



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:02 PM UTC

PDB ID : 4AH7 / pdb_00004ah7
Title : Structure of Wild Type Staphylococcus aureus N-acetylneuraminic acid lyase
in complex with pyruvate
Authors : Timms, N.; Poyakova, A.; Windle, C.L.; Trinh, C.H.; Nelson, A.; Pearson,
A.R.; Berry, A.
Deposited on : 2012-02-03
Resolution : 2.30 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

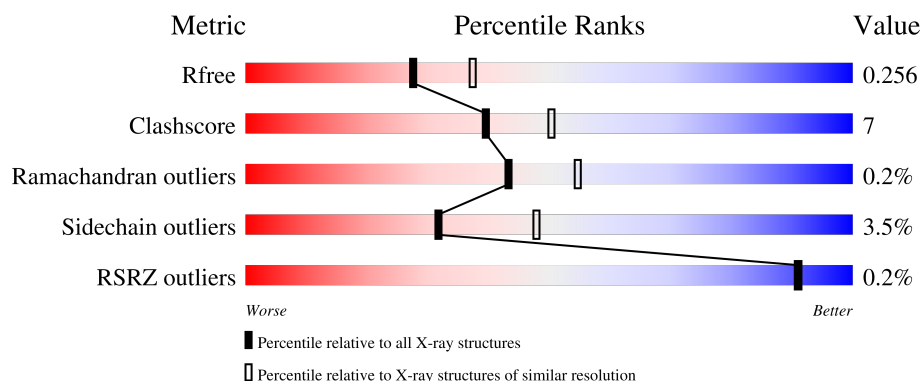
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	298	
1	B	298	
1	C	298	
1	D	298	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9332 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	293	Total	C	N	O	S	0	0	0
			2310	1477	387	443	3			
1	B	295	Total	C	N	O	S	0	0	0
			2315	1486	392	434	3			
1	C	292	Total	C	N	O	S	0	0	0
			2281	1466	381	431	3			
1	D	291	Total	C	N	O	S	0	0	0
			2296	1474	381	438	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP Q2G160
A	-3	HIS	-	expression tag	UNP Q2G160
A	-2	HIS	-	expression tag	UNP Q2G160
A	-1	HIS	-	expression tag	UNP Q2G160
A	0	HIS	-	expression tag	UNP Q2G160
A	1	HIS	-	expression tag	UNP Q2G160
B	-4	HIS	-	expression tag	UNP Q2G160
B	-3	HIS	-	expression tag	UNP Q2G160
B	-2	HIS	-	expression tag	UNP Q2G160
B	-1	HIS	-	expression tag	UNP Q2G160
B	0	HIS	-	expression tag	UNP Q2G160
B	1	HIS	-	expression tag	UNP Q2G160
C	-4	HIS	-	expression tag	UNP Q2G160
C	-3	HIS	-	expression tag	UNP Q2G160
C	-2	HIS	-	expression tag	UNP Q2G160
C	-1	HIS	-	expression tag	UNP Q2G160
C	0	HIS	-	expression tag	UNP Q2G160
C	1	HIS	-	expression tag	UNP Q2G160
D	-4	HIS	-	expression tag	UNP Q2G160
D	-3	HIS	-	expression tag	UNP Q2G160
D	-2	HIS	-	expression tag	UNP Q2G160

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	HIS	-	expression tag	UNP Q2G160
D	0	HIS	-	expression tag	UNP Q2G160
D	1	HIS	-	expression tag	UNP Q2G160

- Molecule 2 is water.

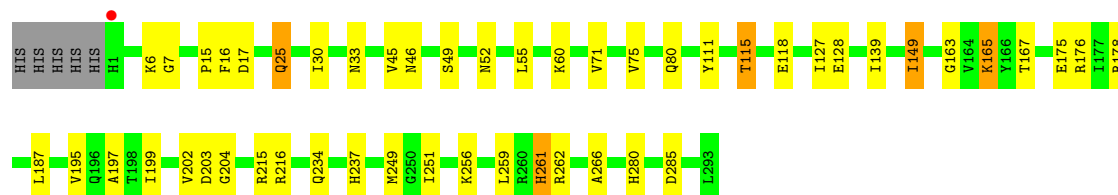
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total 37	O 37	0	0
2	B	33	Total 33	O 33	0	0
2	C	24	Total 24	O 24	0	0
2	D	36	Total 36	O 36	0	0

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: N-ACETYLNEURAMINATE LYASE

Chain A: 



