Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 08:43 pm GMT

PDB ID	:	2YPU
Title	:	human insulin degrading enzyme E111Q in complex with inhibitor compound 41367
Authors	:	Guo, Q.; Deprez-Poulain, R.; Deprez, B.; Tang, W.-J.
Deposited on	:	2012-11-01
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

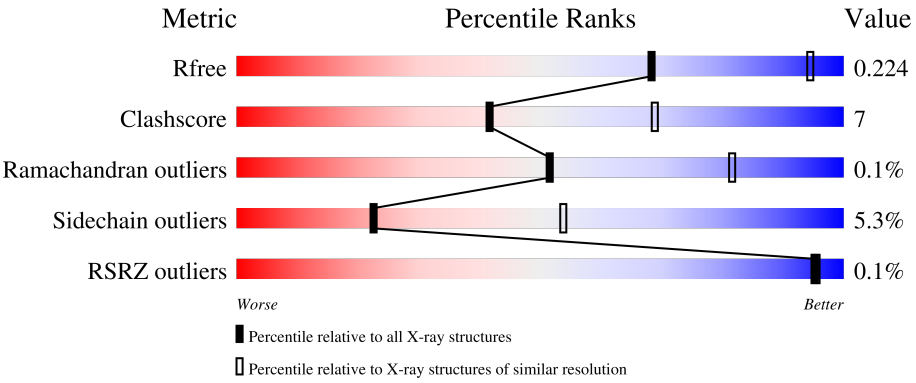
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	990	78% 16%
1	B	990	79% 17%

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	I41	A	1999	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15874 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 INSULIN-DEGRADING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	956	Total	C	N	O	S	0	0	0
			7768	5008	1307	1431	22			
1	B	954	Total	C	N	O	S	0	0	0
			7758	5002	1305	1429	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735

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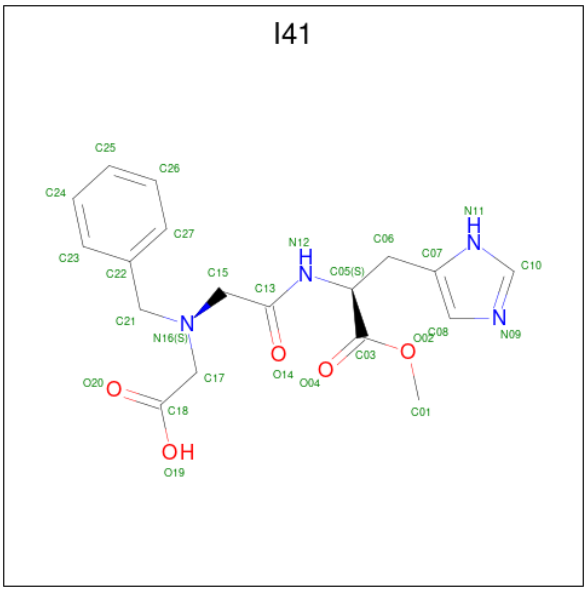
Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is 2-[[2-[[(2S)-3-(3H-IMIDAZOL-4-YL)-1-METHOXY-1-OXO-PROPAN-2-YL]AMINO]-2-OXO-ETHYL]-(PHENYLMETHYL)AMINO]ETHANOIC ACID (three-letter code: I41) (formula: $C_{18}H_{22}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 27 18 4 5	0	0
3	B	1	Total C N O 27 18 4 5	0	0

- Molecule 4 is water.

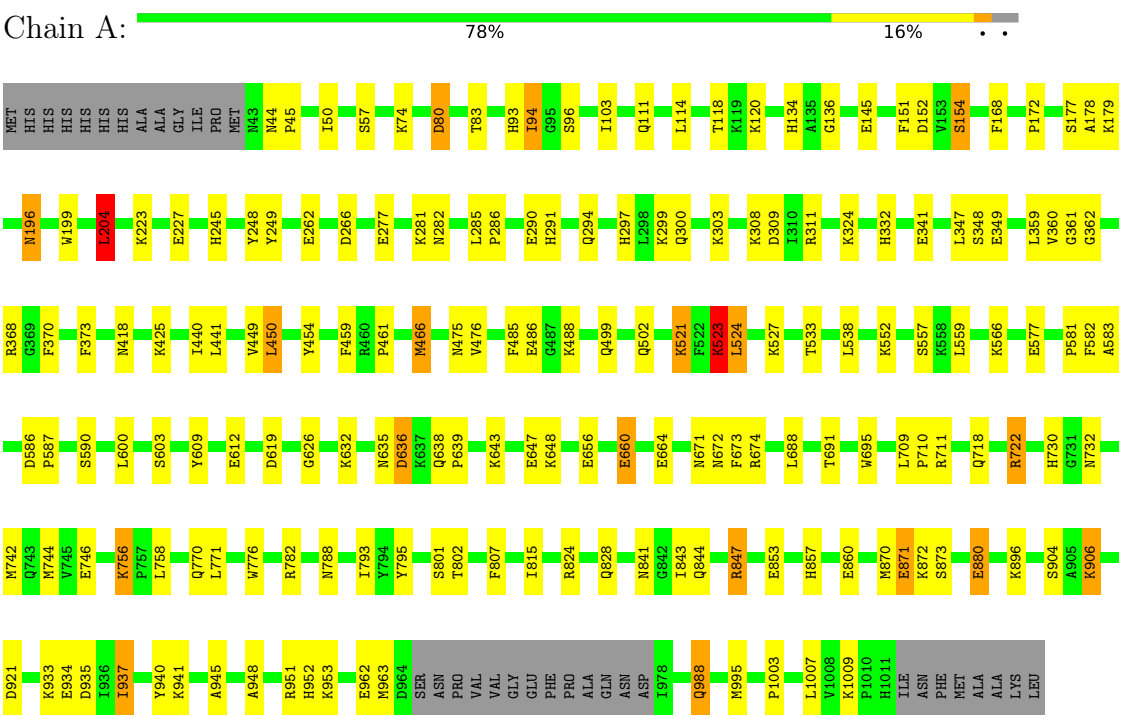
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	178	Total O 178 178	0	0
4	B	114	Total O 114 114	0	0

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.

