



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:22 AM UTC

PDB ID : 4UUI / pdb_00004uui
Title : A case study for twinned data analysis: multiple crystal forms of the enzyme
N-acetyl-neuraminic lyase
Authors : Campeotto, I.; Phillips, S.E.V.; Pearson, A.R.
Deposited on : 2014-07-29
Resolution : 1.79 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

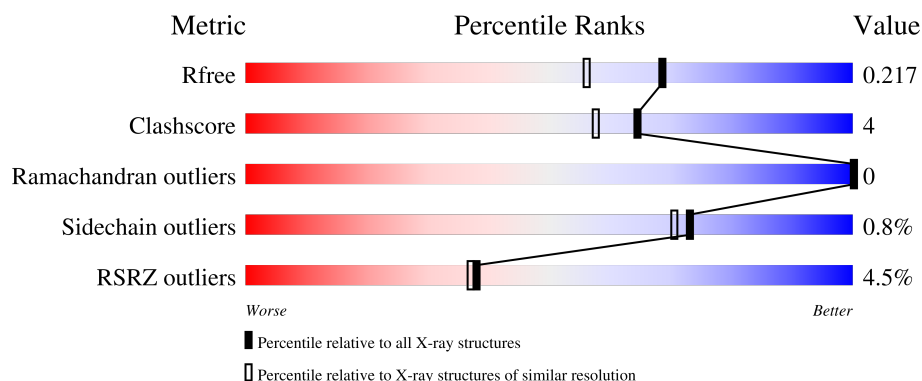
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	6% 88% 10% ..
1	B	304	5% 87% 11% .
1	C	304	3% 89% 9% .
1	D	304	4% 91% 7% .

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
2	PYR	D	1299	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10169 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 N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	6	0
			2357	1503	402	441	11			
1	B	298	Total	C	N	O	S	0	4	0
			2336	1489	400	435	12			
1	C	299	Total	C	N	O	S	0	6	0
			2352	1499	403	439	11			
1	D	299	Total	C	N	O	S	0	4	0
			2338	1489	399	439	11			

There are 40 discrepancies between the modelled and reference sequences:

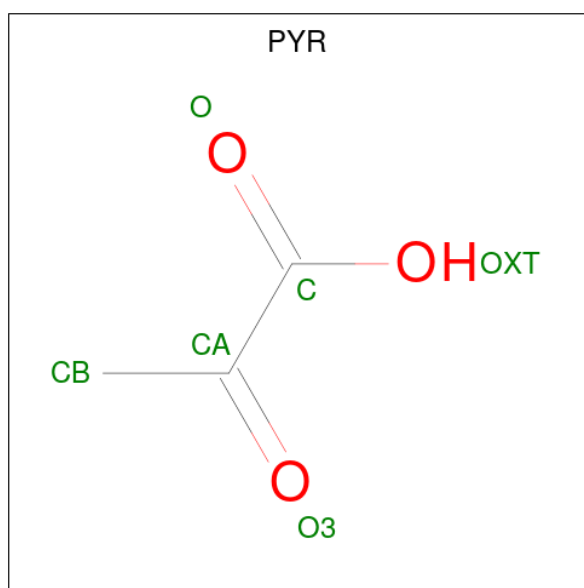
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P0A6L4
A	-5	GLU	-	expression tag	UNP P0A6L4
A	-4	HIS	-	expression tag	UNP P0A6L4
A	-3	HIS	-	expression tag	UNP P0A6L4
A	-2	HIS	-	expression tag	UNP P0A6L4
A	-1	HIS	-	expression tag	UNP P0A6L4
A	0	HIS	-	expression tag	UNP P0A6L4
A	1	HIS	-	expression tag	UNP P0A6L4
A	137	PHE	TYR	engineered mutation	UNP P0A6L4
A	192	ASN	GLU	engineered mutation	UNP P0A6L4
B	-6	MET	-	expression tag	UNP P0A6L4
B	-5	GLU	-	expression tag	UNP P0A6L4
B	-4	HIS	-	expression tag	UNP P0A6L4
B	-3	HIS	-	expression tag	UNP P0A6L4
B	-2	HIS	-	expression tag	UNP P0A6L4
B	-1	HIS	-	expression tag	UNP P0A6L4
B	0	HIS	-	expression tag	UNP P0A6L4
B	1	HIS	-	expression tag	UNP P0A6L4
B	137	PHE	TYR	engineered mutation	UNP P0A6L4
B	192	ASN	GLU	engineered mutation	UNP P0A6L4
C	-6	MET	-	expression tag	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLU	-	expression tag	UNP P0A6L4
C	-4	HIS	-	expression tag	UNP P0A6L4
C	-3	HIS	-	expression tag	UNP P0A6L4
C	-2	HIS	-	expression tag	UNP P0A6L4
C	-1	HIS	-	expression tag	UNP P0A6L4
C	0	HIS	-	expression tag	UNP P0A6L4
C	1	HIS	-	expression tag	UNP P0A6L4
C	137	PHE	TYR	engineered mutation	UNP P0A6L4
C	192	ASN	GLU	engineered mutation	UNP P0A6L4
D	-6	MET	-	expression tag	UNP P0A6L4
D	-5	GLU	-	expression tag	UNP P0A6L4
D	-4	HIS	-	expression tag	UNP P0A6L4
D	-3	HIS	-	expression tag	UNP P0A6L4
D	-2	HIS	-	expression tag	UNP P0A6L4
D	-1	HIS	-	expression tag	UNP P0A6L4
D	0	HIS	-	expression tag	UNP P0A6L4
D	1	HIS	-	expression tag	UNP P0A6L4
D	137	PHE	TYR	engineered mutation	UNP P0A6L4
D	192	ASN	GLU	engineered mutation	UNP P0A6L4

