1.70	0.55
3:E:78:GLU:N	3:E:81:GLU:OE1	2.23	0.55
3:E:190:THR:HA	3:E:227:LYS:HG2	1.87	0.55
4:F:269:GLU:HB3	4:F:270:GLN:HG3	1.88	0.55
3:E:137:GLN:NE2	3:E:207:ARG:O	2.32	0.55
1:A:17:GLU:HB2	1:A:79:LEU:HD12	1.88	0.54
3:C:172:LYS:HA	3:C:179:ILE:HD12	1.90	0.54
4:F:274:VAL:O	7:F:403:HOH:O	2.19	0.54
3:C:80:GLY:HA3	3:C:116:ARG:CZ	2.37	0.54
3:E:153:ARG:HE	3:E:154:GLN:N	2.04	0.54
3:E:188:TYR:O	7:E:405:HOH:O	2.18	0.54
3:E:227:LYS:N	7:E:422:HOH:O	2.40	0.54
3:E:108:ARG:HH11	3:E:108:ARG:HG3	1.73	0.54
3:E:161:LEU:HD22	3:E:163:VAL:HG13	1.90	0.54
3:C:226:ARG:HH21	3:C:229:LYS:HE3	1.72	0.54
2:B:23:LYS:HG3	7:B:303:HOH:O	2.07	0.54
3:E:56:ALA:HB1	3:E:91:LYS:HG3	1.88	0.54
1:L:27:GLN:HG2	1:L:70:THR:HG23	1.89	0.54
3:C:115:PHE:HA	3:C:119:VAL:HG23	1.88	0.54
4:D:262:CYS:HB3	7:D:411:HOH:O	2.08	0.54
2:H:35:VAL:HG21	2:H:107:PHE:CE1	2.43	0.53
1:L:78:ARG:O	1:L:78:ARG:HG3	2.07	0.53
3:E:18:GLY:N	7:E:417:HOH:O	2.36	0.53
3:E:52:ILE:HD13	3:E:67:VAL:HG21	1.90	0.53
2:H:65:GLN:N	7:H:310:HOH:O	2.42	0.53
1:L:152:VAL:HG22	1:L:157:GLN:NE2	2.23	0.53
1:A:110:ARG:HG2	1:A:111:THR:H	1.73	0.53
3:E:16:ILE:HD11	3:E:144:GLY:N	2.23	0.53
3:C:85:GLU:HG3	7:C:439:HOH:O	2.07	0.53
3:E:110:LYS:NZ	3:E:110:LYS:HB2	2.23	0.53
3:E:99:THR:HG23	3:E:101:ASP:H	1.74	0.53
3:E:192:GLN:HA	3:E:225:ALA:HB1	1.89	0.53
3:C:207:ARG:HD2	3:C:212:TYR:CZ	2.44	0.53
3:E:85:GLU:N	7:E:410:HOH:O	2.40	0.53
1:L:84:PHE:CD1	1:L:106:LEU:HG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:PRO:O	7:H:310:HOH:O	2.19	0.53
1:A:150:TRP:O	1:A:156:LEU:HA	2.09	0.53
3:E:52:ILE:HD12	3:E:109:LEU:HD21	1.91	0.53
1:A:27:GLN:HB3	1:A:31:SER:OG	2.09	0.53
3:C:84:HIS:NE2	3:C:113:ILE:HA	2.23	0.53
3:C:194:ASP:OD1	3:C:195:ALA:N	2.42	0.53
3:E:72:ARG:NH1	7:E:401:HOH:O	2.41	0.53
2:H:2:VAL:HG23	2:H:27:TYR:CD1	2.44	0.52
1:A:1:GLU:HG2	1:A:2:ILE:N	2.23	0.52
1:A:93:GLY:HA2	7:A:326:HOH:O	2.10	0.52
2:B:6:GLN:O	2:B:112:GLN:NE2	2.38	0.52
3:C:17:VAL:CG2	3:C:225:ALA:HB2	2.32	0.52
3:C:90:ILE:HD13	3:C:246:SER:HB3	1.91	0.52
2:H:37:VAL:C	7:H:330:HOH:O	2.47	0.52
1:A:69:GLY:HA2	7:A:327:HOH:O	2.09	0.52
3:E:218:VAL:HG12	3:E:233:TYR:CE1	2.44	0.52
3:E:182:ASN:HB3	3:E:239:PHE:HE2	1.74	0.52
3:C:126:GLU:CD	4:D:267:HIS:HE2	2.12	0.52
2:H:193:SER:O	2:H:196:LEU:HD23	2.10	0.52
1:A:52:GLN:NE2	3:E:49:GLU:HG2	2.25	0.51
1:A:140:ASN:OD1	2:B:171:HIS:NE2	2.38	0.51
2:B:11:VAL:HA	2:B:117:THR:O	2.10	0.51
3:E:137:GLN:HE21	3:E:206:THR:HG22	1.75	0.51
3:C:158:LEU:O	7:C:411:HOH:O	2.19	0.51
2:B:24:GLY:O	7:B:307:HOH:O	2.18	0.51
3:C:117:MET:HE1	4:D:303:LEU:O	2.11	0.51
3:C:171:CYS:SG	3:C:179:ILE:HD13	2.49	0.51
4:F:263:ASP:HB2	4:F:288:LYS:O	2.09	0.51
1:L:194:TYR:HE1	1:L:213:ARG:HB2	1.76	0.51
3:C:64:ARG:NH2	3:C:86:VAL:HB	2.11	0.51
4:D:286:ASN:ND2	7:D:406:HOH:O	2.44	0.51
2:H:40:MET:CB	2:H:43:LYS:HD2	2.40	0.51
2:B:2:VAL:HG23	2:B:27:TYR:CD1	2.46	0.51
2:B:90:ASP:HA	7:B:324:HOH:O	2.11	0.51
2:B:150:LYS:HG2	2:B:151:ASP:CG	2.31	0.51
1:A:8:PRO:HG3	1:A:11:LEU:HD13	1.93	0.51
2:B:103:ASN:HB3	3:E:247:MET:SD	2.51	0.51
2:B:136:ARG:HB3	2:B:222:TYR:O	2.10	0.51
3:C:189:ASP:O	3:C:228:GLY:N	2.43	0.51
1:A:32:SER:HA	1:A:72:PHE:HZ	1.75	0.51
1:L:27:GLN:HG2	1:L:70:THR:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:O	1:A:98:PHE:HA	2.11	0.51
1:A:105:LYS:HE2	1:A:107:GLU:HB3	1.93	0.51
1:L:186:ALA:O	1:L:190:LYS:HG3	2.11	0.50
2:B:157:VAL:HG12	2:B:207:HIS:HB2	1.92	0.50
1:A:62:ARG:HH12	1:A:80:GLU:CG	2.25	0.50
3:C:145:PHE:CZ	3:C:158:LEU:HB2	2.46	0.50