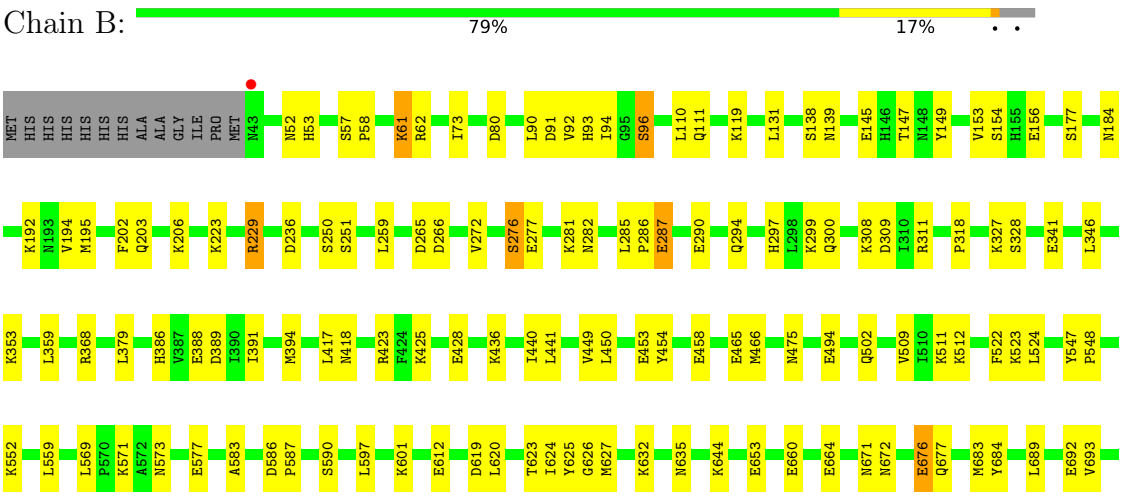
• Molecule 1: INSULIN-DEGRADING ENZYME

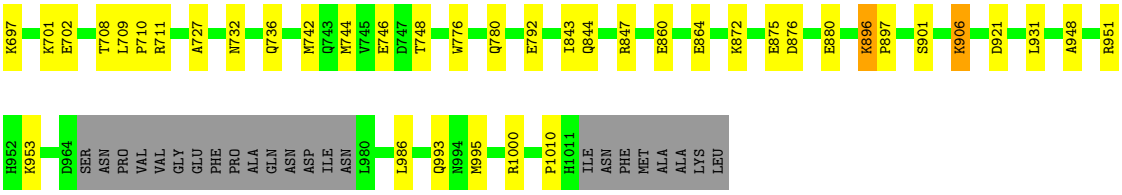
Chain A:



• Molecule 1: INSULIN-DEGRADING ENZYME

Chain B:




K697
K701
E702
T708
L709
P710
R711
A727
N732
Q736
M742
Q743
M744
V745
E746
D747
T748
W776
Q780
E792
I843
Q844
R847
E860
E864
K872
E875
D876
E880
K896
P897
S901
K906
D921
L931
A948
R951
H952
K953
D964
SER
ASN
PRO
VAL
VAL
GLY
GLU
PHE
PRO
ALA
GLN
ASN
ASP
ILE
ASN
L980
L986
Q993
N994
M995
R1000
P1010
H1011
ILE
ASN
PHE
MET
ALA
ALA
LYS
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	262.29Å 262.29Å 90.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.80) 99.9 (49.57-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.22 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.173 , 0.225 0.172 , 0.224	Depositor DCC
R_{free} test set	4383 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15874	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, I41

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	1.05	10/7963 (0.1%)	0.97	9/10779 (0.1%)
1	B	1.03	10/7953 (0.1%)	0.92	5/10765 (0.0%)
All	All	1.04	20/15916 (0.1%)	0.95	14/21544 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	465	GLU	CG-CD	9.96	1.66	1.51
1	B	494	GLU	CG-CD	9.22	1.65	1.51
1	B	577	GLU	CG-CD	7.22	1.62	1.51
1	B	494	GLU	CB-CG	7.12	1.65	1.52
1	A	871	GLU	CG-CD	7.12	1.62	1.51
1	A	880	GLU	CG-CD	7.01	1.62	1.51
1	A	204	LEU	CG-CD2	6.89	1.77	1.51
1	B	465	GLU	CB-CG	6.60	1.64	1.52
1	A	577	GLU	CG-CD	6.51	1.61	1.51
1	B	453	GLU	CB-CG	6.09	1.63	1.52
1	A	178	ALA	CA-CB	-5.97	1.40	1.52
1	B	436	LYS	CD-CE	5.80	1.65	1.51
1	A	523	LYS	CG-CD	5.67	1.71	1.52
1	B	511	LYS	CA-CB	5.58	1.66	1.53
1	B	287	GLU	CG-CD	5.46	1.60	1.51
1	A	673	PHE	CE2-CZ	5.31	1.47	1.37
1	B	660	GLU	CG-CD	5.22	1.59	1.51
1	A	660	GLU	CG-CD	5.13	1.59	1.51
1	A	871	GLU	CB-CG	5.03	1.61	1.52
1	A	523	LYS	CD-CE	5.01	1.63	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	636	ASP	CB-CA-C	-7.28	95.84	110.40
1	A	80	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	466	MET	CG-SD-CE	-6.59	89.66	100.20
1	B	229	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	436	LYS	CD-CE-NZ	5.63	124.66	111.70
1	B	619	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	475	ASN	CB-CA-C	-5.37	99.66	110.40
1	A	847	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	265	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	619	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	94	ILE	CG1-CB-CG2	-5.18	100.01	111.40
1	A	538	LEU	CB-CG-CD1	5.13	119.72	111.00
1	B	92	VAL	CB-CA-C	-5.11	101.70	111.40
1	A	120	LYS	CD-CE-NZ	5.05	123.31	111.70

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	7768	0	7676	117	1
1	B	7758	0	7672	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	21	9	0
3	B	27	0	21	3	0
4	A	178	0	0	12	0
4	B	114	0	0	4	1
All	All	15874	0	15390	216	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 7.

