Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 04:27 AM EDT

PDB ID	:	6NIC
Title	:	Crystal Structure of Medicago truncatula Agmatine Iminohydrolase (Deiminase) in Complex with 6-aminohexanamide
Authors	:	Sekula, B.; Dauter, Z.
Deposited on	:	2018-12-27
Resolution	:	2.20 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:

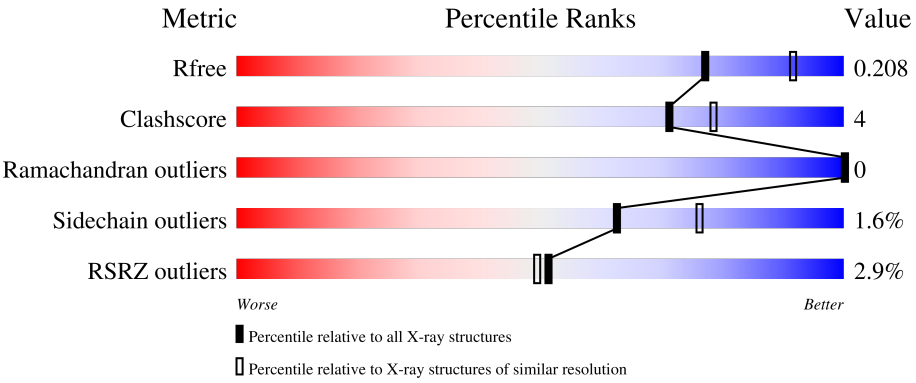
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	367	4% 90% 7% .
1	B	367	4% 89% 8% .
1	C	367	2% 92% 6% .
1	D	367	3% 84% 14% .

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12204 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.

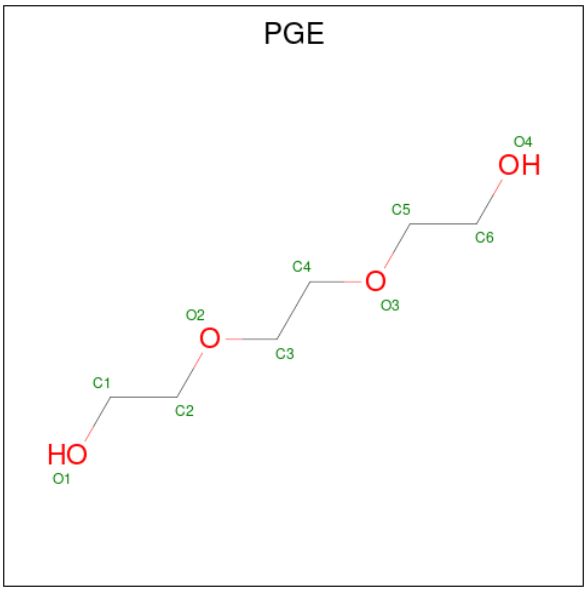
- Molecule 1 is a protein called Porphyromonas-type peptidyl-arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2827	1782	501	531	13			
1	B	356	Total	C	N	O	S	0	0	0
			2827	1782	501	531	13			
1	C	358	Total	C	N	O	S	0	0	0
			2840	1789	503	535	13			
1	D	360	Total	C	N	O	S	0	0	0
			2857	1799	507	538	13			

There are 12 discrepancies between the modelled and reference sequences:

