



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 AM GMT

PDB ID : 2WPB  
Title : CRYSTAL STRUCTURE OF THE E192N MUTANT OF E. COLI N-ACETYLNEURAMINIC ACID LYASE IN COMPLEX WITH PYRUVATE AND THE INHIBITOR (2R,3R)-2,3,4-TRIHYDROXY-N,N-DIPROPYLBU TANAMIDE IN SPACE GROUP P21 CRYSTAL FORM I  
Authors : Campeotto, I.; Bolt, A.H.; Harman, T.A.; Trinh, C.H.; Dennis, C.A.; Phillips, S.E.V.; Pearson, A.R.; Nelson, A.; Berry, A.  
Deposited on : 2009-08-03  
Resolution : 2.05 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

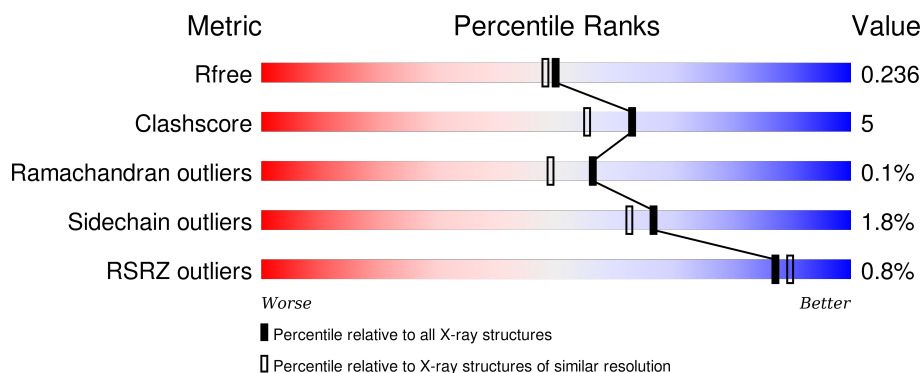
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	<div> <div>%</div> <div>85% 14% ..</div> </div>
1	B	304	<div> <div>%</div> <div>87% 9% ..</div> </div>
1	C	304	<div> <div>%</div> <div>87% 10% .</div> </div>
1	D	304	<div> <div>%</div> <div>86% 10% ..</div> </div>

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	ZZI	A	1298	-	-	-	X
2	ZZI	B	1297	-	-	X	X
2	ZZI	C	1297	-	-	-	X
2	ZZI	D	1297	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9846 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	302	Total	C	N	O	S	0	4	0
			2369	1507	407	444	11			
1	B	295	Total	C	N	O	S	0	3	0
			2296	1463	387	435	11			
1	C	295	Total	C	N	O	S	0	1	0
			2289	1458	388	433	10			
1	D	295	Total	C	N	O	S	0	2	0
			2292	1462	387	432	11			

There are 35 discrepancies between the modelled and reference sequences:

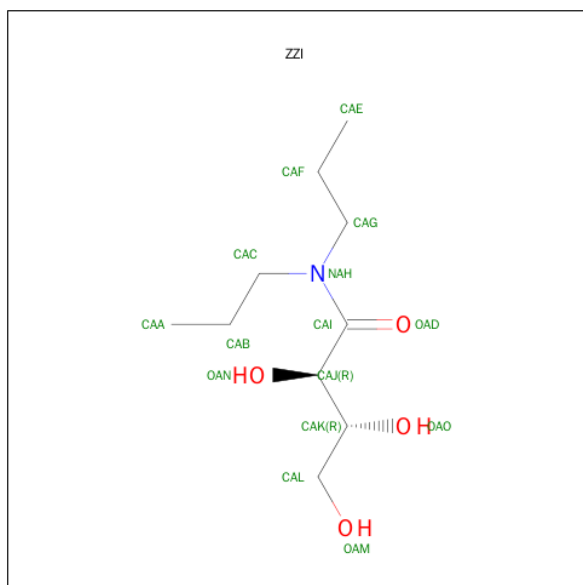
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP P0A6L4
A	-5	GLU	-	EXPRESSION TAG	UNP P0A6L4
A	-4	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-3	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-2	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	-1	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	0	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	1	HIS	-	EXPRESSION TAG	UNP P0A6L4
A	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	192	ASN	GLU	ENGINEERED MUTATION	UNP P0A6L4
C	-6	MET	-	EXPRESSION TAG	UNP P0A6L4
C	-5	GLU	-	EXPRESSION TAG	UNP P0A6L4
C	-4	HIS	-	EXPRESSION TAG	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
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	192	ASN	GLU	ENGINEERED MUTATION	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	192	ASN	GLU	ENGINEERED MUTATION	UNP P0A6L4