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

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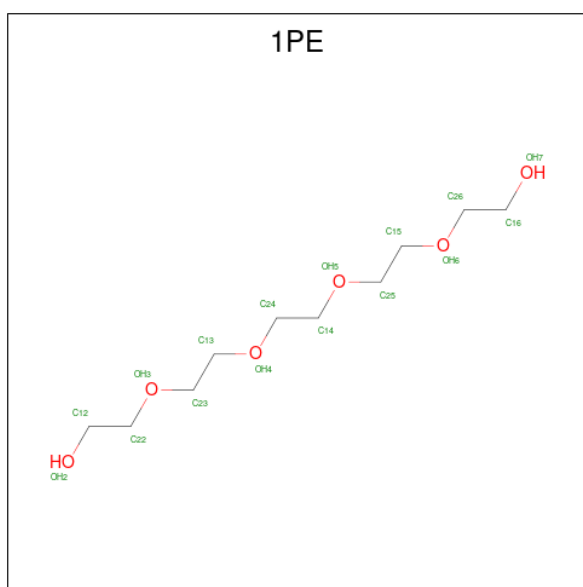
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	Na		0	0
			1	1			

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	5	3		
4	D	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	210	Total	O		0	0
			210	210			
5	B	188	Total	O		0	0
			188	188			

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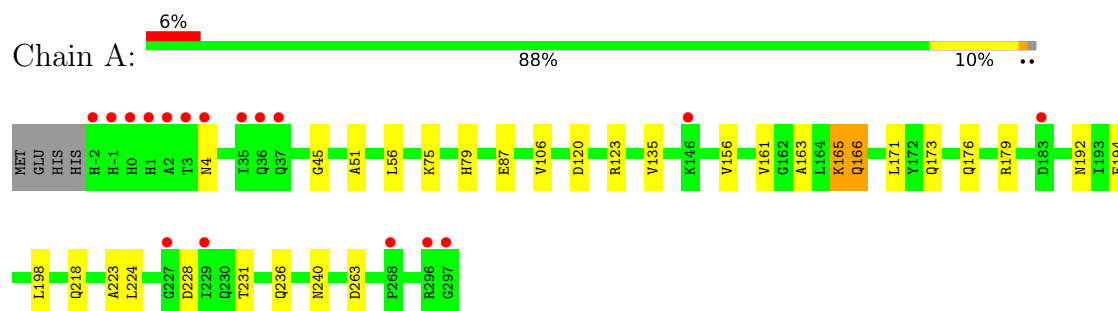
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	172	Total 172	O 172	0	0
5	D	175	Total 175	O 175	0	0