2:B:196:LEU:HD12	2:B:196:LEU:H	1.75	0.50
3:C:207:ARG:NH1	3:C:212:TYR:OH	2.40	0.50
3:E:193:GLU:O	7:E:404:HOH:O	2.18	0.50
2:H:35:VAL:HG11	2:H:107:PHE:CE1	2.46	0.50
1:A:1:GLU:HA	1:A:96:GLN:CG	2.26	0.50
3:E:68:ARG:HD2	3:E:81:GLU:HB3	1.93	0.50
3:C:87:GLU:HG2	3:C:88:VAL:HG23	1.93	0.50
4:D:279:ARG:NH1	7:D:405:HOH:O	2.43	0.50
3:E:17:VAL:HG22	3:E:194:ASP:O	2.12	0.50
1:L:169:ASP:HA	7:L:307:HOH:O	2.12	0.50
2:B:85:SER:O	7:B:310:HOH:O	2.20	0.50
1:L:78:ARG:HG3	7:L:302:HOH:O	2.12	0.50
1:L:78:ARG:NH1	7:L:323:HOH:O	2.45	0.49
1:L:188:TYR:O	1:L:194:TYR:OH	2.29	0.49
1:A:133:SER:OG	7:A:311:HOH:O	2.20	0.49
1:L:30:SER:O	7:L:305:HOH:O	2.20	0.49
2:B:119:SER:HB3	2:B:153:PHE:CZ	2.47	0.49
3:C:166:VAL:HG23	3:C:186:ALA:HA	1.94	0.49
3:C:168:ARG:NH2	3:C:183:MET:O	2.45	0.49
3:E:57:HIS:ND1	3:E:103:ASP:OD2	2.44	0.49
1:L:27:GLN:HE21	1:L:70:THR:HG23	1.78	0.49
2:H:103:ASN:HB3	3:C:247:MET:CE	2.43	0.49
3:C:51:TYR:CG	3:C:247:MET:HE3	2.47	0.49
1:L:177:LEU:HD23	1:L:178:SER:N	2.27	0.49
1:A:32:SER:HA	1:A:72:PHE:CZ	2.48	0.49
3:E:37:GLU:O	3:E:39:GLU:HG3	2.13	0.49
2:H:35:VAL:HG11	2:H:107:PHE:HE1	1.77	0.49
1:L:117:VAL:CG2	1:L:198:VAL:HG21	2.41	0.49
1:L:193:VAL:HG22	7:L:306:HOH:O	2.13	0.49
1:L:28:SER:OG	1:L:29:VAL:N	2.46	0.49
4:D:266:CYS:SG	4:D:273:VAL:HG23	2.53	0.49
3:E:194:ASP:OD1	3:E:195:ALA:N	2.46	0.49
2:H:20:ILE:HD11	2:H:81:LEU:HD23	1.95	0.48
7:H:325:HOH:O	3:C:241:LYS:HE3	2.13	0.48
3:C:217:ILE:HG23	7:C:431:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:165:TYR:HB3	7:E:442:HOH:O	2.12	0.48
1:L:107:GLU:HB2	1:L:168:GLN:OE1	2.14	0.48
3:C:239:PHE:O	3:C:243:ILE:HG13	2.13	0.48
3:E:50:PHE:O	3:E:108:ARG:HA	2.13	0.48
2:H:55:ASP:OD2	3:C:245:ARG:NH2	2.33	0.48
2:B:153:PHE:HE1	7:B:316:HOH:O	1.96	0.48
3:C:149:HIS:O	3:C:152:GLY:N	2.47	0.48
3:E:153:ARG:HE	3:E:153:ARG:HA	1.79	0.48
3:E:182:ASN:HB3	3:E:239:PHE:CE2	2.49	0.48
2:H:35:VAL:HG12	2:H:50:MET:HB3	1.96	0.48
2:B:150:LYS:NZ	2:B:178:GLN:OE1	2.27	0.48
3:E:231:GLY:N	7:E:425:HOH:O	2.45	0.48
2:B:91:THR:O	7:B:308:HOH:O	2.19	0.48
2:H:220:SER:OG	7:H:309:HOH:O	2.19	0.47
2:B:138:THR:OG1	2:B:140:GLU:O	2.15	0.47
3:E:56:ALA:HB2	3:E:104:ILE:O	2.14	0.47
2:H:38:ARG:HE	2:H:46:GLU:CD	2.10	0.47
2:B:169:GLY:N	7:B:328:HOH:O	2.43	0.47
3:E:190:THR:HB	3:E:227:LYS:HE2	1.96	0.47
1:L:33:TYR:CD1	1:L:52:GLN:HG2	2.49	0.47
1:L:94:ASP:HB3	3:C:249:THR:O	2.14	0.47
2:B:101:TYR:O	3:E:244:ASP:OD1	2.32	0.47
4:F:302:THR:O	4:F:303:LEU:HD23	2.14	0.47
1:L:185:LYS:O	1:L:189:GLU:HG3	2.14	0.47
2:H:103:ASN:O	4:D:279:ARG:NH2	2.47	0.47
2:H:148:LEU:HD21	2:H:150:LYS:HD2	1.97	0.47
3:E:168:ARG:O	3:E:171:CYS:HB3	2.14	0.47
1:L:212:ASN:OD1	7:L:306:HOH:O	2.20	0.47
1:A:188:TYR:O	1:A:194:TYR:OH	2.33	0.47
3:C:46:ILE:HA	3:C:52:ILE:HD13	1.95	0.47
3:C:166:VAL:HB	3:C:185:CYS:HB3	1.95	0.47
4:D:265:PHE:HB2	4:D:276:SER:OG	2.14	0.47
4:F:276:SER:HA	4:F:283:LEU:HD11	1.96	0.47
1:L:133:SER:HA	1:L:181:LEU:O	2.15	0.47
2:H:160:SER:OG	2:H:204:ASN:HB2	2.15	0.47
1:A:62:ARG:NH1	1:A:80:GLU:HG2	2.30	0.47
2:B:191:VAL:HG12	2:B:192:PRO:HD2	1.97	0.47
3:C:207:ARG:HB2	3:C:212:TYR:CD2	2.50	0.47
1:A:133:SER:HA	1:A:181:LEU:O	2.15	0.47
2:B:134:CYS:O	7:B:311:HOH:O	2.21	0.47
3:C:125:PRO:HB2	3:C:130:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:64:ARG:HD2	3:E:65:PHE:N	2.28	0.47
3:C:73:ASN:HD22	3:C:76:GLN:H	1.62	0.47
3:E:64:ARG:NH2	3:E:86:VAL:H	2.13	0.47
1:A:32:SER:O	1:A:32:SER:OG	2.33	0.46
3:C:17:VAL:O	3:C:193:GLU:HA	2.15	0.46