- Molecule 2 is (2R,3R)-2,3,4-TRIHYDROXY-N,N-DIPROPYLBUTANAMIDE (three-letter code: ZZI) (formula: C<sub>10</sub>H<sub>21</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		
2	C	1	Total	C	N	O	0	0
			15	10	1	4		
2	D	1	Total	C	N	O	0	0
			15	10	1	4		

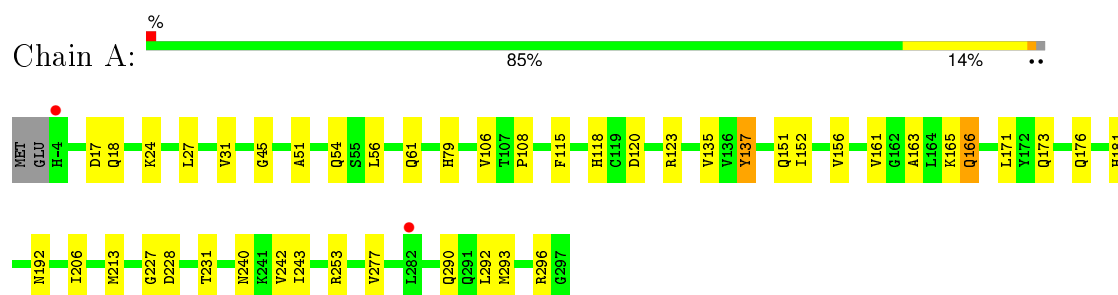
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	129	Total 129	O 129	0	0
3	C	135	Total 135	O 135	0	0
3	D	145	Total 145	O 145	0	0

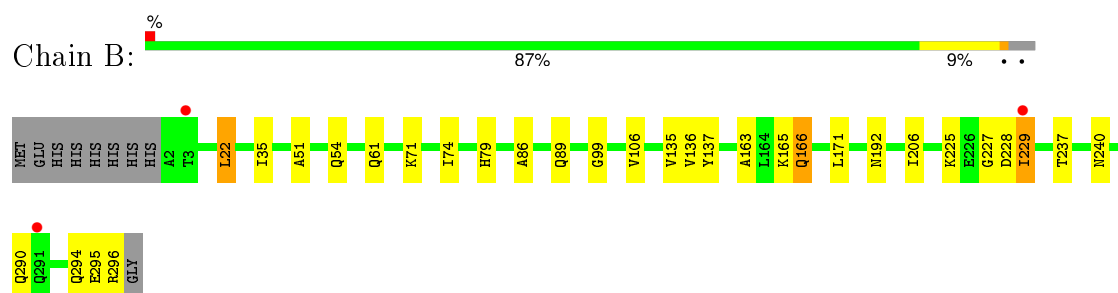
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

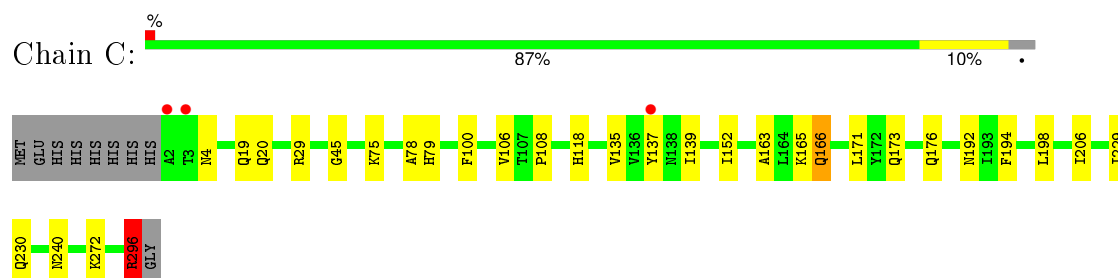
#### • Molecule 1: N-ACETYLNEURAMINATE LYASE