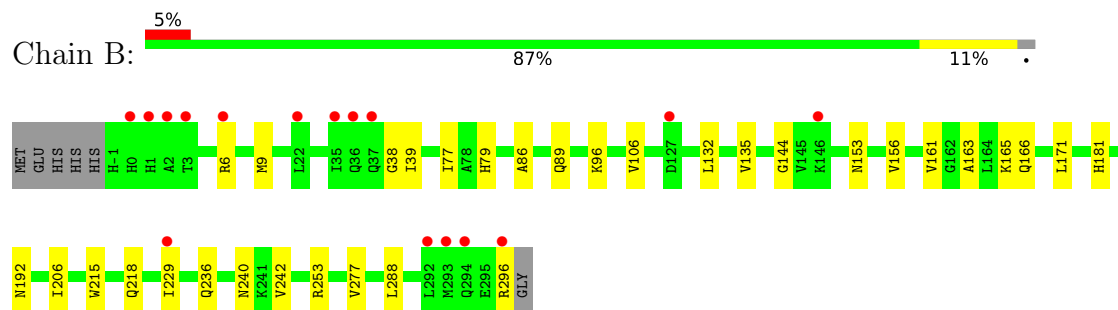
3 Residue-property plots [i](#)

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.

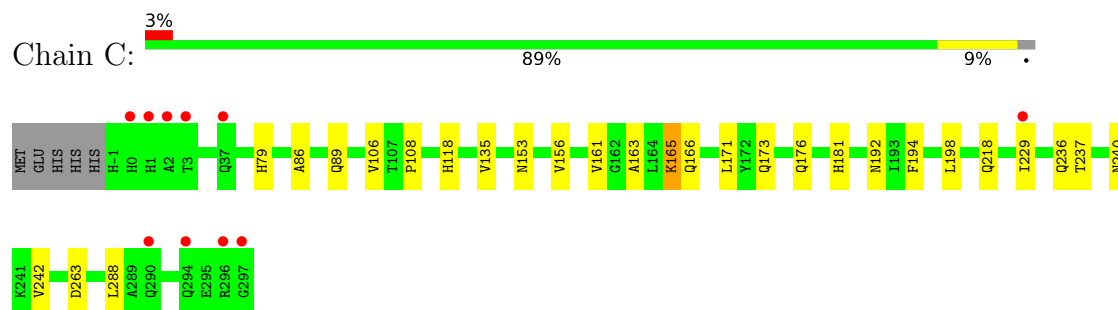
• Molecule 1: N-ACETYLNEURAMINATE LYASE



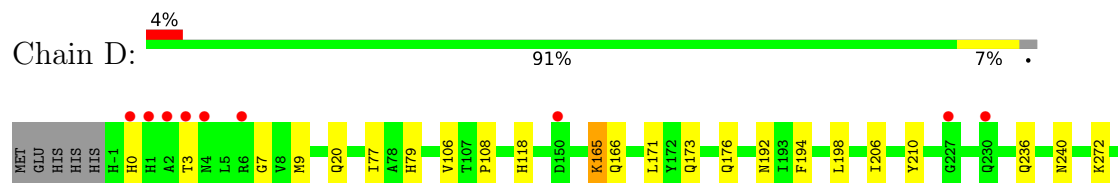
• Molecule 1: N-ACETYLNEURAMINATE LYASE



• Molecule 1: N-ACETYLNEURAMINATE LYASE



• Molecule 1: N-ACETYLNEURAMINATE LYASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.98Å 116.67Å 83.68Å 90.00° 118.06° 90.00°	Depositor
Resolution (Å)	73.85 – 1.79 73.84 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.4 (73.85-1.79) 98.8 (73.84-1.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.6.0105	Depositor
R, R_{free}	0.155 , 0.184 0.189 , 0.217	Depositor DCC
R_{free} test set	6165 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.106 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10169	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PYR, KPI, 1PE