2:B:35:VAL:HG21	2:B:107:PHE:HE1	1.79	0.46
3:E:220:TRP:CE2	3:E:232:ILE:HG21	2.50	0.46
1:A:33:TYR:O	1:A:33:TYR:CD1	2.69	0.46
2:B:137:SER:OG	2:B:138:THR:N	2.48	0.46
1:L:192:LYS:NZ	7:L:329:HOH:O	2.49	0.46
1:A:145:GLU:O	1:A:200:HIS:CD2	2.69	0.46
3:E:159:LYS:NZ	7:E:417:HOH:O	2.48	0.46
4:F:281:TYR:CD1	4:F:292:PRO:HA	2.50	0.46
2:B:35:VAL:HG21	2:B:107:PHE:CE1	2.50	0.46
3:E:23:LYS:HA	3:E:23:LYS:HD3	1.77	0.46
1:L:92:PHE:HA	1:L:97:LEU:O	2.16	0.46
3:E:68:ARG:HA	3:E:82:ALA:O	2.16	0.46
3:C:27:CYS:HB3	7:C:408:HOH:O	2.15	0.45
3:E:150:GLU:O	3:E:151:LYS:HE2	2.17	0.45
1:L:27:GLN:O	1:L:27:GLN:HG3	2.16	0.45
3:E:77:GLU:HB3	7:E:451:HOH:O	2.15	0.45
2:H:136:ARG:HB3	2:H:222:TYR:OXT	2.17	0.45
3:C:222:GLU:O	3:C:226:ARG:HG3	2.15	0.45
1:A:29:VAL:O	1:A:29:VAL:HG23	2.17	0.45
3:C:126:GLU:OE2	4:D:267:HIS:NE2	2.36	0.45
3:E:90:ILE:HD12	3:E:106:VAL:HG23	1.98	0.45
3:E:222:GLU:OE1	7:E:407:HOH:O	2.21	0.45
4:D:253:LYS:HD3	4:D:256:SER:CB	2.47	0.45
1:A:31:SER:HB3	1:A:69:GLY:O	2.17	0.45
1:A:91:GLN:HG2	1:A:92:PHE:N	2.30	0.45
2:B:31:THR:O	2:B:101:TYR:HD1	1.99	0.45
2:H:33:TRP:HB2	2:H:99:LEU:HB3	1.98	0.45
4:F:280:GLY:O	4:F:293:THR:HB	2.17	0.45
1:L:168:GLN:O	7:L:307:HOH:O	2.21	0.45
2:H:103:ASN:HB3	3:C:247:MET:HE2	1.99	0.45
1:A:60:PRO:HG3	1:A:62:ARG:NH2	2.29	0.45
3:C:71:ASP:HA	3:C:81:GLU:HG2	1.98	0.45
3:C:64:ARG:HD2	3:C:65:PHE:H	1.82	0.45
1:A:13:LEU:O	1:A:108:ILE:HA	2.17	0.44
2:B:138:THR:HG21	2:B:193:SER:CB	2.47	0.44
3:C:43:GLY:O	3:C:54:THR:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:VAL:N	7:C:406:HOH:O	2.50	0.44
3:E:24:ASP:OD2	7:E:408:HOH:O	2.21	0.44
3:E:34:ILE:HG21	3:E:68:ARG:NH1	2.31	0.44
2:H:199:LYS:HD2	2:H:201:TYR:CZ	2.51	0.44
2:B:203:CYS:SG	2:B:216:LYS:HB3	2.57	0.44
1:L:183:LEU:HD11	1:L:194:TYR:HE2	1.82	0.44
2:H:35:VAL:HG21	2:H:107:PHE:CD1	2.53	0.44
1:A:24:ARG:NH2	1:A:71:ASP:HB2	2.33	0.44
1:A:116:SER:HB2	1:A:139:ASN:HB3	1.99	0.44
3:E:52:ILE:CD1	3:E:109:LEU:HD21	2.47	0.44
1:L:38:GLN:OE1	1:L:46:ARG:NH2	2.37	0.44
3:C:87:GLU:HB2	3:C:110:LYS:HG2	1.99	0.44
3:E:116:ARG:HG3	3:E:119:VAL:HG23	1.99	0.44
3:E:16:ILE:O	3:E:148:THR:HA	2.17	0.44
3:E:221:GLY:H	5:E:301:0GJ:C	2.31	0.44
4:F:275:CYS:SG	4:F:288:LYS:HB3	2.58	0.44
3:C:195:ALA:O	5:C:301:0GJ:NH1	2.51	0.44
4:F:275:CYS:O	4:F:283:LEU:HD21	2.18	0.44
2:H:18:LEU:O	2:H:82:GLN:HA	2.18	0.44
1:A:60:PRO:CG	1:A:62:ARG:HH21	2.30	0.44
2:B:91:THR:HG23	2:B:117:THR:HA	1.99	0.44
1:A:62:ARG:CG	1:A:76:ILE:HG23	2.48	0.43
3:E:17:VAL:HG21	3:E:225:ALA:HB2	1.99	0.43
1:A:31:SER:O	1:A:32:SER:HB3	2.17	0.43
1:A:169:ASP:HB3	1:A:172:ASP:OD1	2.18	0.43
3:E:51:TYR:HA	3:E:107:LEU:O	2.17	0.43
1:L:127:LEU:HD23	1:L:127:LEU:HA	1.83	0.43
1:A:6:GLN:HA	1:A:22:SER:O	2.19	0.43
3:C:166:VAL:HG21	3:C:230:TYR:CD1	2.54	0.43
4:F:263:ASP:HB2	4:F:289:ALA:HA	2.01	0.43
1:L:12:SER:O	1:L:109:LYS:HE3	2.19	0.43
1:L:110:ARG:HD2	1:L:173:SER:HB2	2.00	0.43
1:L:194:TYR:CE1	1:L:213:ARG:HB2	2.52	0.43
2:H:12:LYS:O	2:H:118:VAL:HA	2.19	0.43
3:C:130:ALA:O	3:C:134:LEU:HB2	2.18	0.43
3:E:74:THR:N	3:E:156:THR:O	2.36	0.43
1:L:2:ILE:HG23	1:L:26:SER:H	1.83	0.43
2:H:207:HIS:HB3	2:H:212:THR:HB	2.01	0.43
1:A:212:ASN:OD1	7:A:312:HOH:O	2.21	0.43
3:E:157:ARG:NH2	7:E:420:HOH:O	2.39	0.43
1:L:157:GLN:HB3	1:L:160:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:168:ARG:NH2	3:E:183:MET:O	2.51	0.43
2:B:33:TRP:HB2	2:B:99:LEU:HB3	2.00	0.43
4:F:262:CYS:HA	4:F:288:LYS:HB2	2.01	0.43
2:H:4:LEU:O	2:H:111:GLY:HA2	2.19	0.43
2:H:51:ILE:HA	2:H:57:PHE:O	2.19	0.43