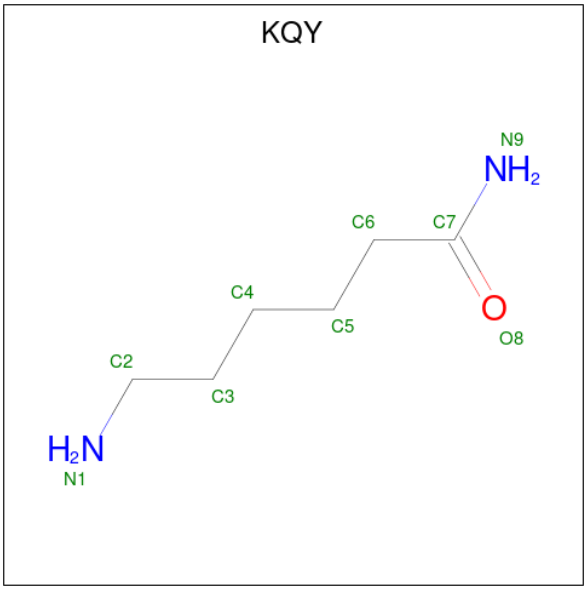
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	SER	-	expression tag	UNP G7JT50
A	9	ASN	-	expression tag	UNP G7JT50
A	10	ALA	-	expression tag	UNP G7JT50
B	8	SER	-	expression tag	UNP G7JT50
B	9	ASN	-	expression tag	UNP G7JT50
B	10	ALA	-	expression tag	UNP G7JT50
C	8	SER	-	expression tag	UNP G7JT50
C	9	ASN	-	expression tag	UNP G7JT50
C	10	ALA	-	expression tag	UNP G7JT50
D	8	SER	-	expression tag	UNP G7JT50
D	9	ASN	-	expression tag	UNP G7JT50
D	10	ALA	-	expression tag	UNP G7JT50

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	A	1	Total C O 10 6 4	0	0

- Molecule 3 is 6-aminohexanamide (three-letter code: KQY) (formula: $C_6H_{14}N_2O$).



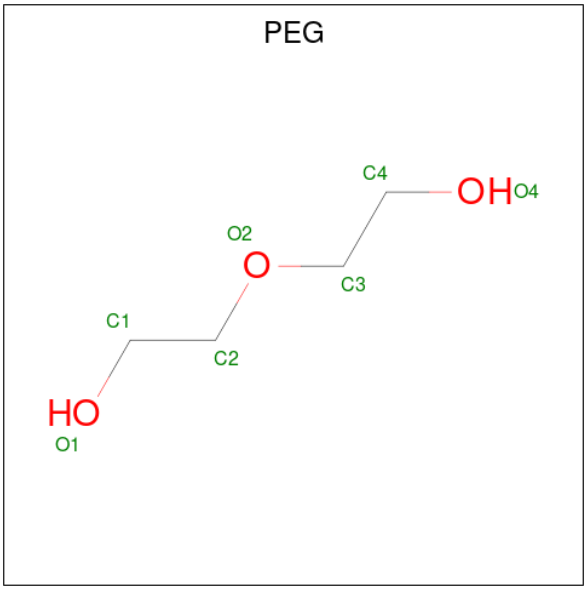
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 6 2 1	0	0
3	C	1	Total C N O 9 6 2 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N O 9 6 2 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