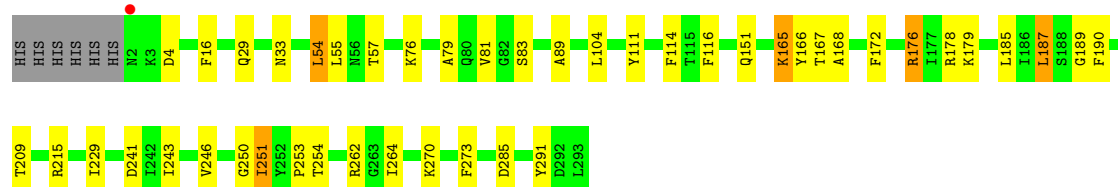
• Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain B: 



• Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain C: 



• Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.29Å 109.86Å 131.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.93 – 2.30 54.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (54.93-2.30) 99.2 (54.93-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.259 0.203 , 0.256	Depositor DCC
R_{free} test set	2659 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9332	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% 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: KPI

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	0.91	2/2338 (0.1%)	1.06	4/3163 (0.1%)
1	B	0.95	2/2346 (0.1%)	1.05	2/3177 (0.1%)
1	C	0.90	1/2309 (0.0%)	1.05	5/3128 (0.2%)
1	D	0.95	4/2324 (0.2%)	1.07	2/3145 (0.1%)
All	All	0.93	9/9317 (0.1%)	1.05	13/12613 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	ASP	C-N	-10.49	1.20	1.33
1	A	285	ASP	C-N	-7.41	1.24	1.33
1	D	285	ASP	C-N	-6.48	1.25	1.33
1	B	285	ASP	C-N	-5.86	1.26	1.33
1	D	158	HIS	CG-CD2	5.65	1.42	1.35
1	A	261	HIS	CG-CD2	5.57	1.42	1.35
1	B	280	HIS	CG-CD2	5.17	1.41	1.35
1	D	158	HIS	ND1-CE1	5.15	1.37	1.32
1	D	280	HIS	CG-CD2	5.06	1.41	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	THR	N-CA-C	6.67	118.20	111.07
1	C	251	ILE	N-CA-C	6.51	116.62	110.30
1	C	172	PHE	N-CA-C	-6.39	103.61	111.40
1	A	251	ILE	N-CA-C	6.35	116.52	110.42
1	D	163	GLY	N-CA-C	6.32	119.09	110.69
1	B	153	SER	N-CA-C	-5.80	104.86	111.07
1	D	207	GLY	N-CA-C	5.80	120.72	110.80
1	A	163	GLY	N-CA-C	5.78	118.38	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	SER	N-CA-C	5.58	118.12	111.71
1	B	207	GLY	N-CA-C	5.34	119.10	110.87
1	A	45	VAL	N-CA-C	5.28	116.19	108.53
1	C	81	VAL	CB-CA-C	-5.17	105.35	111.65
1	C	114	PHE	N-CA-C	5.01	117.16	110.35

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	2310	0	2272	31	0
1	B	2315	0	2270	40	0
1	C	2281	0	2241	29	0
1	D	2296	0	2266	27	0
2	A	37	0	0	2	0
2	B	33	0	0	2	0
2	C	24	0	0	1	0
2	D	36	0	0	0	0
All	All	9332	0	9049	123	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 7.

