



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:25 AM UTC

PDB ID : 2WNN / pdb_00002wnn
Title : Structure of wild type E. coli N-acetylneuraminic acid lyase in complex with pyruvate in space group P21
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 : 2009-07-13
Resolution : 1.65 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

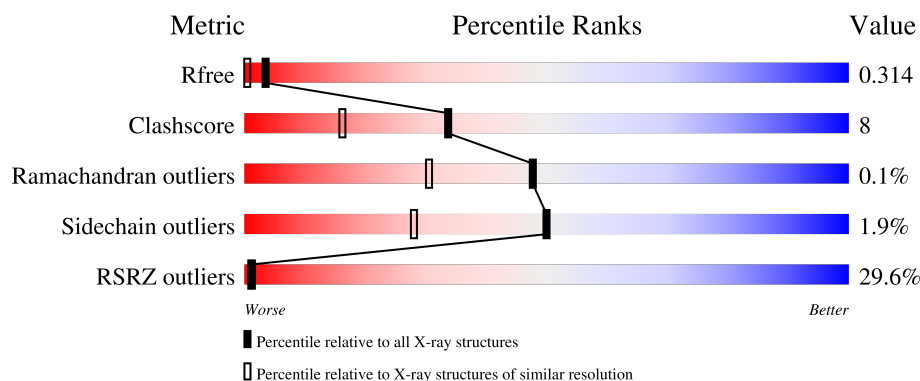
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	303	41% 80% 17% ..
1	B	303	31% 79% 18% .
1	C	303	24% 81% 16% ..
1	D	303	19% 82% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9955 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	296	Total	C	N	O	S	0	2	0
			2298	1467	389	431	11			
1	B	295	Total	C	N	O	S	0	5	0
			2300	1467	384	438	11			
1	C	295	Total	C	N	O	S	0	0	0
			2271	1448	383	430	10			
1	D	297	Total	C	N	O	S	0	2	0
			2297	1464	387	435	11			

There are 32 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
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
C	-6	MET	-	expression tag	UNP P0A6L4
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

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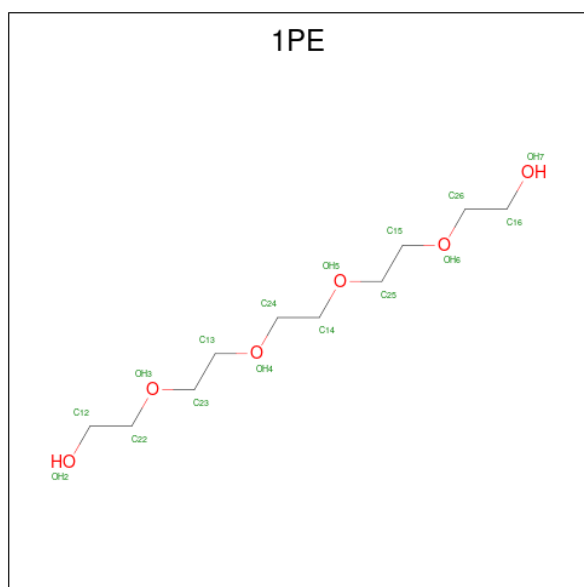
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP P0A6L4
C	0	HIS	-	expression tag	UNP P0A6L4
C	1	HIS	-	expression tag	UNP P0A6L4
D	-6	MET	-	expression tag	UNP P0A6L4
D	-5	GLU	-	expression tag	UNP P0A6L4
D	-4	HIS	-	expression 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

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 7 5 2	0	0
3	B	1	Total C O 16 10 6	0	0