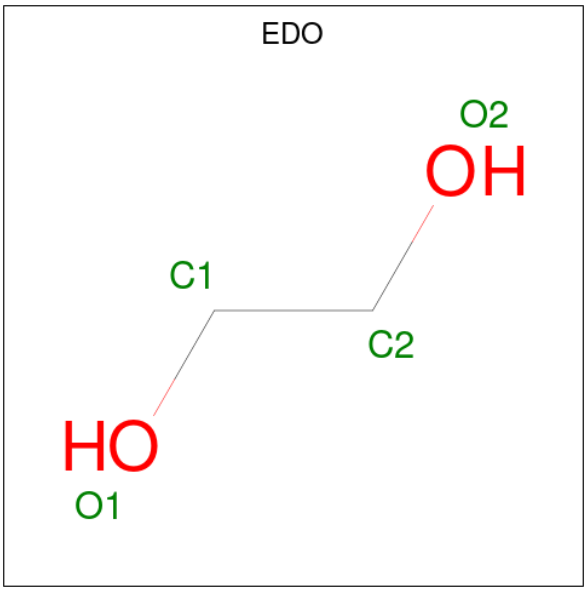


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

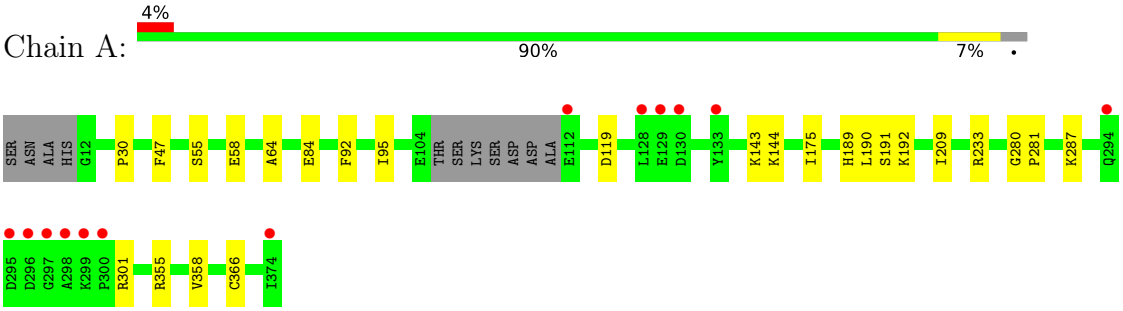
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	220	Total O 220 220	0	0
7	B	90	Total O 90 90	0	0
7	C	299	Total O 299 299	0	0
7	D	164	Total O 164 164	0	0

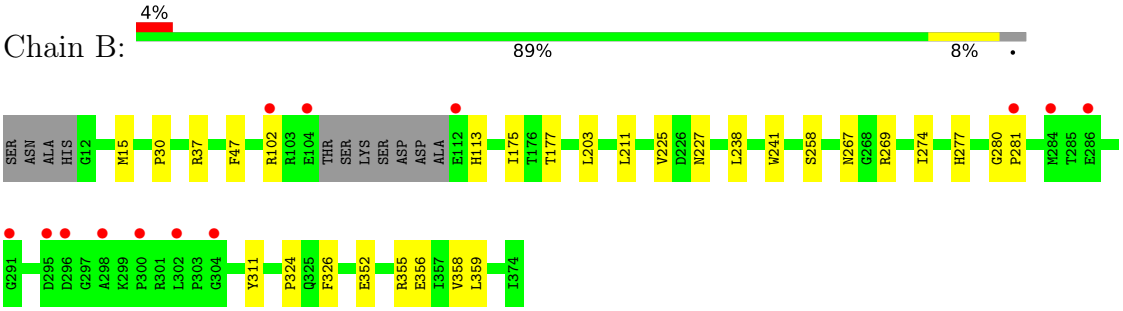
3 Residue-property plots

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.

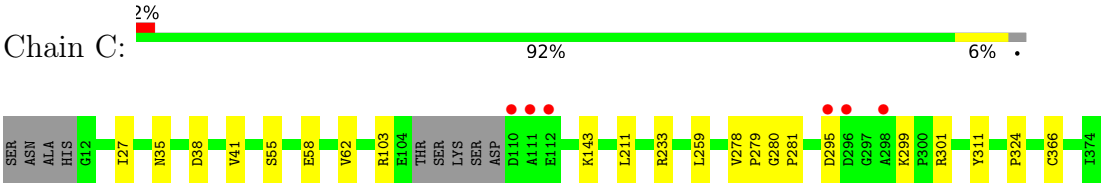
• Molecule 1: Porphyromonas-type peptidyl-arginine deiminase



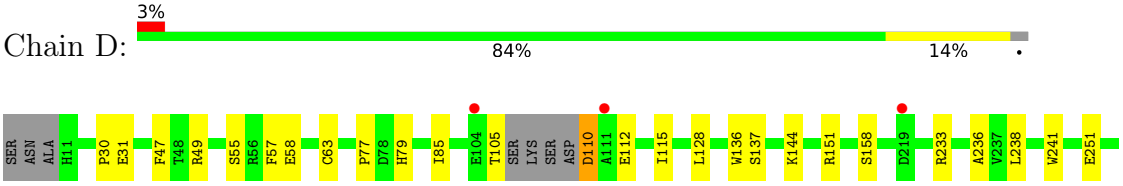
• Molecule 1: Porphyromonas-type peptidyl-arginine deiminase