All (123) 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:115:THR:HG22	1:A:118:GLU:H	1.34	0.92
1:B:71:VAL:HG11	1:B:75:VAL:HG11	1.55	0.87
1:B:71:VAL:CG1	1:B:75:VAL:HG21	2.08	0.84
1:B:256:LYS:HE3	2:B:2030:HOH:O	1.78	0.84
1:C:33:ASN:HD21	1:C:262:ARG:HH11	1.27	0.82
1:D:33:ASN:HD21	1:D:262:ARG:HH11	1.32	0.78
1:B:221:PHE:O	1:B:225:ARG:HG3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:HD21	1:A:262:ARG:HH11	1.30	0.77
1:C:178:ARG:HD3	1:C:178:ARG:O	1.89	0.72
1:C:4:ASP:O	1:C:76:LYS:CE	2.37	0.72
1:A:52:ASN:HA	1:A:55:LEU:HD12	1.74	0.69
1:D:175:GLU:OE1	1:D:176:ARG:HD3	1.92	0.69
1:B:33:ASN:HD21	1:B:262:ARG:HH11	1.42	0.67
1:A:178:ARG:O	1:A:178:ARG:HD3	1.95	0.66
1:B:71:VAL:HG11	1:B:75:VAL:HG21	1.78	0.64
1:A:71:VAL:HB	1:A:75:VAL:HG21	1.79	0.64
1:C:4:ASP:O	1:C:76:LYS:HE2	1.97	0.63
1:C:4:ASP:O	1:C:76:LYS:HE3	1.98	0.63
1:C:185:LEU:HD21	1:C:187:LEU:HD22	1.80	0.63
1:B:71:VAL:HG11	1:B:75:VAL:CG1	2.27	0.62
1:B:178:ARG:O	1:B:178:ARG:HD3	2.00	0.61
1:D:253:PRO:HB3	1:D:269:PRO:HG3	1.80	0.61
1:C:178:ARG:HD3	1:C:178:ARG:C	2.26	0.60
1:A:46:ASN:O	1:A:80:GLN:HB3	2.01	0.60
1:B:68:LYS:HE2	1:B:99:LEU:O	2.03	0.59
1:C:250:GLY:O	1:C:253:PRO:HD2	2.03	0.58
1:B:167:THR:HG22	1:B:189:GLY:HA3	1.85	0.58
1:C:29:GLN:HB3	1:C:264:ILE:HG12	1.87	0.57
1:D:178:ARG:O	1:D:178:ARG:HD3	2.05	0.57
1:C:270:LYS:O	1:C:273:PHE:HB2	2.04	0.57
1:A:175:GLU:OE1	1:A:176:ARG:HD3	2.04	0.57
1:A:178:ARG:HD3	1:A:178:ARG:C	2.28	0.57
1:D:4:ASP:O	1:D:76:LYS:NZ	2.38	0.57
1:A:199:ILE:HB	1:C:229:ILE:HD11	1.86	0.56
1:B:178:ARG:HD3	1:B:178:ARG:C	2.28	0.56
1:B:71:VAL:CG1	1:B:75:VAL:CG2	2.83	0.54
1:B:71:VAL:HG12	1:B:72:GLY:N	2.23	0.54
1:D:46:ASN:HB3	1:D:52:ASN:ND2	2.23	0.54
1:D:175:GLU:OE1	1:D:176:ARG:CD	2.56	0.54
1:D:64:PHE:CE1	1:D:79:ALA:HB1	2.42	0.54
1:C:185:LEU:HD21	1:C:187:LEU:CD2	2.38	0.54
1:A:175:GLU:OE1	1:A:176:ARG:CD	2.57	0.53
1:B:167:THR:O	1:B:190:PHE:CE2	2.63	0.52
1:B:209:THR:HG21	1:B:243:ILE:HG12	1.91	0.52
1:B:131:GLN:O	1:B:160:LYS:HE2	2.10	0.52
1:C:185:LEU:CD2	1:C:187:LEU:HD22	2.40	0.51
1:C:79:ALA:HB3	1:C:104:LEU:HD23	1.91	0.51
2:A:2026:HOH:O	1:C:179:LYS:HE3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ILE:HA	1:A:167:THR:OG1	2.10	0.50
1:B:68:LYS:CE	1:B:99:LEU:O	2.60	0.50
1:C:167:THR:HG22	1:C:189:GLY:HA3	1.94	0.50
1:D:139:ILE:HA	1:D:167:THR:OG1	2.12	0.49
1:A:6:LYS:HG2	1:A:203:ASP:HB3	1.95	0.49
1:A:30:ILE:HG12	1:A:259:LEU:HD13	1.93	0.49
1:D:223:LEU:HB3	1:D:228:GLN:HB2	1.93	0.49
1:D:167:THR:HG22	1:D:189:GLY:HA3	1.95	0.49
1:D:115:THR:OG1	1:D:118:GLU:HG3	2.14	0.48
1:B:71:VAL:HG11	1:B:75:VAL:CB	2.43	0.48
1:C:166:TYR:CZ	1:C:168:ALA:HB3	2.49	0.48
1:D:260:ARG:HA	1:D:264:ILE:O	2.14	0.48
1:B:46:ASN:O	1:B:80:GLN:HB3	2.15	0.47
1:C:246:VAL:HG13	1:C:254:THR:HB	1.95	0.47
1:B:27:LEU:HD23	1:B:66:VAL:HB	1.96	0.47
1:C:116:PHE:CE1	1:C:151:GLN:HB3	2.50	0.46
1:B:241:ASP:OD1	1:D:176:ARG:NH2	2.30	0.46
1:C:176:ARG:HA	1:C:176:ARG:HD2	1.40	0.46
1:A:234:GLN:O	1:A:237:HIS:HB2	2.16	0.46