4:F:258:ASP:N	7:F:407:HOH:O	2.52	0.43
1:L:57:ARG:NH2	7:L:332:HOH:O	2.52	0.42
1:L:107:GLU:OE1	1:L:175:TYR:OH	2.33	0.42
1:A:117:VAL:HA	1:A:137:LEU:O	2.19	0.42
1:A:186:ALA:N	7:A:313:HOH:O	2.23	0.42
4:F:279:ARG:H	4:F:279:ARG:HG2	1.47	0.42
2:H:31:THR:O	2:H:101:TYR:CD2	2.72	0.42
3:C:142:VAL:HG12	7:C:406:HOH:O	2.19	0.42
1:L:48:LEU:HD12	7:L:335:HOH:O	2.19	0.42
1:A:166:THR:HG23	2:B:173:PHE:CE2	2.54	0.42
3:E:33:LEU:HD12	3:E:67:VAL:HG22	2.01	0.42
2:H:131:LEU:HD12	2:H:146:GLY:HA3	2.01	0.42
3:C:115:PHE:HB2	4:D:296:TYR:CD2	2.54	0.42
1:L:26:SER:O	1:L:28:SER:N	2.52	0.42
3:C:35:ASN:OD1	3:C:39:GLU:HG2	2.19	0.42
1:A:49:ILE:CD1	1:A:65:GLY:HA3	2.50	0.42
1:A:55:ARG:HD3	7:A:303:HOH:O	2.20	0.42
2:B:84:SER:O	7:B:312:HOH:O	2.22	0.42
1:L:57:ARG:NE	4:D:291:ILE:HD12	2.35	0.42
1:L:86:VAL:HA	1:L:104:THR:O	2.20	0.42
2:H:178:GLN:N	7:H:304:HOH:O	2.53	0.42
2:B:136:ARG:N	7:B:337:HOH:O	2.52	0.42
2:B:178:GLN:NE2	2:B:182:LEU:HB2	2.35	0.42
4:F:254:LEU:HB3	4:F:273:VAL:CG2	2.49	0.42
2:H:178:GLN:OE1	2:H:184:SER:HB2	2.20	0.42
3:C:99:THR:O	3:C:100:TYR:HB2	2.20	0.42
3:E:153:ARG:HA	3:E:153:ARG:NE	2.35	0.42
1:A:33:TYR:O	1:A:33:TYR:HD1	2.02	0.42
1:A:147:LYS:O	1:A:198:VAL:HA	2.19	0.42
1:L:27:GLN:NE2	1:L:70:THR:HG23	2.35	0.41
1:A:62:ARG:HE	1:A:62:ARG:HB3	1.61	0.41
4:D:253:LYS:N	4:D:257:LEU:HB2	2.35	0.41
3:E:157:ARG:NH1	7:E:420:HOH:O	2.41	0.41
1:L:38:GLN:HB2	1:L:48:LEU:HD11	2.02	0.41
2:B:94:TYR:HD2	7:B:301:HOH:O	2.03	0.41
3:C:78:GLU:H	3:C:81:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:CYS:SG	3:C:160:MET:HB3	2.60	0.41
2:H:199:LYS:HE2	2:H:199:LYS:HB2	1.77	0.41
2:B:136:ARG:NE	2:B:220:SER:HB2	2.33	0.41
3:C:30:GLN:HB2	7:C:408:HOH:O	2.21	0.41
3:E:153:ARG:NE	3:E:154:GLN:H	2.12	0.41
3:E:240:LEU:HA	3:E:240:LEU:HD23	1.91	0.41
1:L:92:PHE:CE2	1:L:97:LEU:HA	2.55	0.41
1:L:169:ASP:O	1:L:173:SER:HA	2.21	0.41
2:H:103:ASN:C	4:D:279:ARG:HH21	2.24	0.41
2:H:222:TYR:OH	7:H:302:HOH:O	2.10	0.41
3:C:68:ARG:NH2	3:C:71:ASP:OD1	2.48	0.41
3:E:197:GLN:HG3	5:E:301:0GJ:O1	2.21	0.41
2:H:137:SER:C	2:H:138:THR:HG1	2.15	0.41
1:A:62:ARG:NH1	1:A:80:GLU:CG	2.84	0.41
2:B:83:TRP:HB3	7:B:346:HOH:O	2.21	0.41
4:D:260:GLY:HA3	4:D:273:VAL:HG21	2.03	0.41
3:E:17:VAL:HG13	3:E:196:CYS:HB2	2.02	0.41
3:E:180:THR:CG2	3:E:181:GLN:N	2.84	0.41
1:L:105:LYS:HE3	7:L:331:HOH:O	2.20	0.41
1:L:183:LEU:HD12	1:L:188:TYR:HD2	1.85	0.41
2:H:220:SER:HB3	2:H:222:TYR:O	2.20	0.41
3:C:16:ILE:HA	3:C:195:ALA:HA	2.02	0.41
3:C:98:GLU:H	3:C:98:GLU:HG3	1.70	0.41
4:D:253:LYS:HD3	4:D:256:SER:HB2	2.02	0.41
3:E:195:ALA:HB3	5:E:301:0GJ:NH1	2.36	0.41
3:C:35:ASN:HD21	3:C:39:GLU:HG2	1.86	0.41
4:D:255:CYS:HB2	4:D:268:GLU:OE2	2.20	0.41
1:L:50:TYR:HE2	4:D:279:ARG:HH11	1.69	0.40
1:A:13:LEU:O	1:A:109:LYS:N	2.40	0.40
2:B:178:GLN:HB3	7:B:335:HOH:O	2.21	0.40
2:B:28:SER:HA	4:F:269:GLU:CG	2.51	0.40
3:E:16:ILE:HG23	3:E:161:LEU:HD12	2.03	0.40
3:E:87:GLU:HB3	3:E:108:ARG:O	2.20	0.40
1:A:209:LYS:HA	1:A:209:LYS:HD3	1.85	0.40
3:C:207:ARG:NH2	7:C:427:HOH:O	2.54	0.40
3:E:90:ILE:HB	3:E:106:VAL:HG23	2.03	0.40
3:E:195:ALA:HB3	5:E:301:0GJ:HH11	1.86	0.40
1:L:24:ARG:HA	1:L:70:THR:O	2.22	0.40
2:H:101:TYR:HD1	3:C:244:ASP:CG	2.25	0.40
2:B:13:LYS:HB2	2:B:16:GLU:HG3	2.03	0.40
3:E:46:ILE:HG23	7:E:424:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:270:GLN:NE2	7:F:402:HOH:O	2.17	0.40
1:L:27:GLN:HB3	1:L:69:GLY:C	2.42	0.40
1:A:90:GLN:HA	1:A:99:THR:O	2.21	0.40
3:C:117:MET:O	3:C:118:ASN:HB2	2.21	0.40