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	0.58	1/2404 (0.0%)	0.80	2/3253 (0.1%)
1	B	0.53	0/2376	0.74	0/3213
1	C	0.55	0/2398	0.75	0/3243
1	D	0.55	0/2378	0.77	1/3217 (0.0%)
All	All	0.55	1/9556 (0.0%)	0.76	3/12926 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLN	CA-C	9.80	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLN	CA-C-O	11.08	132.59	120.63
1	A	218	GLN	N-CA-C	8.54	121.66	111.33
1	D	7	GLY	N-CA-C	5.33	117.95	110.38

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	2357	0	2381	21	0
1	B	2336	0	2363	22	0
1	C	2352	0	2382	18	0
1	D	2338	0	2356	17	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	B	1	0	0	0	0
4	B	8	0	9	2	0
4	D	8	0	9	0	0
5	A	210	0	0	1	0
5	B	188	0	0	0	0
5	C	172	0	0	1	0
5	D	175	0	0	1	0
All	All	10169	0	9500	74	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 (74) 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:9[B]:MET:HE3	1:D:77:ILE:CD1	1.92	0.98
1:D:9[B]:MET:HE3	1:D:77:ILE:HD11	1.46	0.95
1:D:9[B]:MET:CE	1:D:77:ILE:HD11	1.97	0.95
1:D:20:GLN:HE22	1:D:272:LYS:H	1.19	0.90
1:A:223:ALA:HB1	1:A:231[A]:THR:HG23	1.71	0.73
1:A:4:ASN:HD22	1:A:75:LYS:NZ	1.88	0.71
1:A:224:LEU:O	1:C:229:ILE:HD12	1.92	0.69
1:C:173:GLN:HA	1:C:176:GLN:HE21	1.59	0.67
1:A:4:ASN:HD22	1:A:75:LYS:HZ2	1.42	0.66
1:A:223:ALA:CB	1:A:231[A]:THR:HG23	2.26	0.66
1:D:9[B]:MET:HE3	1:D:77:ILE:HD12	1.77	0.65
1:C:79:HIS:HE1	1:C:106:VAL:H	1.43	0.64
1:A:79:HIS:HE1	1:A:106:VAL:H	1.47	0.62
1:A:173:GLN:HA	1:A:176:GLN:HE21	1.64	0.62
1:B:79:HIS:HE1	1:B:106:VAL:H	1.49	0.60
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.68	0.59
1:C:165:KPI:H1B	5:C:2114:HOH:O	2.05	0.57
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.86	0.56
1:B:9[B]:MET:HE2	1:B:77:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLY:O	1:B:218[B]:GLN:NE2	2.39	0.55
1:A:223:ALA:HB1	1:A:231[A]:THR:CG2	2.35	0.55
1:C:156:VAL:HA	1:C:161:VAL:HG11	1.89	0.54
1:C:86:ALA:HA	1:C:89:GLN:HE21	1.73	0.54
1:D:20:GLN:HE22	1:D:272:LYS:N	1.96	0.53
1:D:79:HIS:HE1	1:D:106:VAL:H	1.56	0.53
1:D:194:PHE:CE2	1:D:198:LEU:HD11	2.44	0.52
1:B:242:VAL:HG13	1:B:288:LEU:HD21	1.91	0.52
1:C:192:ASN:HA	1:C:240:ASN:HD21	1.78	0.49
1:A:135:VAL:HG22	1:A:163:ALA:HB3	1.95	0.49
1:B:144:GLY:HA2	4:B:1298:1PE:H122	1.95	0.48
1:D:236:GLN:HE21	1:D:240:ASN:ND2	2.12	0.48