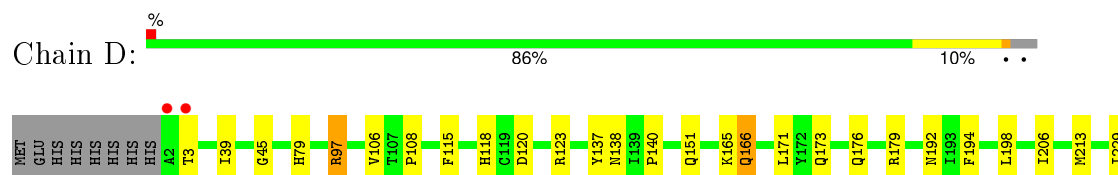
#### • Molecule 1: N-ACETYLNEURAMINATE LYASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	57.02Å 143.74Å 84.30Å 90.00° 109.90° 90.00°	Depositor
Resolution (Å)	71.88 – 2.05 71.87 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (71.88-2.05) 99.2 (71.87-2.05)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0097	Depositor
R, $R_{free}$	0.190 , 0.234 0.192 , 0.236	Depositor DCC
$R_{free}$ test set	4017 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.9	EDS
Estimated twinning fraction	0.938 for H,K,L 0.062 for -H,-K,H+L 0.119 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.938 for H,K,L 0.062 for -H,-K,H+L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 79739 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: KPI, ZZI

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	0.54	0/2412	0.62	1/3264 (0.0%)
1	B	0.58	0/2330	0.65	0/3153
1	C	0.57	0/2317	0.68	3/3136 (0.1%)
1	D	0.58	0/2323	0.68	2/3143 (0.1%)
All	All	0.57	0/9382	0.66	6/12696 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	D	97	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	29	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	29	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	296	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	17	ASP	CB-CG-OD1	5.28	123.06	118.30