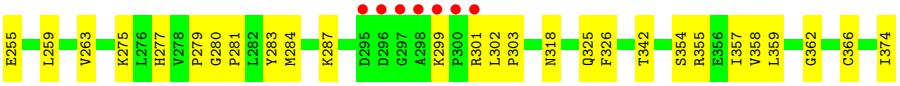


• Molecule 1: Porphyromonas-type peptidyl-arginine deiminase



• Molecule 1: Porphyromonas-type peptidyl-arginine deiminase




E255
L259
V263
K275
L276
H277
V278
P279
G280
P281
L282
Y283
M284
K287
D295
D296
G297
A298
K299
P300
R301
L302
P303
N318
Q325
F326
T342
S354
R355
E356
I357
V358
L359
G362
C366
I374

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	142.44Å 142.44Å 345.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.19 – 2.20 49.59 – 2.20	Depositor EDS
% Data completeness (in resolution range)	76.2 (50.19-2.20) 76.2 (49.59-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.165 , 0.204 0.174 , 0.208	Depositor DCC
R_{free} test set	1232 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12204	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: PGE, PEG, KQY, EDO, 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	0.92	0/2901	0.91	0/3938
1	B	0.77	0/2901	0.82	0/3938
1	C	0.97	0/2914	0.93	0/3956
1	D	0.93	0/2932	0.96	0/3981
All	All	0.90	0/11648	0.91	0/15813