1:B:9[B]:MET:HE2	1:B:77:ILE:CD1	2.44	0.48
1:C:218[B]:GLN:HE21	1:C:218[B]:GLN:HA	1.79	0.48
1:A:120:ASP:OD1	1:A:123:ARG:NH1	2.46	0.48
1:A:166:GLN:HE21	1:A:166:GLN:HA	1.77	0.48
1:B:236:GLN:HE21	1:B:240:ASN:HD21	1.61	0.47
1:A:228:ASP:CG	1:A:231[A]:THR:HG22	2.39	0.47
1:C:108:PRO:HD2	1:C:118:HIS:HD2	1.79	0.47
1:C:153:ASN:OD1	1:C:181:HIS:HE1	1.98	0.46
1:B:192:ASN:HA	1:B:240:ASN:HD21	1.81	0.46
1:B:236:GLN:HE21	1:B:240:ASN:ND2	2.14	0.45
1:B:96:LYS:HD3	1:B:132:LEU:HD13	1.99	0.45
1:B:153:ASN:OD1	1:B:181:HIS:HE1	1.99	0.45
1:D:165:KPI:H1B	5:D:2120:HOH:O	2.15	0.45
1:C:194:PHE:CE2	1:C:198:LEU:HD11	2.53	0.44
1:D:192:ASN:HA	1:D:240:ASN:HD21	1.83	0.44
1:C:135:VAL:HG22	1:C:163:ALA:HB3	1.98	0.44
1:B:39:ILE:HA	1:B:218[B]:GLN:NE2	2.33	0.44
1:B:39:ILE:HA	1:B:218[B]:GLN:HE22	1.82	0.44
1:C:79:HIS:CE1	1:C:106:VAL:H	2.31	0.44
1:B:86:ALA:HA	1:B:89:GLN:HE21	1.83	0.44
1:B:135:VAL:HG22	1:B:163:ALA:HB3	1.99	0.43
1:A:165:KPI:H1B	5:A:2141:HOH:O	2.16	0.43
1:A:56:LEU:HD11	1:A:87:GLU:HG2	2.01	0.43
1:A:156:VAL:HA	1:A:161:VAL:HG11	2.00	0.43
1:C:242:VAL:HG13	1:C:288:LEU:HD21	2.00	0.43
1:D:0:HIS:O	1:D:3:THR:HG23	2.19	0.43
1:B:253:ARG:HG3	1:B:277:VAL:HG22	2.00	0.42
1:B:171:LEU:HD12	1:D:171:LEU:HD12	2.01	0.42
1:A:179:ARG:HD3	1:C:237:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLN:HE21	1:C:166:GLN:HA	1.85	0.42
1:C:236:GLN:HE21	1:C:240:ASN:ND2	2.17	0.42
1:A:192:ASN:HA	1:A:240:ASN:HD21	1.84	0.42
1:B:215:TRP:CE3	1:B:296:ARG:HD3	2.55	0.42
1:D:108:PRO:HD2	1:D:118:HIS:HD2	1.85	0.41
1:A:194:PHE:CE2	1:A:198:LEU:HD11	2.55	0.41
1:A:236:GLN:HE21	1:A:240:ASN:ND2	2.18	0.41
1:B:156:VAL:HA	1:B:161:VAL:HG11	2.01	0.41
1:B:38:GLY:C	1:B:218[B]:GLN:HE22	2.29	0.41
1:B:144:GLY:CA	4:B:1298:1PE:H122	2.51	0.41
1:A:45:GLY:O	1:A:51:ALA:HB2	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	303/304 (100%)	299 (99%)	4 (1%)	0	100	100
1	B	299/304 (98%)	295 (99%)	4 (1%)	0	100	100
1	C	302/304 (99%)	297 (98%)	5 (2%)	0	100	100
1	D	300/304 (99%)	294 (98%)	6 (2%)	0	100	100
All	All	1204/1216 (99%)	1185 (98%)	19 (2%)	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	252/250 (101%)	250 (99%)	2 (1%)	73	70
1	B	249/250 (100%)	246 (99%)	3 (1%)	63	57
1	C	251/250 (100%)	250 (100%)	1 (0%)	84	83
1	D	249/250 (100%)	247 (99%)	2 (1%)	73	70
All	All	1001/1000 (100%)	993 (99%)	8 (1%)	73	70