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	2369	0	2374	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2296	0	2318	18	0
1	C	2289	0	2307	21	0
1	D	2292	0	2314	23	0
2	A	15	0	21	4	0
2	B	15	0	21	8	0
2	C	15	0	21	4	0
2	D	15	0	21	0	0
3	A	131	0	0	1	0
3	B	129	0	0	1	0
3	C	135	0	0	1	0
3	D	145	0	0	2	0
All	All	9846	0	9397	99	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 5.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1298:ZZI:HAF1	2:A:1298:ZZI:HAJ	1.43	1.00
2:B:1297:ZZI:HAG2	2:B:1297:ZZI:CAK	2.02	0.89
1:C:20[B]:GLN:HE22	1:C:272:LYS:H	1.15	0.88
2:B:1297:ZZI:HAK	2:B:1297:ZZI:CAG	2.02	0.88
2:B:1297:ZZI:HAK	2:B:1297:ZZI:CAF	2.08	0.83
2:C:1297:ZZI:HAJ	2:C:1297:ZZI:HAE2	1.62	0.81
1:B:229:ILE:HG21	3:D:2113:HOH:O	1.81	0.80
1:C:173:GLN:HA	1:C:176:GLN:HE21	1.50	0.76
2:B:1297:ZZI:HAK	2:B:1297:ZZI:HAF1	1.68	0.73
1:A:79:HIS:HE1	1:A:106:VAL:H	1.38	0.72
1:C:166:GLN:HE21	1:C:166:GLN:HA	1.55	0.72
1:D:97:ARG:NH2	3:D:2055:HOH:O	2.15	0.72
1:A:173:GLN:HA	1:A:176:GLN:HE21	1.56	0.70
2:B:1297:ZZI:HAK	2:B:1297:ZZI:HAG2	1.66	0.69
1:A:243:ILE:HG23	2:A:1298:ZZI:HAE2	1.75	0.68
1:C:194:PHE:CE2	1:C:198:LEU:HD11	2.29	0.67
2:B:1297:ZZI:CAK	2:B:1297:ZZI:CAG	2.66	0.66
1:C:152:ILE:HD11	3:C:2078:HOH:O	1.95	0.66
1:D:213[B]:MET:HE1	1:D:292:LEU:HD21	1.77	0.65
1:D:166:GLN:HA	1:D:166:GLN:HE21	1.63	0.63
1:A:166:GLN:HA	1:A:166:GLN:HE21	1.62	0.63
1:B:171:LEU:HD12	1:D:171:LEU:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLN:O	1:B:294:GLN:HG2	1.99	0.62
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.64	0.62
1:D:79:HIS:HE1	1:D:106:VAL:H	1.47	0.61
1:A:192:ASN:HD21	2:A:1298:ZZI:CAB	2.15	0.60
2:B:1297:ZZI:HAN	2:B:1297:ZZI:HAM	1.50	0.60
1:A:120:ASP:OD1	1:A:123:ARG:NH1	2.35	0.60
1:B:79:HIS:HE1	1:B:106:VAL:H	1.49	0.59
2:C:1297:ZZI:HAJ	2:C:1297:ZZI:CAE	2.33	0.59
1:C:296:ARG:CG	1:C:296:ARG:HH11	2.16	0.59
1:C:20[B]:GLN:NE2	1:C:272:LYS:H	1.95	0.59
1:C:79:HIS:HE1	1:C:106:VAL:H	1.51	0.58
1:B:86:ALA:HA	1:B:89:GLN:HE21	1.69	0.56
1:B:227:GLY:HA2	1:D:229:ILE:HD12	1.86	0.56
1:A:227:GLY:HA2	1:C:229:ILE:HD12	1.85	0.56
1:C:296:ARG:HG3	1:C:296:ARG:HH11	1.71	0.55
1:B:51:ALA:HA	1:B:54:GLN:HE21	1.71	0.55
1:A:51:ALA:HA	1:A:54:GLN:HE21	1.72	0.55
1:B:22:LEU:HD12	1:B:61:GLN:NE2	2.21	0.55
1:B:295:GLU:O	1:B:296:ARG:CG	2.56	0.53
1:C:19:GLN:O	1:C:20[B]:GLN:HB2	2.09	0.53
1:A:213[B]:MET:CE	1:A:292:LEU:HD21	2.39	0.52
1:A:192:ASN:HA	1:A:240:ASN:HD21	1.75	0.52
2:B:1297:ZZI:HAG2	2:B:1297:ZZI:OAO	2.09	0.52
1:C:4:ASN:HD22	1:C:75:LYS:NZ	2.09	0.51
1:A:135:VAL:HG22	1:A:163:ALA:HB3	1.93	0.51
1:D:213[B]:MET:CE	1:D:242:VAL:HG21	2.41	0.51
1:A:253:ARG:HG3	1:A:277:VAL:HG22	1.93	0.50
1:D:165:KPI:H1A	1:D:206:ILE:HG22	1.91	0.50
1:C:108:PRO:HD2	1:C:118:HIS:HD2	1.76	0.50
1:D:108:PRO:HD2	1:D:118:HIS:HD2	1.77	0.49
1:A:108:PRO:HD2	1:A:118:HIS:HD2	1.77	0.49
2:C:1297:ZZI:HAJ	2:C:1297:ZZI:CAF	2.43	0.48
1:D:138:ASN:ND2	1:D:140:PRO:HD3	2.27	0.48
1:B:237:THR:HG23	1:D:179:ARG:HD3	1.95	0.48
1:B:166:GLN:HE21	1:B:166:GLN:HA	1.78	0.48
1:C:165:KPI:H1A	1:C:206:ILE:HG22	1.95	0.48
1:D:115:PHE:CE1	1:D:151:GLN:HB3	2.50	0.47
2:A:1298:ZZI:CAF	2:A:1298:ZZI:HAJ	2.20	0.47
1:D:213[B]:MET:CE	1:D:292:LEU:HD21	2.42	0.47
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.96	0.47
1:B:295:GLU:O	1:B:296:ARG:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213[B]:MET:HE1	1:A:242:VAL:HG21	1.97	0.46
1:A:137:TYR:CD1	1:A:165:KPI:HD	2.51	0.46
1:B:136:VAL:HG12	3:B:2069:HOH:O	2.16	0.46
1:B:192:ASN:HA	1:B:240:ASN:HD21	1.82	0.45
1:C:135:VAL:HG22	1:C:163:ALA:HB3	1.98	0.45
1:D:45:GLY:O	1:D:79:HIS:HD2	2.00	0.45
1:A:45:GLY:O	1:A:79:HIS:HD2	2.00	0.44
1:A:228:ASP:OD2	1:A:231:THR:OG1	2.26	0.44
1:D:137:TYR:CD1	1:D:165:KPI:HD	2.52	0.44
1:D:236:GLN:HE21	1:D:240:ASN:ND2	2.15	0.44
1:A:115:PHE:CE1	1:A:151:GLN:HB3	2.53	0.44
1:D:213[B]:MET:HE3	1:D:242:VAL:HG11	1.99	0.44
1:A:290:GLN:HA	1:A:293:MET:HE3	2.00	0.44
1:A:152:ILE:O	1:A:156:VAL:HG22	2.18	0.43
1:D:236:GLN:HE21	1:D:240:ASN:HD21	1.65	0.43
1:A:213[B]:MET:HE2	1:A:292:LEU:HD21	2.01	0.43
1:A:24:LYS:CE	1:A:61[A]:GLN:NE2	2.81	0.43
1:B:165:KPI:H1A	1:B:206:ILE:HG22	2.01	0.43
1:B:135:VAL:HG22	1:B:163:ALA:HB3	1.99	0.43
1:C:78:ALA:HB2	1:C:100:PHE:CD2	2.54	0.43
1:C:192:ASN:HA	1:C:240:ASN:HD21	1.84	0.43
1:D:194:PHE:CE2	1:D:198:LEU:HD11	2.55	0.42
1:B:71:LYS:HE2	1:B:99:GLY:HA3	2.01	0.42
1:A:156:VAL:HA	1:A:161:VAL:HG11	2.01	0.42
1:A:165:KPI:H1A	1:A:206:ILE:HG22	2.01	0.42
1:B:35:ILE:HG12	1:B:74:ILE:HD13	2.02	0.42
1:C:45:GLY:O	1:C:79:HIS:HD2	2.02	0.42
1:D:192:ASN:HA	1:D:240:ASN:HD21	1.84	0.42
1:A:213[B]:MET:HE3	1:A:213[B]:MET:HB3	1.76	0.41
1:A:181:HIS:HD2	3:A:2028:HOH:O	2.03	0.41
2:C:1297:ZZI:OAO	2:C:1297:ZZI:HAG1	2.20	0.41
1:D:39:ILE:HA	1:D:39:ILE:HD12	1.93	0.41
1:C:139:ILE:O	1:C:139:ILE:HG23	2.20	0.41
1:D:120:ASP:OD1	1:D:123:ARG:NH1	2.52	0.41
1:C:194:PHE:CZ	1:C:198:LEU:HD11	2.56	0.40
1:A:27:LEU:O	1:A:31:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/304 (100%)	296 (98%)	7 (2%)	0	100	100
1	B	295/304 (97%)	288 (98%)	7 (2%)	0	100	100
1	C	293/304 (96%)	286 (98%)	7 (2%)	0	100	100
1	D	294/304 (97%)	288 (98%)	5 (2%)	1 (0%)	46	36
All	All	1185/1216 (98%)	1158 (98%)	26 (2%)	1 (0%)	56	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	THR