All (4) 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)
7:H:328:HOH:O	7:B:312:HOH:O[1_565]	1.98	0.22
7:C:434:HOH:O	7:E:420:HOH:O[2_556]	2.05	0.15
7:C:477:HOH:O	7:E:463:HOH:O[2_556]	2.06	0.14
7:H:351:HOH:O	7:B:313:HOH:O[1_565]	2.08	0.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/216 (99%)	205 (96%)	8 (4%)	1 (0%)	29	52
1	L	214/216 (99%)	204 (95%)	8 (4%)	2 (1%)	17	35
2	B	220/222 (99%)	211 (96%)	7 (3%)	2 (1%)	17	35
2	H	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	29	52
3	C	232/241 (96%)	224 (97%)	7 (3%)	1 (0%)	34	57
3	E	232/241 (96%)	223 (96%)	8 (3%)	1 (0%)	34	57
4	D	50/58 (86%)	46 (92%)	4 (8%)	0	100	100
4	F	49/58 (84%)	46 (94%)	3 (6%)	0	100	100
All	All	1431/1474 (97%)	1370 (96%)	53 (4%)	8 (1%)	25	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	28	SER
1	L	32	SER
2	H	100	HIS
1	A	30	SER
2	B	101	TYR
3	C	189	ASP
3	E	189	ASP
2	B	102	TYR