All (216) 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:204:LEU:CD2	1:A:204:LEU:CG	1.77	1.60
1:B:309:ASP:H	1:B:672:ASN:HD21	1.12	0.95
1:A:332:HIS:HD2	3:A:1999:I41:C01	1.80	0.94
1:B:184:ASN:HD21	1:B:223:LYS:NZ	1.67	0.93
1:A:74:LYS:NZ	4:A:2009:HOH:O	2.01	0.92
1:A:309:ASP:H	1:A:672:ASN:HD21	1.19	0.90
1:B:597:LEU:HD11	1:B:627:MET:HG2	1.53	0.90
1:B:96:SER:HB3	4:B:2008:HOH:O	1.71	0.89
1:B:847:ARG:NH1	4:B:2103:HOH:O	1.83	0.84
1:A:776:TRP:CD1	1:A:953:LYS:HG2	2.15	0.82
1:A:332:HIS:CD2	3:A:1999:I41:C01	2.63	0.81
1:A:635:ASN:ND2	1:A:732:ASN:HD22	1.79	0.81
1:B:93:HIS:HE1	1:B:368:ARG:HH21	1.29	0.80
1:A:988:GLN:HB2	4:A:2174:HOH:O	1.82	0.80
1:B:184:ASN:HD21	1:B:223:LYS:HZ2	1.27	0.79
1:B:309:ASP:H	1:B:672:ASN:ND2	1.82	0.77
1:A:332:HIS:CD2	3:A:1999:I41:H011	2.21	0.76
1:A:857:HIS:HD2	4:A:2159:HOH:O	1.69	0.76
1:A:988:GLN:CB	4:A:2174:HOH:O	2.33	0.76
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.69	0.75
1:A:635:ASN:HD21	1:A:732:ASN:HD22	1.35	0.74
3:B:1999:I41:O14	3:B:1999:I41:C18	2.37	0.73
1:B:671:ASN:OD1	1:B:701:LYS:HD3	1.87	0.73
1:B:93:HIS:CE1	1:B:368:ARG:HH21	2.07	0.72
1:B:635:ASN:ND2	1:B:732:ASN:HD22	1.88	0.72
1:A:300:GLN:HE21	1:A:502:GLN:HE21	1.40	0.69
1:B:711:ARG:HG3	4:B:2098:HOH:O	1.92	0.68
1:A:204:LEU:CD2	1:A:204:LEU:HG	2.12	0.68
1:B:184:ASN:ND2	1:B:223:LYS:NZ	2.39	0.68
1:A:196:ASN:HD21	1:A:199:TRP:HD1	1.42	0.68
1:A:196:ASN:ND2	1:A:199:TRP:HD1	1.91	0.67
1:B:635:ASN:HD21	1:B:732:ASN:HD22	1.42	0.66
3:A:1999:I41:C08	4:A:2177:HOH:O	2.43	0.65
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.32	0.65
1:A:309:ASP:H	1:A:672:ASN:ND2	1.91	0.65
1:B:776:TRP:CD1	1:B:953:LYS:HD3	2.33	0.64
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.81	0.63
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.81	0.62
1:A:204:LEU:CD2	1:A:204:LEU:CD1	2.75	0.61
1:A:93:HIS:HE1	1:A:368:ARG:HH21	1.49	0.61
1:A:583:ALA:CB	1:A:626:GLY:HA2	2.31	0.60
1:A:308:LYS:HE3	1:A:672:ASN:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLN:NE2	1:A:502:GLN:HE21	1.99	0.60
1:A:557:SER:HB2	1:A:742:MET:CE	2.32	0.60
3:B:1999:I41:O14	3:B:1999:I41:O20	2.20	0.59
1:B:623:THR:HG22	1:B:624:ILE:N	2.18	0.59
1:A:776:TRP:NE1	1:A:953:LYS:HE2	2.18	0.58
1:B:689:LEU:CD2	1:B:995:MET:HG2	2.34	0.58
1:A:1007:LEU:HD12	1:B:1000:ARG:HG2	1.86	0.58
1:B:266:ASP:HB2	4:B:2040:HOH:O	2.02	0.58
1:A:359:LEU:O	3:A:1999:I41:H10	2.04	0.58
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.86	0.57
1:B:341:GLU:OE2	3:B:1999:I41:H10	2.04	0.57
1:A:843:ILE:HG22	1:A:844:GLN:H	1.70	0.57
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.87	0.56
1:A:795:TYR:CE1	1:A:953:LYS:HD2	2.40	0.56
1:B:689:LEU:HD23	1:B:995:MET:HG2	1.86	0.56
1:A:782:ARG:HH12	1:A:963:MET:H	1.54	0.56
1:A:223:LYS:HE2	1:A:227:GLU:OE2	2.06	0.55
1:B:300:GLN:HE21	1:B:502:GLN:HE21	1.55	0.55
1:B:184:ASN:ND2	1:B:223:LYS:HZ3	2.02	0.55
1:A:660:GLU:HG3	4:A:2126:HOH:O	2.06	0.55
1:A:671:ASN:O	1:A:674:ARG:HG2	2.07	0.55
1:B:559:LEU:HD22	1:B:742:MET:HB2	1.88	0.54
1:A:933:LYS:O	1:A:937:ILE:HG12	2.07	0.54
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.89	0.54
1:B:294:GLN:H	1:B:297:HIS:HD2	1.55	0.54
1:A:632:LYS:HD2	4:A:2118:HOH:O	2.07	0.54
1:A:636:ASP:O	1:A:636:ASP:OD1	2.27	0.53
1:A:691:THR:HG23	1:A:841:ASN:HD21	1.73	0.53
1:A:557:SER:HB2	1:A:742:MET:HE3	1.89	0.53
1:A:940:TYR:CE2	1:A:945:ALA:HB2	2.43	0.53
1:B:52:ASN:O	1:B:53:HIS:C	2.46	0.53
1:A:523:LYS:HD3	1:A:524:LEU:N	2.24	0.53
1:B:727:ALA:HB3	1:B:742:MET:CE	2.39	0.52
1:A:94:ILE:HG13	1:A:248:TYR:HB3	1.92	0.52
1:A:988:GLN:HB3	4:A:2174:HOH:O	2.06	0.52
1:A:303:LYS:HD3	1:A:485:PHE:CE1	2.44	0.52
1:B:285:LEU:HD12	1:B:286:PRO:CD	2.39	0.52
1:A:937:ILE:HG22	1:A:941:LYS:HD2	1.93	0.51
1:A:294:GLN:H	1:A:297:HIS:HD2	1.57	0.51
1:B:388:GLU:OE2	1:B:509:VAL:HG22	2.11	0.51
1:B:308:LYS:HD3	1:B:672:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASP:HB2	1:A:587:PRO:HD2	1.92	0.50
1:A:722:ARG:HB2	1:A:758:LEU:HD23	1.91	0.50
1:A:722:ARG:HB2	1:A:758:LEU:CD2	2.41	0.50
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.92	0.50
1:B:93:HIS:HE1	1:B:368:ARG:NH2	2.05	0.50
1:B:93:HIS:HD2	1:B:145:GLU:O	1.93	0.50
1:B:184:ASN:ND2	1:B:223:LYS:HZ2	2.02	0.50
1:A:332:HIS:HD2	3:A:1999:I41:H012	1.73	0.50
1:A:801:SER:O	1:A:802:THR:C	2.50	0.50
1:B:583:ALA:CB	1:B:626:GLY:HA2	2.42	0.49
1:A:533:THR:N	1:A:636:ASP:OD2	2.39	0.49
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.94	0.49
1:A:285:LEU:HD12	1:A:286:PRO:HD2	1.93	0.49
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.45	0.49
1:B:864:GLU:OE2	1:B:953:LYS:HE3	2.12	0.49
1:B:906:LYS:HE3	1:B:921:ASP:OD2	2.13	0.49
1:B:147:THR:HG22	1:B:149:TYR:CE1	2.47	0.49
1:B:272:VAL:O	1:B:276:SER:OG	2.30	0.49
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.94	0.49
1:B:623:THR:HG22	1:B:625:TYR:H	1.78	0.49
1:A:290:GLU:HB3	4:A:2049:HOH:O	2.12	0.49
1:A:843:ILE:HG22	1:A:844:GLN:N	2.27	0.49
1:B:328:SER:HB2	1:B:458:GLU:O	2.12	0.49
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.94	0.49