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/250 (101%)	247 (98%)	5 (2%)	63	58
1	B	245/250 (98%)	239 (98%)	6 (2%)	57	50
1	C	243/250 (97%)	239 (98%)	4 (2%)	70	67
1	D	243/250 (97%)	240 (99%)	3 (1%)	78	76
All	All	983/1000 (98%)	965 (98%)	18 (2%)	66	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	56	LEU
1	A	137	TYR
1	A	166	GLN
1	A	296	ARG
1	B	22	LEU
1	B	137	TYR
1	B	166	GLN
1	B	225	LYS
1	B	228	ASP
1	B	229	ILE
1	C	137	TYR
1	C	166	GLN
1	C	230	GLN
1	C	296	ARG
1	D	166	GLN
1	D	230	GLN
1	D	234	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	79	HIS
1	A	118	HIS
1	A	138	ASN
1	A	166	GLN
1	A	176	GLN
1	A	181	HIS
1	A	192	ASN
1	A	240	ASN
1	A	260	HIS
1	B	32	GLN
1	B	37	GLN
1	B	54	GLN
1	B	61	GLN
1	B	79	HIS
1	B	89	GLN
1	B	118	HIS
1	B	138	ASN
1	B	166	GLN
1	B	181	HIS
1	B	240	ASN