5.3.2 Protein sidechains (i)

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	189/189 (100%)	178 (94%)	11 (6%)	20	40
1	L	189/189 (100%)	181 (96%)	8 (4%)	30	55
2	B	194/194 (100%)	181 (93%)	13 (7%)	16	33
2	H	194/194 (100%)	185 (95%)	9 (5%)	27	51
3	C	196/204 (96%)	187 (95%)	9 (5%)	27	51
3	E	196/204 (96%)	188 (96%)	8 (4%)	30	56
4	D	43/50 (86%)	40 (93%)	3 (7%)	15	30
4	F	42/50 (84%)	41 (98%)	1 (2%)	49	74
All	All	1243/1274 (98%)	1181 (95%)	62 (5%)	24	47

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14	SER
1	L	31	SER
1	L	68	SER
1	L	75	THR
1	L	95	SER
1	L	96	GLN
1	L	107	GLU
1	L	177	LEU

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Mol	Chain	Res	Type
2	H	100	HIS
2	H	101	TYR
2	H	104	SER
2	H	115	LEU
2	H	139	SER
2	H	141	SER
2	H	148	LEU
2	H	158	THR
2	H	186	SER
1	A	3	VAL
1	A	34	LEU
1	A	78	ARG
1	A	92	PHE
1	A	95	SER
1	A	97	LEU
1	A	107	GLU
1	A	111	THR
1	A	148	VAL
1	A	156	LEU
1	A	171	LYS
2	B	25	SER
2	B	35	VAL
2	B	74	LYS
2	B	104	SER
2	B	135	SER
2	B	148	LEU
2	B	166	LEU
2	B	194	SER
2	B	198	THR
2	B	200	THR
2	B	210	SER
2	B	216	LYS
2	B	221	LYS
3	C	60	TYR
3	C	65	PHE
3	C	97	LYS
3	C	106	VAL
3	C	111	THR
3	C	116	ARG
3	C	200	SER
3	C	210	ASP
3	C	248	LYS

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Mol	Chain	Res	Type
4	D	257	LEU
4	D	279	ARG
4	D	288	LYS
3	E	33	LEU
3	E	97	LYS
3	E	108	ARG
3	E	154	GLN
3	E	173	LEU
3	E	177	PHE
3	E	207	ARG
3	E	248	LYS
4	F	263	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
3	C	137	GLN
3	E	197	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	0GJ	C	301	-	20,24,25	3.22	6 (30%)	23,30,31	1.91	4 (17%)
5	0GJ	E	301	-	20,24,25	3.22	6 (30%)	23,30,31	1.50	4 (17%)

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
5	0GJ	C	301	-	-	10/27/29/31	-
5	0GJ	E	301	-	-	7/27/29/31	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	0GJ	C-N1	8.74	1.52	1.33
5	E	301	0GJ	C-N1	8.60	1.52	1.33
5	E	301	0GJ	C1-N2	7.38	1.49	1.34
5	C	301	0GJ	C1-N2	6.85	1.48	1.34
5	C	301	0GJ	CZ-NE	6.74	1.46	1.33
5	E	301	0GJ	CZ-NE	6.72	1.46	1.33
5	C	301	0GJ	CB1-CA2	2.67	1.58	1.52
5	E	301	0GJ	O1-C1	-2.49	1.18	1.23
5	C	301	0GJ	O1-C1	-2.41	1.18	1.23
5	E	301	0GJ	CZ-NH2	-2.18	1.23	1.32
5	C	301	0GJ	CZ-NH2	-2.11	1.23	1.32
5	E	301	0GJ	CD1-NE	2.03	1.50	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	301	0GJ	CB1-CA2-C2	5.71	122.44	112.51
5	C	301	0GJ	O2-C2-C3	-3.87	98.29	109.74
5	E	301	0GJ	CB1-CA2-C2	-3.33	106.72	112.51
5	C	301	0GJ	CG1-CB1-CA2	-3.11	107.57	113.93
5	E	301	0GJ	CA-C-N1	3.08	125.65	115.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	301	0GJ	CA1-C1-N2	2.78	122.74	116.10
5	C	301	0GJ	CA1-N1-C	2.73	128.13	121.37
5	E	301	0GJ	O-C-N1	-2.53	117.56	122.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	0GJ	O-C-CA-N
5	C	301	0GJ	N1-C-CA-N
5	C	301	0GJ	O-C-CA-CB
5	C	301	0GJ	N1-C-CA-CB
5	C	301	0GJ	C3-C2-CA2-N2
5	C	301	0GJ	O2-C2-CA2-CB1
5	C	301	0GJ	C3-C2-CA2-CB1
5	C	301	0GJ	N2-CA2-CB1-CG1
5	E	301	0GJ	N1-C-CA-N
5	E	301	0GJ	O-C-CA-CB
5	E	301	0GJ	N1-C-CA-CB
5	E	301	0GJ	N2-CA2-CB1-CG1
5	C	301	0GJ	NE-CD1-CG1-CB1
5	E	301	0GJ	NE-CD1-CG1-CB1
5	E	301	0GJ	C2-CA2-CB1-CG1
5	E	301	0GJ	O-C-CA-N
5	C	301	0GJ	O2-C2-CA2-N2

There are no ring outliers.

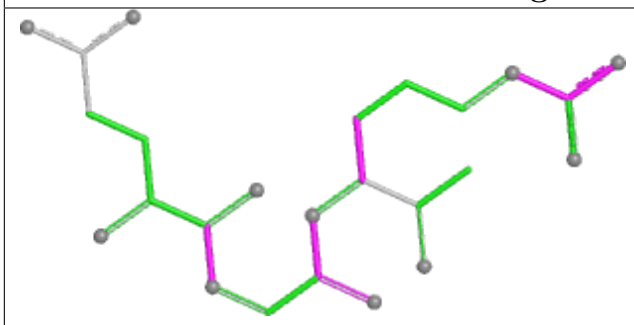
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	301	0GJ	4	0
5	E	301	0GJ	7	0

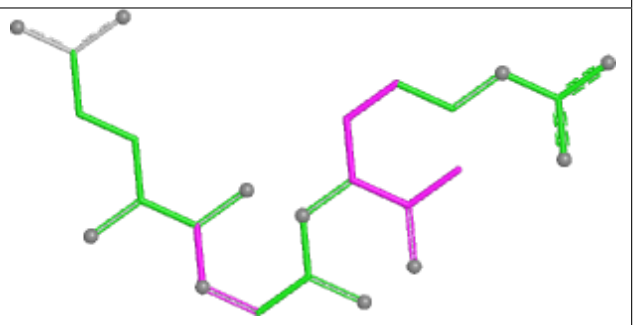
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