1:B:776:TRP:NE1	1:B:953:LYS:HD3	2.28	0.48
1:A:136:GLY:HA3	1:A:152:ASP:O	2.14	0.48
1:A:418:ASN:HB3	1:A:454:TYR:O	2.13	0.48
1:A:857:HIS:CD2	4:A:2159:HOH:O	2.54	0.48
1:B:601:LYS:NZ	1:B:620:LEU:O	2.36	0.48
1:A:196:ASN:ND2	1:A:199:TRP:CD1	2.79	0.48
1:B:547:TYR:HB3	1:B:548:PRO:CD	2.43	0.48
1:A:880:GLU:HB2	4:A:2163:HOH:O	2.13	0.48
1:A:245:HIS:O	1:A:249:TYR:HB2	2.14	0.48
1:A:586:ASP:HA	1:A:695:TRP:CZ2	2.48	0.48
1:A:793:ILE:O	1:A:847:ARG:HA	2.14	0.47
1:B:727:ALA:HB3	1:B:742:MET:HE1	1.95	0.47
1:B:559:LEU:HD13	1:B:742:MET:CE	2.44	0.47
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.14	0.47
1:B:236:ASP:OD1	1:B:236:ASP:C	2.53	0.47
1:A:93:HIS:HD2	1:A:145:GLU:O	1.97	0.47
1:A:583:ALA:HB2	1:A:626:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:GLU:OE1	1:B:676:GLU:HA	2.14	0.47
1:B:418:ASN:HB3	1:B:454:TYR:O	2.15	0.46
1:A:93:HIS:CE1	1:A:368:ARG:HH21	2.31	0.46
1:A:262:GLU:HB3	1:A:266:ASP:HB2	1.98	0.46
1:A:718:GLN:HE22	1:B:711:ARG:HH12	1.62	0.46
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.98	0.46
1:B:346:LEU:HA	1:B:522:PHE:CE1	2.50	0.46
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.41	0.46
1:B:860:GLU:OE1	1:B:953:LYS:NZ	2.49	0.46
1:A:134:HIS:O	1:A:154:SER:HB3	2.15	0.46
1:A:643:LYS:HE2	1:A:647:GLU:OE1	2.16	0.46
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.39	0.46
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.46	0.46
1:B:202:PHE:CZ	1:B:206:LYS:HE3	2.51	0.45
1:B:843:ILE:HG22	1:B:844:GLN:H	1.80	0.45
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.73	0.45
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.98	0.45
1:A:756:LYS:HB2	1:A:756:LYS:HE2	1.41	0.45
1:B:61:LYS:HD3	1:B:61:LYS:HA	1.76	0.45
1:B:559:LEU:HD13	1:B:742:MET:HE2	1.97	0.45
1:B:194:VAL:HG12	1:B:195:MET:HG2	1.99	0.45
1:A:151:PHE:CD1	1:A:151:PHE:C	2.89	0.45
1:A:581:PRO:HG2	1:A:582:PHE:CD2	2.52	0.45
1:B:684:TYR:OH	1:B:697:LYS:HG2	2.17	0.45
1:B:300:GLN:NE2	1:B:502:GLN:HE21	2.15	0.45
1:A:360:VAL:HA	3:A:1999:I41:H10	1.99	0.45
1:B:552:LYS:HB3	1:B:559:LEU:HB3	1.99	0.45
1:A:857:HIS:O	1:A:860:GLU:HB2	2.17	0.45
1:A:94:ILE:HD12	1:A:94:ILE:HG23	1.53	0.44
1:B:573:ASN:OD1	1:B:632:LYS:HG2	2.17	0.44
1:A:559:LEU:HD22	1:A:742:MET:HB2	1.99	0.44
1:B:110:LEU:C	1:B:110:LEU:HD23	2.38	0.44
1:A:359:LEU:C	1:A:359:LEU:HD23	2.38	0.44
1:B:843:ILE:HG22	1:B:844:GLN:N	2.31	0.44
1:A:80:ASP:O	1:A:83:THR:HG22	2.18	0.44
1:A:341:GLU:HG2	1:A:347:LEU:HD23	2.00	0.44
1:A:688:LEU:HD13	1:A:995:MET:HE1	1.99	0.44
1:A:449:VAL:HG23	1:A:450:LEU:HD13	2.00	0.44
1:A:730:HIS:HD2	1:A:904:SER:OG	2.01	0.44
1:B:864:GLU:HG3	1:B:986:LEU:HD21	1.99	0.43
1:A:782:ARG:NH1	1:A:963:MET:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:PHE:HE1	1:A:935:ASP:HB3	1.83	0.43
1:B:683:MET:HA	1:B:792:GLU:OE1	2.19	0.43
1:A:552:LYS:NZ	1:A:746:GLU:OE2	2.50	0.43
1:B:391:ILE:O	1:B:394:MET:HB2	2.19	0.43
1:A:362:GLY:HA2	1:A:373:PHE:CZ	2.54	0.43
1:A:557:SER:HB2	1:A:742:MET:HE2	2.01	0.43
1:A:948:ALA:HB3	1:A:951:ARG:HB2	2.00	0.43
1:B:583:ALA:HB2	1:B:626:GLY:HA2	2.01	0.43
1:B:623:THR:N	1:B:626:GLY:O	2.44	0.43
1:A:824:ARG:O	1:A:828:GLN:HA	2.19	0.43
1:B:692:GLU:HG2	1:B:693:VAL:HG23	2.01	0.43
1:B:708:THR:HB	1:B:710:PRO:HD2	2.01	0.42
1:A:299:LYS:HE3	1:A:299:LYS:HB2	1.89	0.42
1:A:638:GLN:N	1:A:639:PRO:CD	2.82	0.42
1:A:776:TRP:HA	1:A:953:LYS:O	2.18	0.42
1:B:931:LEU:HD23	1:B:931:LEU:HA	1.81	0.42
1:A:349:GLU:OE1	1:A:521:LYS:HG2	2.19	0.42
1:A:459:PHE:CE2	1:A:461:PRO:HG3	2.55	0.42
1:B:62:ARG:HG2	1:B:80:ASP:HB2	2.00	0.42
1:B:294:GLN:H	1:B:297:HIS:CD2	2.35	0.42
1:A:118:THR:HG22	1:A:172:PRO:HA	2.01	0.42
1:B:58:PRO:HG2	1:B:423:ARG:HG3	2.00	0.42
1:B:672:ASN:HD22	1:B:672:ASN:HA	1.60	0.42
1:A:360:VAL:HA	3:A:1999:I41:C10	2.50	0.42
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.23	0.42
1:B:153:VAL:HG22	1:B:154:SER:N	2.35	0.41
1:A:361:GLY:H	3:A:1999:I41:H11	1.68	0.41
1:A:744:MET:O	1:A:744:MET:HG2	2.20	0.41
1:B:90:LEU:HD23	1:B:91:ASP:N	2.35	0.41
1:A:179:LYS:HE3	1:A:179:LYS:HB3	1.91	0.41
1:A:600:LEU:CD1	1:A:648:LYS:HB3	2.49	0.41
1:A:586:ASP:HB2	1:A:587:PRO:CD	2.50	0.41
1:A:788:ASN:ND2	4:A:2027:HOH:O	2.53	0.41
1:A:44:ASN:HA	1:A:45:PRO:HD2	1.82	0.41
1:B:359:LEU:C	1:B:359:LEU:HD23	2.42	0.41
1:B:586:ASP:HB2	1:B:587:PRO:HD2	2.03	0.41
1:B:623:THR:CG2	1:B:624:ILE:N	2.82	0.41
1:B:386:HIS:HD2	1:B:389:ASP:OD2	2.03	0.41
1:B:896:LYS:HA	1:B:897:PRO:HD2	1.90	0.41
1:B:259:LEU:C	1:B:259:LEU:HD23	2.42	0.40
1:A:281:LYS:HZ3	1:A:281:LYS:HG3	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:HA	1:A:756:LYS:O	2.21	0.40
1:B:559:LEU:HD22	1:B:742:MET:CB	2.50	0.40
1:B:569:LEU:O	1:B:571:LYS:N	2.54	0.40
1:A:770:GLN:HB3	1:A:1003:PRO:HB2	2.03	0.40
1:B:203:GLN:O	1:B:203:GLN:HG3	2.21	0.40
1:B:318:PRO:HD2	1:B:475:ASN:O	2.22	0.40
1:B:948:ALA:HB3	1:B:951:ARG:HB2	2.02	0.40
1:A:341:GLU:HB2	1:A:609:TYR:CD1	2.57	0.40
1:A:425:LYS:HB3	1:A:425:LYS:NZ	2.37	0.40
1:B:309:ASP:N	1:B:672:ASN:HD21	1.95	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:A:934:GLU:CB	4:B:2001:HOH:O[5_555]	1.50	0.70