1:C:165:KPI:H1B	2:C:2011:HOH:O	2.15	0.46
1:B:17:ASP:OD1	1:B:17:ASP:C	2.59	0.46
1:B:241:ASP:OD2	1:B:291:TYR:OH	2.29	0.46
1:D:176:ARG:HA	1:D:176:ARG:HD2	1.52	0.46
1:A:178:ARG:NH2	1:A:203:ASP:OD2	2.47	0.45
1:B:71:VAL:HG11	1:B:75:VAL:CG2	2.44	0.45
1:B:290:LYS:HE2	1:B:291:TYR:CZ	2.50	0.45
1:A:197:ALA:O	1:A:202:VAL:HG13	2.17	0.45
1:B:10:ALA:HB2	1:B:40:LEU:HD13	1.99	0.45
1:B:178:ARG:C	1:B:178:ARG:CD	2.90	0.45
1:D:178:ARG:O	1:D:178:ARG:CD	2.64	0.45
1:C:167:THR:O	1:C:190:PHE:CE2	2.70	0.45
1:A:52:ASN:ND2	1:A:60:LYS:HG2	2.32	0.44
1:B:178:ARG:O	1:B:178:ARG:CD	2.65	0.44
1:B:59:GLN:O	1:B:62:GLN:HB3	2.18	0.44
1:A:115:THR:HG22	1:A:118:GLU:N	2.17	0.44
1:D:9:TYR:HB2	1:D:206:ILE:HG12	1.99	0.44
1:A:16:PHE:CZ	1:A:55:LEU:HD21	2.54	0.43
1:A:256:LYS:HB3	1:A:266:ALA:HB1	2.00	0.43
1:B:176:ARG:HA	1:B:176:ARG:HD2	1.67	0.43
1:A:195:VAL:O	1:A:199:ILE:HG23	2.18	0.43
1:D:168:ALA:O	1:D:190:PHE:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ASP:OD2	1:C:291:TYR:OH	2.32	0.43
1:D:5:LEU:HD23	1:D:5:LEU:HA	1.87	0.43
1:A:165:KPI:H1B	2:A:2012:HOH:O	2.18	0.42
1:B:221:PHE:O	1:B:225:ARG:CG	2.60	0.42
1:D:290:LYS:HD3	1:D:291:TYR:CE2	2.54	0.42
1:A:17:ASP:C	1:A:17:ASP:OD1	2.62	0.42
1:D:158:HIS:CE1	1:D:160:LYS:HB2	2.54	0.42
1:B:44:TYR:CD1	1:B:206:ILE:HD13	2.54	0.42
1:B:112:TYR:CE2	1:C:54:LEU:HD13	2.54	0.42
1:B:132:ASN:OD1	1:B:133:ASN:N	2.51	0.42
1:C:246:VAL:HG12	1:C:251:ILE:HA	2.02	0.42
1:A:7:GLY:O	1:A:204:GLY:HA3	2.20	0.42
1:B:28:LYS:O	1:B:32:GLN:HG3	2.18	0.42
1:A:25:GLN:H	1:A:25:GLN:CD	2.28	0.41
1:C:83:SER:HB3	1:C:89:ALA:HB2	2.02	0.41
1:A:149:ILE:H	1:A:149:ILE:HG13	1.61	0.41
1:D:127:ILE:HD11	1:D:161:ILE:HG13	2.02	0.41
1:A:127:ILE:O	1:A:128:GLU:C	2.61	0.41
1:D:10:ALA:HB2	1:D:40:LEU:CD1	2.50	0.41
1:B:112:TYR:HE2	1:C:54:LEU:HD13	1.86	0.41
1:D:79:ALA:HB2	1:D:101:TYR:CD2	2.56	0.41
1:D:107:VAL:HA	1:D:137:TYR:HB3	2.01	0.41
1:B:71:VAL:CG1	1:B:72:GLY:N	2.82	0.41
1:D:12:LEU:HD21	1:D:27:LEU:HD11	2.01	0.41
1:A:176:ARG:HA	1:A:176:ARG:HD2	1.69	0.41
1:B:163:GLY:HA3	1:B:185:LEU:O	2.20	0.41
1:B:165:KPI:H1B	2:B:2014:HOH:O	2.21	0.41
1:A:33:ASN:HD21	1:A:262:ARG:NH1	2.06	0.40
1:A:15:PRO:HD3	1:A:30:ILE:HD12	2.02	0.40
1:A:249:MET:HE2	1:A:280:HIS:HB3	2.03	0.40
1:C:209:THR:HG21	1:C:243:ILE:HG12	2.03	0.40
1:B:61:LYS:NZ	1:B:91:GLU:OE2	2.55	0.40
1:D:7:GLY:O	1:D:204:GLY:HA3	2.22	0.40
1:C:16:PHE:CE2	1:C:55:LEU:HD21	2.56	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	290/298 (97%)	285 (98%)	4 (1%)	1 (0%)	36	46
1	B	292/298 (98%)	285 (98%)	7 (2%)	0	100	100
1	C	289/298 (97%)	279 (96%)	9 (3%)	1 (0%)	36	46
1	D	288/298 (97%)	282 (98%)	6 (2%)	0	100	100
All	All	1159/1192 (97%)	1131 (98%)	26 (2%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	111	TYR
1	A	111	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/253 (95%)	233 (97%)	7 (3%)	37	55
1	B	237/253 (94%)	227 (96%)	10 (4%)	26	40
1	C	234/253 (92%)	230 (98%)	4 (2%)	53	72
1	D	239/253 (94%)	227 (95%)	12 (5%)	22	33
All	All	950/1012 (94%)	917 (96%)	33 (4%)	32	48