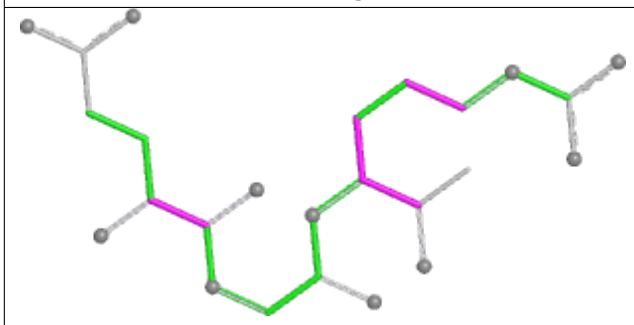
Ligand 0GJ C 301



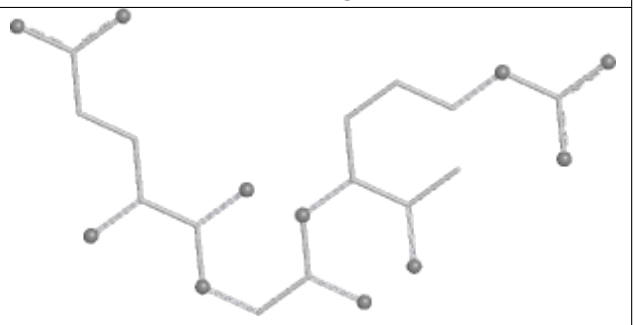
Bond lengths



Bond angles

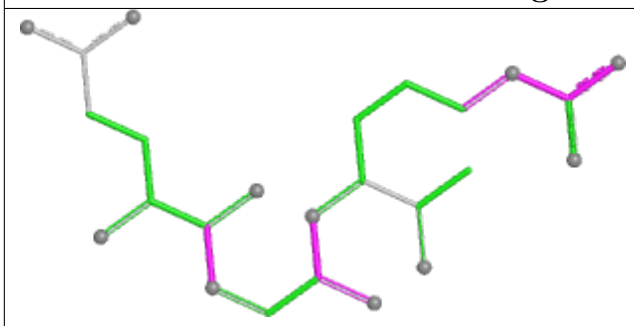


Torsions

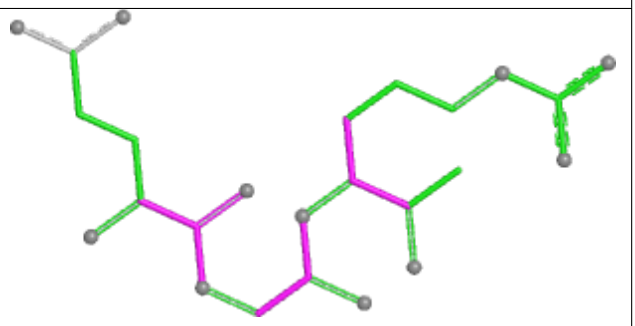


Rings

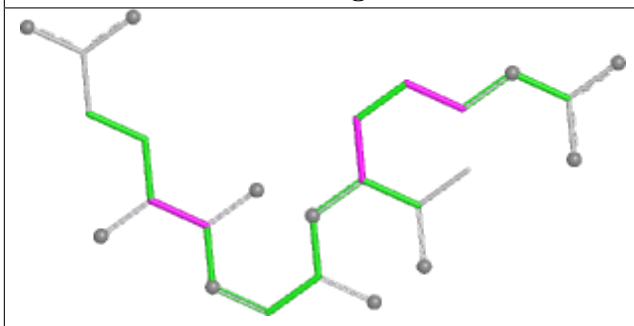
Ligand 0GJ E 301



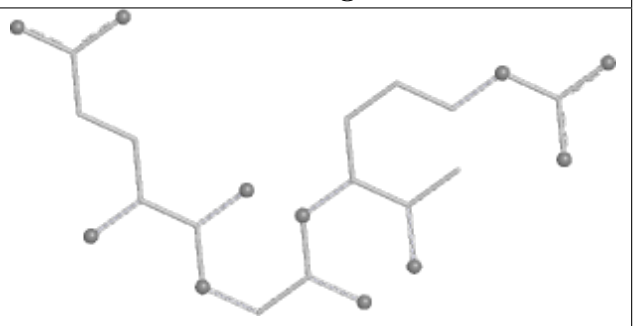
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	216/216 (100%)	-0.14	2 (0%) 84 82	36, 55, 70, 80	0
1	L	216/216 (100%)	-0.31	4 (1%) 66 62	27, 50, 66, 71	0
2	B	222/222 (100%)	-0.36	3 (1%) 75 71	24, 41, 69, 87	0
2	H	222/222 (100%)	-0.41	0 100 100	27, 39, 62, 75	0
3	C	234/241 (97%)	-0.40	0 100 100	26, 40, 57, 74	0
3	E	234/241 (97%)	-0.34	0 100 100	34, 47, 66, 85	0
4	D	52/58 (89%)	-0.15	0 100 100	36, 47, 63, 73	0
4	F	51/58 (87%)	-0.25	0 100 100	34, 44, 54, 63	0
All	All	1447/1474 (98%)	-0.32	9 (0%) 89 88	24, 45, 66, 87	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	PHE	3.2
2	B	138	THR	3.1
1	L	2	ILE	3.0
2	B	139	SER	2.9
1	L	94	ASP	2.7
1	A	42	GLY	2.7
1	L	93	GLY	2.6
2	B	222	TYR	2.3
1	L	8	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