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	952/990 (96%)	912 (96%)	39 (4%)	1 (0%)	51	81
1	B	950/990 (96%)	910 (96%)	39 (4%)	1 (0%)	51	81
All	All	1902/1980 (96%)	1822 (96%)	78 (4%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1010	PRO
1	A	103	ILE

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	837/879 (95%)	796 (95%)	41 (5%)	25 57
1	B	837/879 (95%)	790 (94%)	47 (6%)	21 51
All	All	1674/1758 (95%)	1586 (95%)	88 (5%)	22 54

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	57	SER
1	A	96	SER
1	A	111	GLN
1	A	154	SER
1	A	177	SER
1	A	196	ASN
1	A	204	LEU
1	A	277	GLU
1	A	282	ASN
1	A	324	LYS
1	A	348	SER
1	A	440	ILE
1	A	450	LEU
1	A	466	MET
1	A	476	VAL
1	A	486	GLU
1	A	488	LYS
1	A	499	GLN
1	A	521	LYS
1	A	523	LYS
1	A	524	LEU
1	A	527	LYS
1	A	566	LYS
1	A	590	SER
1	A	603	SER
1	A	612	GLU

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Mol	Chain	Res	Type
1	A	656	GLU
1	A	711	ARG
1	A	722	ARG
1	A	756	LYS
1	A	853	GLU
1	A	871	GLU
1	A	872	LYS
1	A	873	SER
1	A	896	LYS
1	A	906	LYS
1	A	937	ILE
1	A	962	GLU
1	A	988	GLN
1	A	1009	LYS
1	B	57	SER
1	B	61	LYS
1	B	94	ILE
1	B	96	SER
1	B	111	GLN
1	B	119	LYS
1	B	139	ASN
1	B	156	GLU
1	B	177	SER
1	B	192	LYS
1	B	229	ARG
1	B	250	SER
1	B	276	SER
1	B	277	GLU
1	B	281	LYS
1	B	282	ASN
1	B	287	GLU
1	B	290	GLU
1	B	299	LYS
1	B	327	LYS
1	B	353	LYS
1	B	440	ILE
1	B	450	LEU
1	B	466	MET
1	B	512	LYS
1	B	523	LYS
1	B	524	LEU
1	B	590	SER