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2827	0	2710	16	0
1	B	2827	0	2710	18	0
1	C	2840	0	2719	12	0
1	D	2857	0	2733	33	0
2	A	20	0	28	4	0
3	A	9	0	0	2	0
3	C	9	0	0	2	0
3	D	9	0	0	4	0
4	A	14	0	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	4	0	6	0	0
6	D	4	0	6	2	0
7	A	220	0	0	1	0
7	B	90	0	0	0	0
7	C	299	0	0	0	0
7	D	164	0	0	5	0
All	All	12204	0	10942	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (79) 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:D:366:CYS:SG	3:D:402:KQY:C7	2.50	0.99
1:B:15:MET:HE2	1:B:203:LEU:HD22	1.52	0.90
1:A:366:CYS:SG	3:A:403:KQY:C7	2.62	0.87
1:C:366:CYS:SG	3:C:402:KQY:C7	2.64	0.86
1:B:15:MET:CE	1:B:203:LEU:HD22	2.11	0.80
1:B:267:ASN:HD22	1:B:269:ARG:NH2	1.82	0.76
1:D:366:CYS:SG	3:D:402:KQY:C6	2.74	0.75
1:C:35:ASN:OD1	1:C:301:ARG:NH1	2.20	0.73
1:D:144:LYS:HD3	7:D:656:HOH:O	1.90	0.72
1:A:192:LYS:H	2:A:401:PGE:H62	1.56	0.71
1:C:366:CYS:SG	3:C:402:KQY:N9	2.71	0.64
1:B:311:TYR:HA	1:B:324:PRO:HG2	1.82	0.61
1:A:366:CYS:SG	3:A:403:KQY:N9	2.73	0.61
1:B:326:PHE:HE2	1:B:358:VAL:HG21	1.66	0.60
1:C:301:ARG:NH2	1:C:301:ARG:HG3	2.16	0.59
1:C:301:ARG:HG3	1:C:301:ARG:HH21	1.67	0.59
1:D:55:SER:HA	1:D:58:GLU:O	2.04	0.57
1:D:115:ILE:HB	1:D:374:ILE:HG21	1.89	0.55
1:D:233:ARG:HG2	1:D:236:ALA:HB3	1.89	0.54
1:A:144:LYS:HD2	7:A:655:HOH:O	2.09	0.53
1:A:280:GLY:HA3	1:A:281:PRO:C	2.29	0.52
1:B:241:TRP:O	1:B:277:HIS:HA	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ARG:NH2	7:D:501:HOH:O	2.30	0.52
1:C:278:VAL:HB	1:C:279:PRO:HD2	1.92	0.51
1:D:280:GLY:HA3	1:D:281:PRO:C	2.30	0.51
1:D:136:TRP:CE2	6:D:401:EDO:H12	2.45	0.51
1:D:241:TRP:CE2	1:D:275:LYS:HE3	2.45	0.51
1:D:137:SER:HB3	6:D:401:EDO:H21	1.93	0.51
1:A:355:ARG:HA	1:A:358:VAL:HG22	1.94	0.50
1:D:302:LEU:HD12	1:D:303:PRO:HD2	1.93	0.50
1:B:280:GLY:HA3	1:B:281:PRO:C	2.31	0.50
1:A:189:HIS:CD2	1:A:190:LEU:HG	2.47	0.49
1:C:211:LEU:HD12	1:C:259:LEU:HD23	1.93	0.49
1:D:302:LEU:CD1	1:D:303:PRO:HD2	2.42	0.49
1:A:64:ALA:O	1:A:84:GLU:HA	2.12	0.49
1:A:192:LYS:N	2:A:401:PGE:H62	2.27	0.48
1:A:191:SER:HB2	2:A:401:PGE:H62	1.94	0.48
1:D:105:THR:HB	7:D:644:HOH:O	2.12	0.48
1:B:30:PRO:HD3	1:B:47:PHE:CD2	2.50	0.47
1:C:280:GLY:HA3	1:C:281:PRO:C	2.35	0.47
1:D:325:GLN:O	1:D:354:SER:HB2	2.15	0.47
1:D:49:ARG:HG3	1:D:49:ARG:NH1	2.30	0.47
1:D:110:ASP:N	1:D:110:ASP:OD1	2.47	0.46
1:C:38:ASP:O	1:C:41:VAL:HG12	2.15	0.46
1:C:55:SER:HA	1:C:58:GLU:O	2.15	0.46
1:D:279:PRO:HG3	1:D:326:PHE:CD2	2.49	0.46
1:B:177:THR:HA	1:B:211:LEU:O	2.15	0.46
1:A:175:ILE:HG22	1:A:209:ILE:HB	1.96	0.46
1:A:191:SER:HB2	2:A:401:PGE:C6	2.45	0.46
1:B:30:PRO:HD3	1:B:47:PHE:CE2	2.51	0.45
1:B:352:GLU:O	1:B:352:GLU:HG3	2.15	0.45
1:D:366:CYS:SG	3:D:402:KQY:N9	2.89	0.45
1:B:238:LEU:HA	1:B:274:ILE:O	2.17	0.45
1:D:355:ARG:O	1:D:359:LEU:HG	2.16	0.45
1:D:366:CYS:HB3	3:D:402:KQY:C6	2.48	0.44
1:B:102:ARG:NH2	1:B:113:HIS:O	2.51	0.43
1:D:77:PRO:HB2	1:D:79:HIS:CE1	2.52	0.43
1:D:326:PHE:HE1	1:D:358:VAL:HG21	1.83	0.43
1:D:128:LEU:HD23	1:D:128:LEU:HA	1.81	0.43
1:D:151:ARG:NE	7:D:501:HOH:O	2.40	0.43