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	263	ASP
1	B	6	ARG
1	B	166	GLN
1	B	229	ILE
1	C	263	ASP
1	D	166	GLN
1	D	210	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	18	GLN
1	A	34	ASN
1	A	79	HIS
1	A	118	HIS
1	A	138	ASN
1	A	166	GLN
1	A	176	GLN
1	A	188	ASN
1	A	211	ASN
1	A	240	ASN
1	B	32	GLN
1	B	37	GLN
1	B	79	HIS
1	B	89	GLN
1	B	90	GLN
1	B	118	HIS

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Mol	Chain	Res	Type
1	B	138	ASN
1	B	166	GLN
1	B	181	HIS
1	B	240	ASN
1	C	0	HIS
1	C	19	GLN
1	C	34	ASN
1	C	37	GLN
1	C	61	GLN
1	C	79	HIS
1	C	89	GLN
1	C	90	GLN
1	C	118	HIS
1	C	166	GLN
1	C	176	GLN
1	C	181	HIS
1	C	211	ASN
1	C	240	ASN
1	C	294	GLN
1	D	20	GLN
1	D	34	ASN
1	D	37	GLN
1	D	79	HIS
1	D	118	HIS
1	D	138	ASN
1	D	166	GLN
1	D	176	GLN
1	D	181	HIS
1	D	211	ASN
1	D	240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KPI	B	165	1	11,13,14	1.05	0	9,15,17	1.29	2 (22%)
1	KPI	A	165	1	11,13,14	1.10	1 (9%)	9,15,17	1.22	1 (11%)
1	KPI	C	165	1	11,13,14	1.11	1 (9%)	9,15,17	1.14	1 (11%)
1	KPI	D	165	1	11,13,14	1.04	0	9,15,17	1.07	1 (11%)

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
1	KPI	B	165	1	-	0/13/14/16	-
1	KPI	A	165	1	-	2/13/14/16	-
1	KPI	C	165	1	-	1/13/14/16	-
1	KPI	D	165	1	-	2/13/14/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	165	KPI	O1-CX2	-2.70	1.23	1.30
1	A	165	KPI	O1-CX2	-2.15	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	KPI	C1-CX1-CX2	2.84	120.79	118.11
1	A	165	KPI	C1-CX1-CX2	2.81	120.76	118.11
1	D	165	KPI	O2-CX2-CX1	-2.16	118.71	121.35
1	B	165	KPI	O2-CX2-CX1	-2.14	118.74	121.35
1	C	165	KPI	C1-CX1-CX2	2.06	120.06	118.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	165	KPI	C1-CX1-NZ-CE
1	A	165	KPI	CX2-CX1-NZ-CE
1	D	165	KPI	C1-CX1-NZ-CE
1	D	165	KPI	CX2-CX1-NZ-CE
1	C	165	KPI	C1-CX1-NZ-CE

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	165	KPI	1	0
1	C	165	KPI	1	0
1	D	165	KPI	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
2	PYR	D	1299	-	5,5,5	3.13	3 (60%)	3,6,6	1.38	1 (33%)
4	1PE	D	1298	-	7,7,15	0.66	0	6,6,14	0.69	0
2	PYR	A	1298	-	5,5,5	3.13	3 (60%)	3,6,6	1.55	1 (33%)
4	1PE	B	1298	-	7,7,15	0.64	0	6,6,14	0.39	0
2	PYR	C	1298	-	5,5,5	3.19	3 (60%)	3,6,6	1.44	1 (33%)
2	PYR	B	1299	-	5,5,5	3.16	3 (60%)	3,6,6	1.31	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
2	PYR	D	1299	-	-	3/4/4/4	-
4	1PE	D	1298	-	-	4/5/5/13	-
2	PYR	A	1298	-	-	0/4/4/4	-
4	1PE	B	1298	-	-	3/5/5/13	-
2	PYR	C	1298	-	-	0/4/4/4	-
2	PYR	B	1299	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1299	PYR	CA-C	-4.73	1.38	1.54
2	B	1299	PYR	CA-C	-4.64	1.39	1.54
2	A	1298	PYR	CA-C	-4.51	1.39	1.54
2	C	1298	PYR	CA-C	-4.37	1.39	1.54
2	C	1298	PYR	O-C	4.04	1.32	1.22
2	C	1298	PYR	O3-CA	3.92	1.32	1.23
2	A	1298	PYR	O-C	3.83	1.32	1.22
2	B	1299	PYR	O-C	3.82	1.32	1.22
2	D	1299	PYR	O-C	3.73	1.31	1.22
2	B	1299	PYR	O3-CA	3.72	1.31	1.23
2	A	1298	PYR	O3-CA	3.69	1.31	1.23
2	D	1299	PYR	O3-CA	3.54	1.31	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1298	PYR	OXT-C-CA	2.33	120.04	113.59
2	D	1299	PYR	OXT-C-CA	2.09	119.39	113.59
2	C	1298	PYR	OXT-C-CA	2.01	119.17	113.59