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Mol	Chain	Res	Type
1	B	612	GLU
1	B	644	LYS
1	B	653	GLU
1	B	676	GLU
1	B	677	GLN
1	B	702	GLU
1	B	736	GLN
1	B	744	MET
1	B	746	GLU
1	B	748	THR
1	B	780	GLN
1	B	872	LYS
1	B	875	GLU
1	B	876	ASP
1	B	880	GLU
1	B	896	LYS
1	B	901	SER
1	B	906	LYS
1	B	993	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	111	GLN
1	A	231	ASN
1	A	239	GLN
1	A	297	HIS
1	A	300	GLN
1	A	332	HIS
1	A	407	GLN
1	A	635	ASN
1	A	672	ASN
1	A	677	GLN
1	A	730	HIS
1	A	788	ASN
1	A	841	ASN
1	A	857	HIS
1	B	52	ASN
1	B	93	HIS
1	B	129	GLN
1	B	139	ASN

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Mol	Chain	Res	Type
1	B	184	ASN
1	B	232	GLN
1	B	282	ASN
1	B	297	HIS
1	B	300	GLN
1	B	386	HIS
1	B	407	GLN
1	B	635	ASN
1	B	672	ASN
1	B	677	GLN
1	B	730	HIS
1	B	781	GLN
1	B	841	ASN
1	B	914	GLN
1	B	922	ASN
1	B	993	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
3	I41	B	1999	-	24,28,28	1.80	5 (20%)	30,36,36	1.95	9 (30%)
3	I41	A	1999	-	24,28,28	1.74	3 (12%)	30,36,36	1.82	4 (13%)

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	I41	B	1999	-	-	10/26/26/26	0/2/2/2
3	I41	A	1999	-	-	15/26/26/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1999	I41	O02-C03	6.00	1.47	1.33
3	B	1999	I41	O02-C03	5.81	1.47	1.33
3	B	1999	I41	C15-N16	2.53	1.52	1.47
3	B	1999	I41	C17-C18	2.47	1.56	1.51
3	B	1999	I41	C15-C13	2.37	1.56	1.52
3	B	1999	I41	C21-C22	2.29	1.55	1.51
3	A	1999	I41	C23-C22	2.21	1.43	1.38
3	A	1999	I41	C27-C22	2.03	1.43	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1999	I41	O02-C03-C05	5.96	126.78	111.52
3	A	1999	I41	O02-C03-O04	-4.97	114.12	123.84
3	B	1999	I41	O02-C03-C05	4.11	122.04	111.52
3	B	1999	I41	O14-C13-N12	-3.98	116.24	122.95
3	B	1999	I41	C06-C05-N12	3.93	119.08	110.79
3	B	1999	I41	O02-C03-O04	-3.83	116.35	123.84
3	B	1999	I41	C01-O02-C03	3.53	123.92	115.94
3	B	1999	I41	C15-C13-N12	3.03	122.14	115.31
3	B	1999	I41	O19-C18-C17	2.91	124.92	113.45
3	A	1999	I41	C06-C05-N12	-2.79	104.90	110.79
3	B	1999	I41	O19-C18-O20	-2.73	116.50	123.30
3	A	1999	I41	C21-N16-C17	-2.52	106.64	112.02
3	B	1999	I41	C22-C21-N16	2.20	117.39	113.12

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1999	I41	C05-C06-C07-C08
3	A	1999	I41	C05-C06-C07-N11
3	A	1999	I41	N16-C17-C18-O19
3	A	1999	I41	N16-C17-C18-O20
3	B	1999	I41	N12-C05-C06-C07
3	B	1999	I41	C05-C06-C07-N11
3	B	1999	I41	C13-C15-N16-C17
3	A	1999	I41	C03-C05-C06-C07
3	B	1999	I41	C03-C05-C06-C07
3	A	1999	I41	C18-C17-N16-C15
3	A	1999	I41	C05-C03-O02-C01
3	B	1999	I41	N16-C17-C18-O20
3	A	1999	I41	O02-C03-C05-N12
3	A	1999	I41	N12-C13-C15-N16
3	A	1999	I41	O02-C03-C05-C06
3	A	1999	I41	O04-C03-C05-N12
3	B	1999	I41	N16-C17-C18-O19
3	A	1999	I41	O04-C03-O02-C01
3	A	1999	I41	O14-C13-C15-N16
3	B	1999	I41	O02-C03-C05-N12
3	B	1999	I41	O04-C03-C05-N12
3	A	1999	I41	O04-C03-C05-C06
3	A	1999	I41	N12-C05-C06-C07
3	B	1999	I41	N12-C13-C15-N16
3	B	1999	I41	O14-C13-C15-N16

There are no ring outliers.

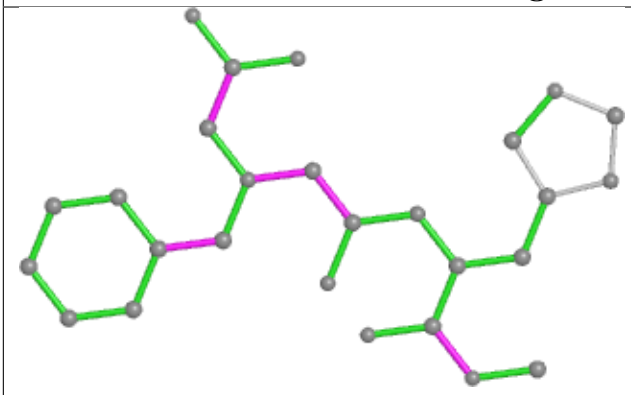
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1999	I41	3	0
3	A	1999	I41	9	0