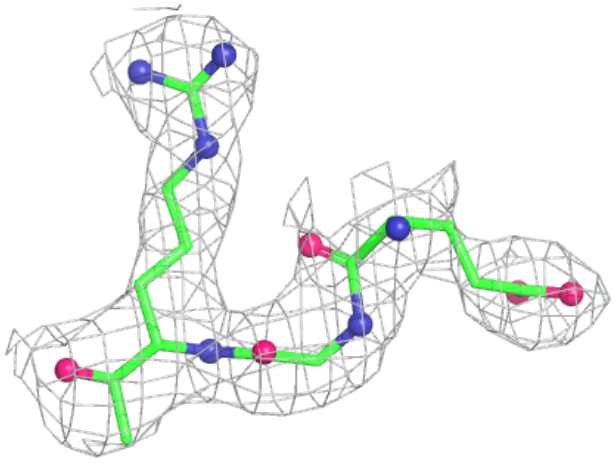
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

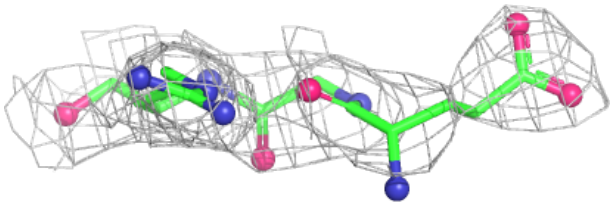
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	0GJ	E	301	25/26	0.94	0.21	45,51,60,60	0
5	0GJ	C	301	25/26	0.95	0.15	35,38,42,44	0
6	CA	E	302	1/1	0.95	0.06	53,53,53,53	0
6	CA	C	302	1/1	0.98	0.05	46,46,46,46	0

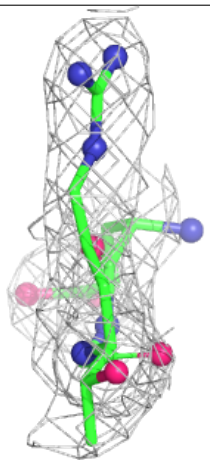
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0GJ E 301:

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

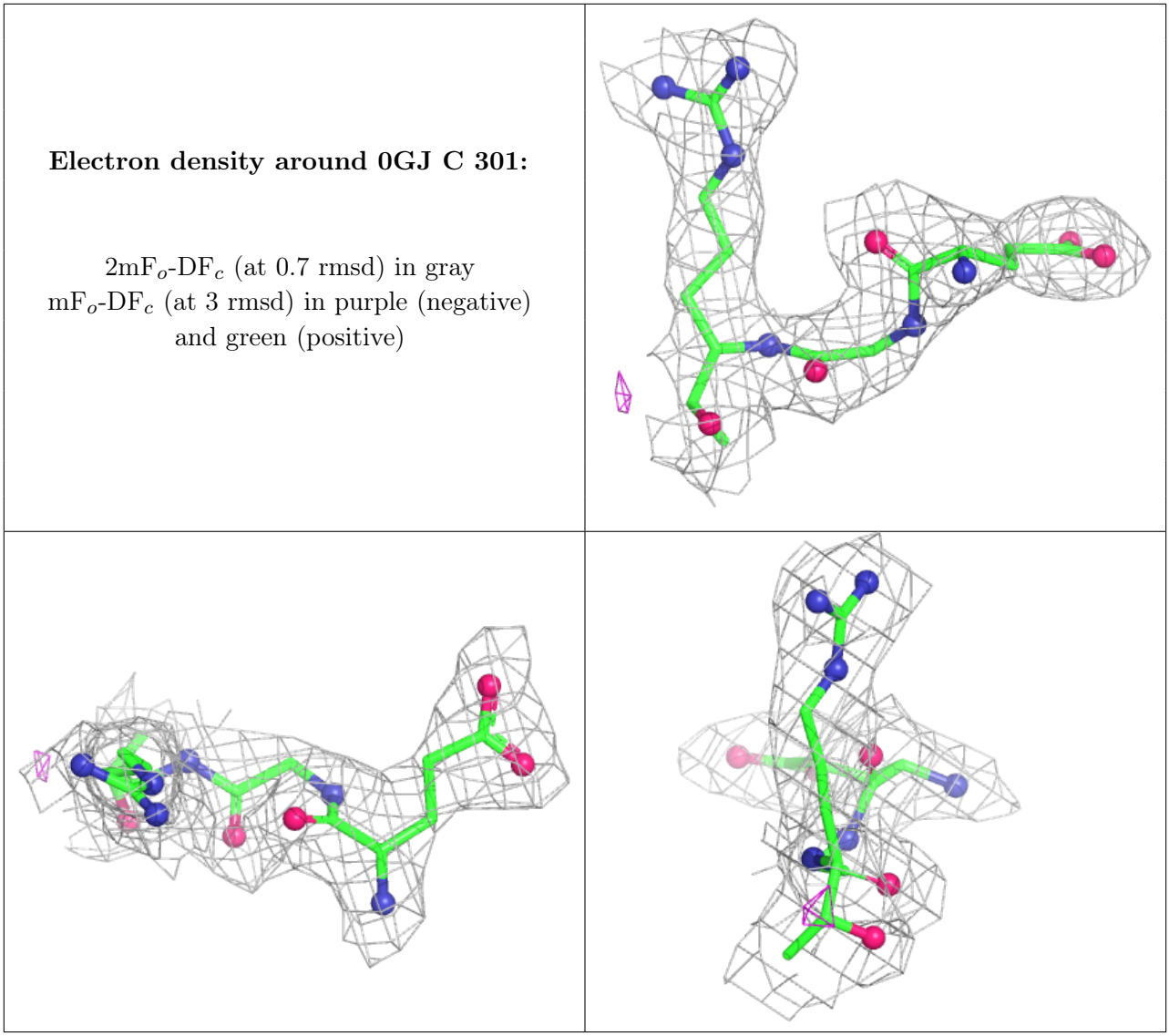






Electron density around 0GJ C 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.