1:A:119:ASP:HA	1:A:143:LYS:HD2	2.01	0.43
1:B:175:ILE:HG22	1:B:225:VAL:HG21	2.01	0.43
1:A:55:SER:HA	1:A:58:GLU:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:PRO:HD3	1:D:47:PHE:CD2	2.54	0.42
1:B:15:MET:HE2	1:B:15:MET:HB2	1.98	0.42
1:D:63:CYS:HB3	1:D:85:ILE:HB	2.02	0.42
1:D:357:ILE:HG22	1:D:362:GLY:O	2.20	0.42
1:B:37:ARG:HH21	1:B:356:GLU:CD	2.23	0.41
1:A:30:PRO:HD3	1:A:47:PHE:CD2	2.56	0.41
1:B:355:ARG:O	1:B:359:LEU:HG	2.20	0.41
1:A:92:PHE:CE1	1:A:95:ILE:HD11	2.55	0.41
1:B:267:ASN:ND2	1:B:269:ARG:NH2	2.60	0.41
1:D:281:PRO:HB2	1:D:283:TYR:CE2	2.55	0.41
1:C:27:ILE:O	1:C:62:VAL:HA	2.21	0.41
1:D:238:LEU:HD11	1:D:342:THR:HG21	2.02	0.41
1:D:251:GLU:O	1:D:255:GLU:HB2	2.21	0.41
1:D:277:HIS:HE1	7:D:601:HOH:O	2.04	0.41
1:C:311:TYR:HA	1:C:324:PRO:HG2	2.02	0.41
1:D:57:PHE:HB3	1:D:318:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	352/367 (96%)	340 (97%)	12 (3%)	0	100	100
1	B	352/367 (96%)	336 (96%)	16 (4%)	0	100	100
1	C	354/367 (96%)	344 (97%)	10 (3%)	0	100	100
1	D	356/367 (97%)	336 (94%)	20 (6%)	0	100	100
All	All	1414/1468 (96%)	1356 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	303/312 (97%)	300 (99%)	3 (1%)	76 86
1	B	303/312 (97%)	301 (99%)	2 (1%)	84 91
1	C	304/312 (97%)	299 (98%)	5 (2%)	62 76
1	D	306/312 (98%)	296 (97%)	10 (3%)	38 49
All	All	1216/1248 (97%)	1196 (98%)	20 (2%)	62 76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	ARG
1	A	287	LYS
1	A	301	ARG
1	B	227	ASN
1	B	258	SER
1	C	103	ARG
1	C	143	LYS
1	C	233	ARG
1	C	295	ASP
1	C	299	LYS
1	D	31	GLU
1	D	110	ASP
1	D	112	GLU
1	D	158	SER
1	D	259	LEU
1	D	263	VAL
1	D	284	MET
1	D	287	LYS
1	D	299	LYS
1	D	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	267	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	KQY	C	402	-	8,8,8	1.65	2 (25%)	8,8,8	1.42	2 (25%)
6	EDO	D	401	-	3,3,3	0.47	0	2,2,2	0.58	0
2	PGE	A	401	-	9,9,9	0.88	0	8,8,8	0.93	0
4	PEG	A	405	-	6,6,6	0.66	0	5,5,5	0.74	0
3	KQY	D	402	-	8,8,8	1.43	2 (25%)	8,8,8	1.42	2 (25%)
2	PGE	A	402	-	9,9,9	0.94	0	8,8,8	0.77	0
4	PEG	B	401	-	6,6,6	0.71	0	5,5,5	0.54	0
3	KQY	A	403	-	8,8,8	1.26	1 (12%)	8,8,8	2.22	3 (37%)
4	PEG	A	404	-	6,6,6	0.55	0	5,5,5	0.13	0
6	EDO	C	401	-	3,3,3	1.04	0	2,2,2	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KQY	C	402	-	-	0/6/6/6	-
6	EDO	D	401	-	-	1/1/1/1	-
2	PGE	A	401	-	-	2/7/7/7	-
4	PEG	A	405	-	-	3/4/4/4	-
3	KQY	D	402	-	-	0/6/6/6	-
2	PGE	A	402	-	-	6/7/7/7	-
4	PEG	B	401	-	-	0/4/4/4	-
3	KQY	A	403	-	-	0/6/6/6	-
4	PEG	A	404	-	-	1/4/4/4	-
6	EDO	C	401	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	KQY	C7-N9	3.83	1.45	1.32
3	D	402	KQY	C7-N9	3.18	1.43	1.32
3	A	403	KQY	C7-N9	2.85	1.42	1.32
3	D	402	KQY	O8-C7	2.15	1.30	1.24
3	C	402	KQY	O8-C7	2.04	1.30	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	KQY	O8-C7-C6	4.10	133.11	121.07
3	A	403	KQY	C5-C6-C7	3.72	122.14	113.79
3	D	402	KQY	O8-C7-C6	2.58	128.65	121.07
3	C	402	KQY	O8-C7-C6	2.39	128.10	121.07
3	C	402	KQY	C5-C6-C7	2.30	118.95	113.79
3	A	403	KQY	O8-C7-N9	-2.21	116.46	122.50
3	D	402	KQY	C5-C6-C7	2.16	118.64	113.79