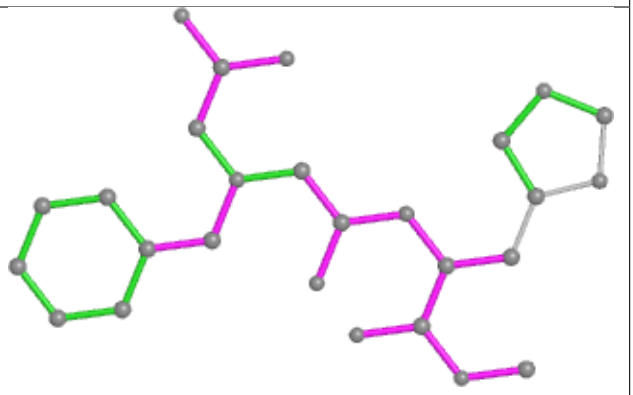
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

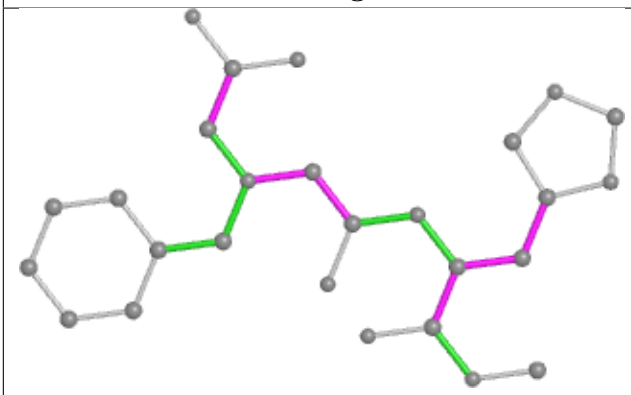
Ligand I41 B 1999



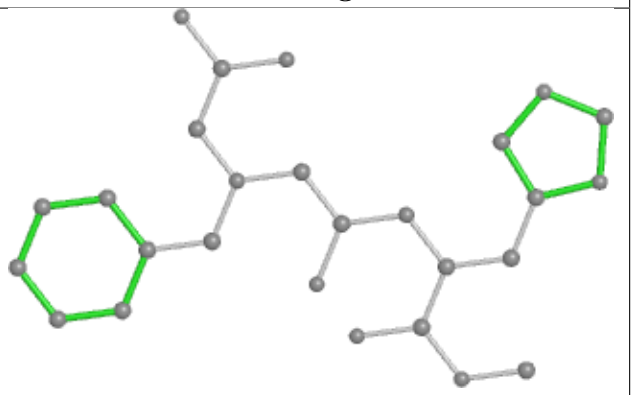
Bond lengths



Bond angles

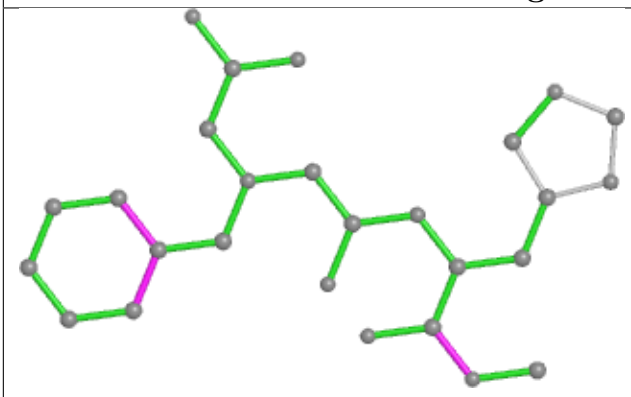


Torsions

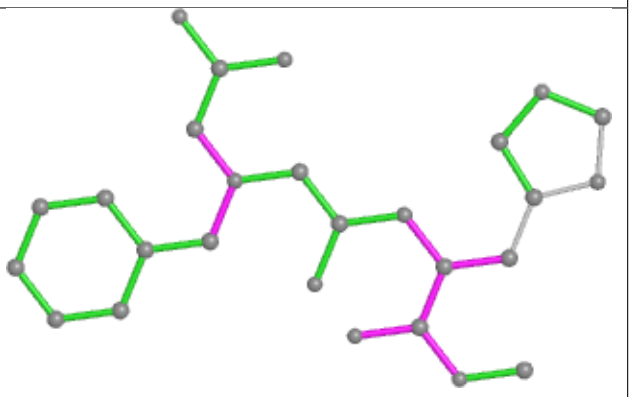


Rings

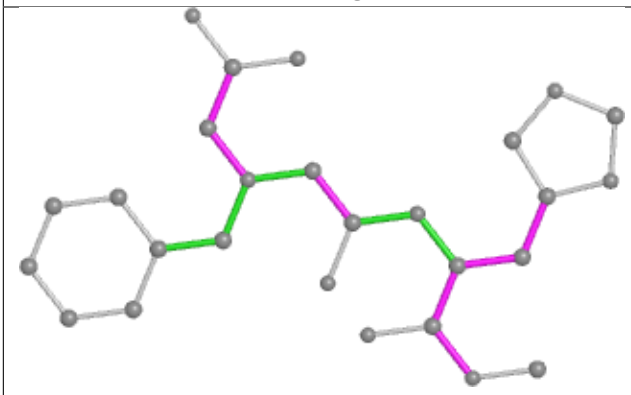
Ligand I41 A 1999



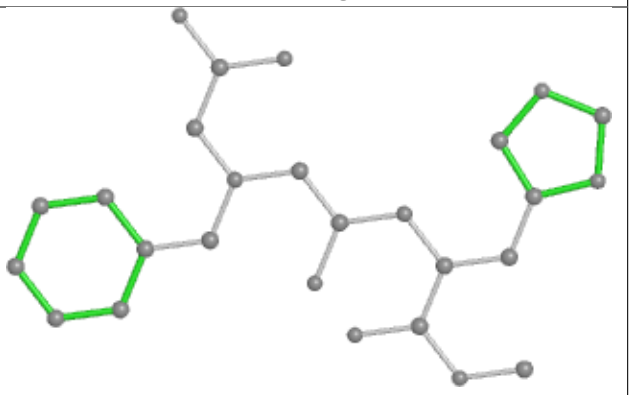
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	956/990 (96%)	-0.51	0 100 100	14, 27, 43, 64	0
1	B	954/990 (96%)	-0.44	1 (0%) 95 95	17, 32, 47, 68	0
All	All	1910/1980 (96%)	-0.47	1 (0%) 95 95	14, 30, 45, 68	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	43	ASN	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

There are no monosaccharides in this entry.