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	115	THR
1	A	149	ILE
1	A	187	LEU
1	A	215	ARG
1	A	216	ARG
1	A	261	HIS
1	B	25	GLN
1	B	160	LYS
1	B	162	VAL
1	B	173	LEU
1	B	176	ARG
1	B	178	ARG
1	B	187	LEU
1	B	215	ARG
1	B	228	GLN
1	B	261	HIS
1	C	54	LEU
1	C	176	ARG
1	C	187	LEU
1	C	215	ARG
1	D	4	ASP
1	D	54	LEU
1	D	73	ASP
1	D	76	LYS
1	D	176	ARG
1	D	178	ARG
1	D	187	LEU
1	D	190	PHE
1	D	215	ARG
1	D	218	ARG
1	D	246	VAL
1	D	260	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	52	ASN
1	A	226	GLN
1	B	33	ASN
1	B	261	HIS
1	C	33	ASN

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Mol	Chain	Res	Type
1	C	52	ASN
1	D	33	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	C	165	1	11,13,14	1.32	2 (18%)	9,15,17	3.63	3 (33%)
1	KPI	A	165	1	11,13,14	1.53	2 (18%)	9,15,17	1.69	1 (11%)
1	KPI	B	165	1	11,13,14	1.58	2 (18%)	9,15,17	2.02	2 (22%)
1	KPI	D	165	1	11,13,14	1.35	1 (9%)	9,15,17	1.98	3 (33%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	KPI	CX2-CX1	4.07	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	165	KPI	CX2-CX1	3.19	1.53	1.49
1	A	165	KPI	CX2-CX1	3.07	1.53	1.49
1	C	165	KPI	C1-CX1	2.78	1.55	1.49
1	A	165	KPI	C1-CX1	2.65	1.55	1.49
1	C	165	KPI	CX2-CX1	2.36	1.52	1.49
1	B	165	KPI	C1-CX1	2.07	1.53	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	KPI	O2-CX2-CX1	-9.58	109.64	121.35
1	B	165	KPI	O2-CX2-CX1	-5.07	115.15	121.35
1	A	165	KPI	O2-CX2-CX1	-4.10	116.34	121.35
1	D	165	KPI	O2-CX2-CX1	-4.04	116.42	121.35
1	C	165	KPI	O1-CX2-CX1	3.71	124.40	116.50
1	C	165	KPI	C1-CX1-CX2	3.11	121.05	118.11
1	D	165	KPI	C1-CX1-CX2	3.07	121.01	118.11
1	B	165	KPI	O1-CX2-CX1	2.50	121.82	116.50
1	D	165	KPI	CD-CE-NZ	-2.07	107.00	110.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	165	KPI	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	285:ASP	C	286:GLN	N	1.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	292/298 (97%)	-0.34	1 (0%) 90 90	11, 18, 27, 44	0
1	B	294/298 (98%)	-0.36	0 100 100	10, 17, 25, 33	0
1	C	291/298 (97%)	-0.22	1 (0%) 90 90	11, 19, 31, 42	0
1	D	290/298 (97%)	-0.42	0 100 100	10, 15, 24, 44	0
All	All	1167/1192 (97%)	-0.33	2 (0%) 91 91	10, 17, 27, 44	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ASN	2.1
1	A	1	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KPI	C	165	14/15	0.94	0.07	13,14,16,18	0
1	KPI	A	165	14/15	0.95	0.07	12,13,14,14	0
1	KPI	B	165	14/15	0.96	0.06	11,12,14,14	0
1	KPI	D	165	14/15	0.96	0.06	11,11,13,13	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.