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1299	PYR	OXT-C-CA-CB
2	D	1299	PYR	OXT-C-CA-CB
4	B	1298	1PE	C13-C23-OH3-C22
4	D	1298	1PE	OH4-C13-C23-OH3
4	D	1298	1PE	OH2-C12-C22-OH3

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Mol	Chain	Res	Type	Atoms
4	D	1298	1PE	C12-C22-OH3-C23
2	B	1299	PYR	O-C-CA-CB
2	D	1299	PYR	O-C-CA-CB
4	B	1298	1PE	C12-C22-OH3-C23
4	B	1298	1PE	OH4-C13-C23-OH3
4	D	1298	1PE	C13-C23-OH3-C22
2	D	1299	PYR	O-C-CA-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1298	1PE	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	299/304 (98%)	0.17	17 (5%)	29 28	8, 14, 30, 47	8 (2%)
1	B	297/304 (97%)	0.27	16 (5%)	31 30	7, 14, 29, 52	6 (2%)
1	C	298/304 (98%)	0.11	10 (3%)	48 48	6, 13, 29, 55	6 (2%)
1	D	298/304 (98%)	0.18	11 (3%)	45 45	9, 14, 27, 52	4 (1%)
All	All	1192/1216 (98%)	0.18	54 (4%)	38 37	6, 14, 29, 55	24 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	5.8
1	D	0	HIS	4.7
1	A	0	HIS	4.4
1	C	1	HIS	4.4
1	C	297	GLY	4.1
1	D	3	THR	4.1
1	C	0	HIS	3.9
1	B	1	HIS	3.9
1	A	3	THR	3.8
1	C	296	ARG	3.7
1	D	1	HIS	3.7
1	B	2	ALA	3.7
1	D	2	ALA	3.4
1	B	22	LEU	3.4
1	C	290	GLN	3.3
1	B	3	THR	3.3
1	B	294	GLN	3.2
1	C	3	THR	3.2
1	A	1	HIS	3.2
1	D	296	ARG	3.2
1	B	296	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	229	ILE	3.0
1	A	2	ALA	3.0
1	B	293[A]	MET	3.0
1	A	36	GLN	2.9
1	A	-2	HIS	2.8
1	C	229	ILE	2.8
1	B	6	ARG	2.7
1	A	4	ASN	2.7
1	A	35[A]	ILE	2.7
1	A	183	ASP	2.7
1	C	294	GLN	2.7
1	D	150	ASP	2.6
1	C	2	ALA	2.6
1	A	297	GLY	2.5
1	A	296	ARG	2.5
1	D	4	ASN	2.4
1	D	297	GLY	2.4
1	A	268	PRO	2.4
1	A	37	GLN	2.3
1	A	-1	HIS	2.3
1	B	36	GLN	2.3
1	B	37	GLN	2.3
1	D	230	GLN	2.3
1	C	37	GLN	2.2
1	B	146	LYS	2.2
1	A	146	LYS	2.1
1	A	227	GLY	2.1
1	B	292	LEU	2.1
1	B	35	ILE	2.1
1	D	6	ARG	2.1
1	D	227	GLY	2.0
1	A	229	ILE	2.0
1	B	127	ASP	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KPI	A	165	14/15	0.95	0.06	11,12,13,14	0
1	KPI	B	165	14/15	0.95	0.06	11,12,13,13	0
1	KPI	C	165	14/15	0.95	0.07	9,10,11,12	0
1	KPI	D	165	14/15	0.95	0.07	11,12,13,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PYR	C	1298	6/6	0.75	0.18	32,34,36,36	0
2	PYR	D	1299	6/6	0.76	0.20	32,35,37,40	0
3	NA	B	1297	1/1	0.77	0.15	30,30,30,30	0
4	1PE	B	1298	8/16	0.78	0.16	28,29,30,33	0
2	PYR	A	1298	6/6	0.81	0.15	24,26,27,28	0
2	PYR	B	1299	6/6	0.83	0.14	28,31,32,33	0
4	1PE	D	1298	8/16	0.87	0.13	27,28,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.