6.4 Ligands

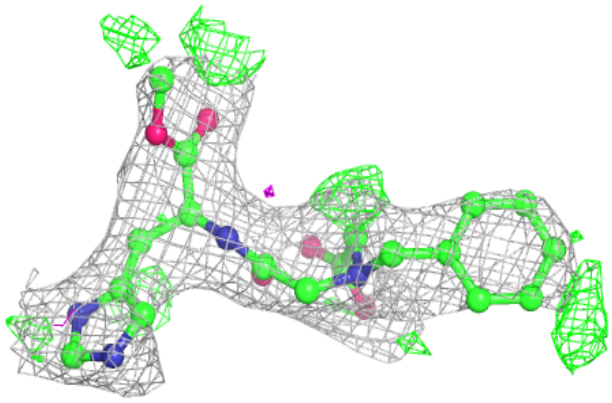
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

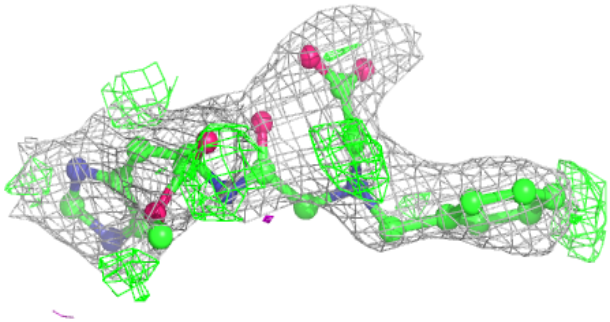
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	I41	B	1999	27/27	0.86	0.26	53,63,76,76	0
3	I41	A	1999	27/27	0.87	0.26	35,56,83,84	0
2	ZN	A	1998	1/1	0.99	0.12	31,31,31,31	0
2	ZN	B	1998	1/1	0.99	0.12	33,33,33,33	0

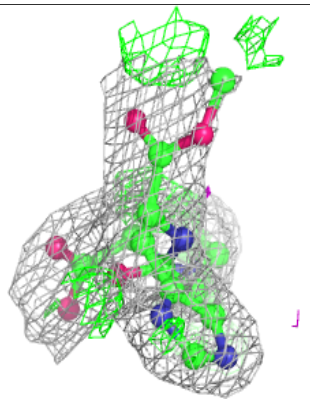
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I41 B 1999:

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

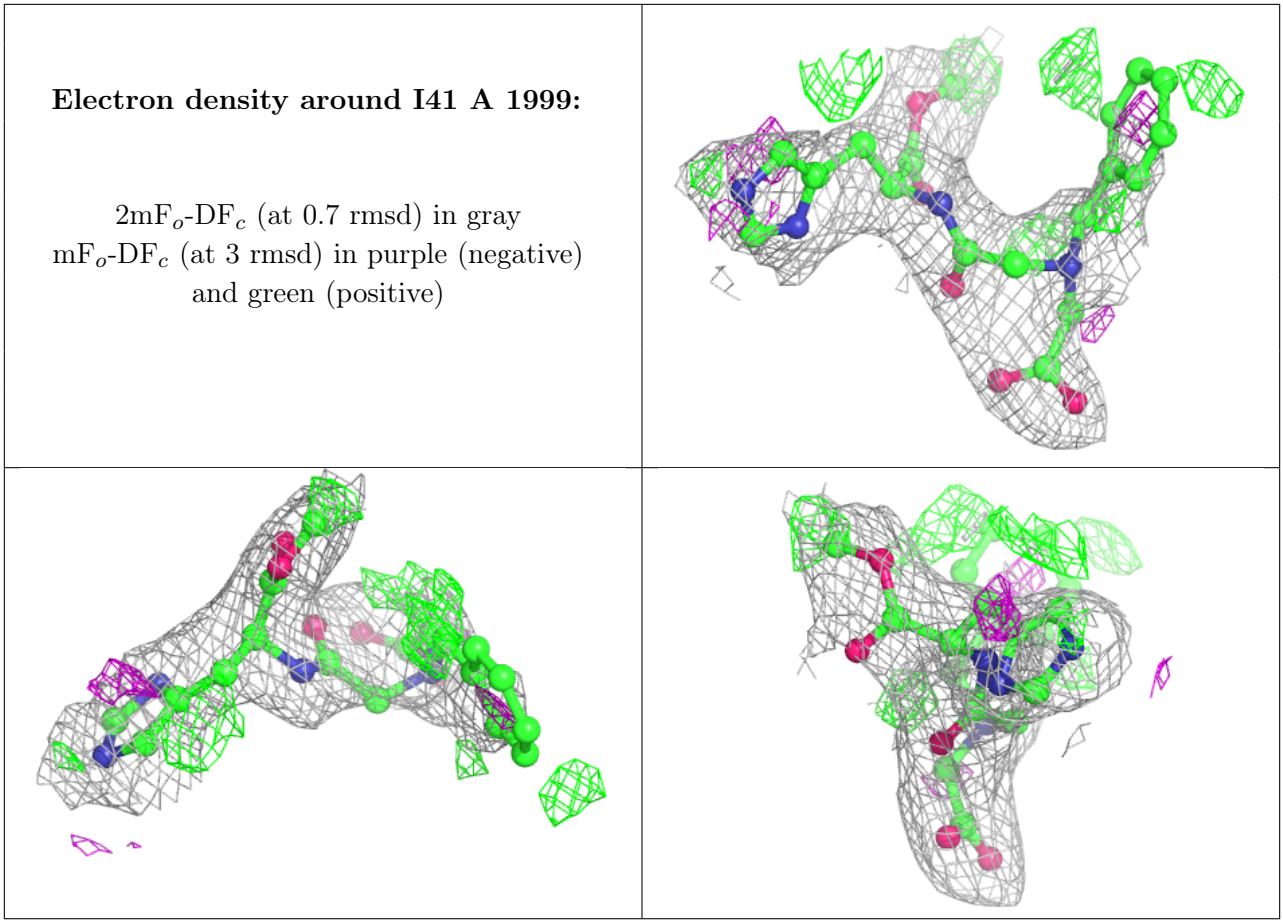






Electron density around I41 A 1999:

$2mF_o$-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.