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	PEG	C4-C3-O2-C2
2	A	402	PGE	O2-C3-C4-O3
4	A	405	PEG	O2-C3-C4-O4
2	A	402	PGE	O3-C5-C6-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	401	PGE	C6-C5-O3-C4
2	A	401	PGE	O3-C5-C6-O4
6	D	401	EDO	O1-C1-C2-O2
4	A	405	PEG	O1-C1-C2-O2
6	C	401	EDO	O1-C1-C2-O2
2	A	402	PGE	C6-C5-O3-C4
2	A	402	PGE	C4-C3-O2-C2
2	A	402	PGE	C3-C4-O3-C5
2	A	402	PGE	C1-C2-O2-C3
4	A	404	PEG	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	KQY	2	0
6	D	401	EDO	2	0
2	A	401	PGE	4	0
3	D	402	KQY	4	0
3	A	403	KQY	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	356/367 (97%)	-0.46	13 (3%)	41	39	16, 27, 62, 111	0
1	B	356/367 (97%)	-0.35	13 (3%)	41	39	26, 45, 73, 103	0
1	C	358/367 (97%)	-0.72	6 (1%)	70	68	13, 21, 48, 110	0
1	D	360/367 (98%)	-0.45	10 (2%)	53	51	17, 31, 70, 123	0
All	All	1430/1468 (97%)	-0.50	42 (2%)	51	49	13, 30, 69, 123	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	LYS	8.6
1	D	300	PRO	6.6
1	A	298	ALA	5.5
1	A	296	ASP	5.3
1	B	298	ALA	5.1
1	B	296	ASP	4.6
1	D	301	ARG	4.5
1	C	111	ALA	4.5
1	C	110	ASP	4.2
1	B	302	LEU	4.1
1	C	295	ASP	3.7
1	D	296	ASP	3.5
1	A	297	GLY	3.1
1	B	295	ASP	3.1
1	A	129	GLU	3.0
1	A	294	GLN	3.0
1	C	296	ASP	3.0
1	B	300	PRO	3.0
1	C	298	ALA	2.9
1	B	286	GLU	2.8
1	B	104	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	297	GLY	2.8
1	A	295	ASP	2.7
1	D	219	ASP	2.7
1	C	112	GLU	2.7
1	A	300	PRO	2.6
1	D	295	ASP	2.6
1	D	298	ALA	2.5
1	A	299	LYS	2.4
1	B	291	GLY	2.3
1	B	102	ARG	2.3
1	A	130	ASP	2.3
1	A	133	TYR	2.2
1	A	374	ILE	2.1
1	A	128	LEU	2.1
1	B	112	GLU	2.1
1	B	304	GLY	2.1
1	D	111	ALA	2.0
1	D	104	GLU	2.0
1	B	281	PRO	2.0
1	B	284	MET	2.0
1	A	112	GLU	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 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
4	PEG	A	405	7/7	0.59	0.18	67,74,79,82	0
4	PEG	A	404	7/7	0.83	0.14	66,71,73,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PGE	A	402	10/10	0.83	0.16	47,53,59,60	0
3	KQY	C	402	9/9	0.87	0.17	26,27,36,38	0
3	KQY	D	402	9/9	0.88	0.16	28,32,43,47	0
6	EDO	C	401	4/4	0.88	0.16	39,49,50,51	0
2	PGE	A	401	10/10	0.91	0.18	40,50,56,56	0
4	PEG	B	401	7/7	0.92	0.13	47,51,53,57	0
3	KQY	A	403	9/9	0.92	0.14	29,31,45,50	0
6	EDO	D	401	4/4	0.98	0.15	35,39,41,43	0
5	NA	C	403	1/1	0.99	0.12	26,26,26,26	0
5	NA	D	403	1/1	0.99	0.06	33,33,33,33	0
5	NA	A	406	1/1	0.99	0.06	33,33,33,33	0
5	NA	B	402	1/1	0.99	0.07	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.