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Mol	Chain	Res	Type
1	B	260	HIS
1	C	4	ASN
1	C	37	GLN
1	C	79	HIS
1	C	89	GLN
1	C	118	HIS
1	C	138	ASN
1	C	166	GLN
1	C	176	GLN
1	C	181	HIS
1	C	218	GLN
1	C	230	GLN
1	C	240	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	230	GLN
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	A	165	1	10,13,14	1.43	1 (10%)	9,15,17	0.75	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KPI	B	165	1	10,13,14	1.65	1 (10%)	9,15,17	0.91	0
1	KPI	C	165	1	10,13,14	1.72	1 (10%)	9,15,17	0.86	0
1	KPI	D	165	1	10,13,14	1.74	1 (10%)	9,15,17	0.87	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
1	KPI	A	165	1	-	0/8/14/16	0/0/0/0
1	KPI	B	165	1	-	0/8/14/16	0/0/0/0
1	KPI	C	165	1	-	0/8/14/16	0/0/0/0
1	KPI	D	165	1	-	0/8/14/16	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	KPI	CX1-NZ	3.97	1.35	1.29
1	B	165	KPI	CX1-NZ	4.33	1.35	1.29
1	C	165	KPI	CX1-NZ	4.65	1.36	1.29
1	D	165	KPI	CX1-NZ	5.02	1.37	1.29

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	165	KPI	2	0
1	B	165	KPI	1	0
1	C	165	KPI	1	0
1	D	165	KPI	2	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands 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
2	ZZI	A	1298	-	14,14,14	0.89	1 (7%)	14,17,17	0.80	0
2	ZZI	B	1297	-	14,14,14	1.39	2 (14%)	14,17,17	1.43	2 (14%)
2	ZZI	C	1297	-	14,14,14	0.62	0	14,17,17	0.61	0
2	ZZI	D	1297	-	14,14,14	0.76	1 (7%)	14,17,17	0.75	1 (7%)

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	ZZI	A	1298	-	-	0/20/20/20	0/0/0/0
2	ZZI	B	1297	-	-	0/20/20/20	0/0/0/0
2	ZZI	C	1297	-	-	0/20/20/20	0/0/0/0
2	ZZI	D	1297	-	-	0/20/20/20	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1297	ZZI	CAJ-CAI	2.05	1.55	1.53
2	A	1298	ZZI	OAN-CAJ	2.32	1.46	1.42
2	B	1297	ZZI	CAK-CAJ	3.16	1.56	1.53
2	B	1297	ZZI	CAJ-CAI	3.54	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1297	ZZI	OAN-CAJ-CAI	2.07	111.81	108.53
2	B	1297	ZZI	CAK-CAJ-CAI	3.15	117.14	110.10
2	B	1297	ZZI	CAL-CAK-CAJ	3.65	118.02	111.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1298	ZZI	4	0
2	B	1297	ZZI	8	0
2	C	1297	ZZI	4	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	301/304 (99%)	-0.31	2 (0%) 89 91	19, 28, 46, 67	0
1	B	294/304 (96%)	-0.31	3 (1%) 84 87	19, 27, 39, 58	0
1	C	294/304 (96%)	-0.39	3 (1%) 84 87	16, 25, 40, 54	0
1	D	294/304 (96%)	-0.39	2 (0%) 89 91	16, 25, 39, 55	0
All	All	1183/1216 (97%)	-0.35	10 (0%) 87 90	16, 26, 41, 67	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	6.5
1	C	3	THR	4.3
1	A	-4	HIS	3.7
1	B	3	THR	3.4
1	B	229	ILE	2.8
1	A	282	LEU	2.7
1	D	3	THR	2.4
1	D	2	ALA	2.3
1	B	291	GLN	2.3
1	C	137	TYR	2.1

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	C	165	14/15	0.93	0.14	-	23,24,27,27	0
1	KPI	A	165	14/15	0.95	0.11	-	19,20,23,23	0
1	KPI	D	165	14/15	0.93	0.12	-	22,24,28,29	0
1	KPI	B	165	14/15	0.93	0.14	-	18,22,24,24	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZZI	C	1297	15/15	0.59	0.30	15.41	44,58,61,62	0
2	ZZI	A	1298	15/15	0.78	0.22	9.83	34,42,44,45	0
2	ZZI	B	1297	15/15	0.73	0.26	8.87	44,54,56,56	0
2	ZZI	D	1297	15/15	0.86	0.20	7.78	41,48,50,50	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.