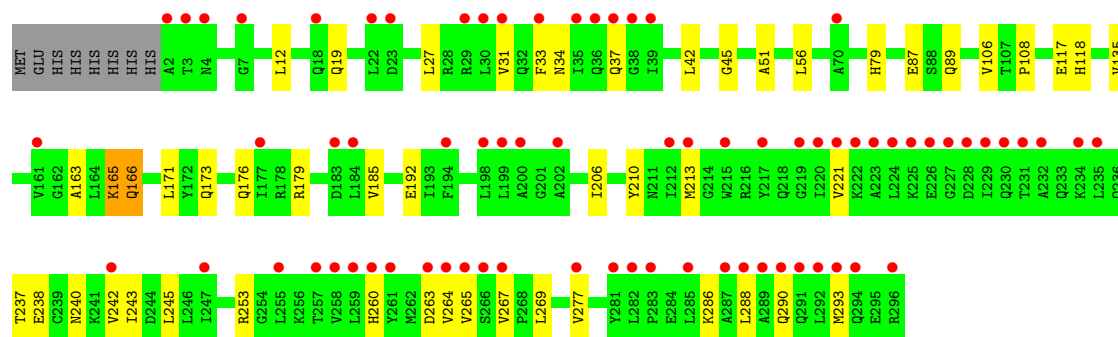
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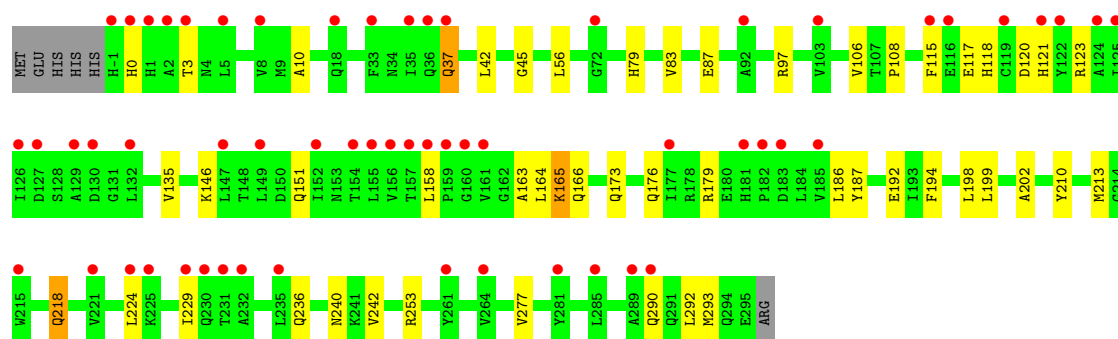
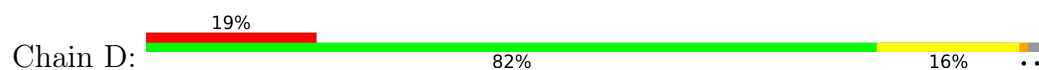
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			7	5	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total	O	0	0
			172	172		
4	B	195	Total	O	0	0
			195	195		
4	C	188	Total	O	0	0
			188	188		
4	D	203	Total	O	0	0
			203	203		



● 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	54.69Å 142.46Å 83.63Å 90.00° 109.16° 90.00°	Depositor
Resolution (Å)	79.07 – 1.65 78.99 – 1.65	Depositor EDS
% Data completeness (in resolution range)	90.6 (79.07-1.65) 94.2 (78.99-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.5.0097	Depositor
R, R_{free}	0.210 , 0.249 0.266 , 0.314	Depositor DCC
R_{free} test set	15656 reflections (10.77%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.666 for H,K,L 0.334 for -H,-K,H+L	Depositor
Outliers	0 of 136539 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9955	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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, NA, 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	0.73	0/2332	0.92	2/3157 (0.1%)
1	B	0.74	0/2340	0.96	2/3166 (0.1%)
1	C	0.82	0/2296	0.94	2/3108 (0.1%)
1	D	0.79	0/2329	0.92	1/3151 (0.0%)
All	All	0.77	0/9297	0.94	7/12582 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	185	VAL	N-CA-C	-5.70	101.32	108.84
1	B	83	VAL	N-CA-C	-5.53	105.11	110.42
1	B	7	GLY	N-CA-C	5.50	119.02	110.88
1	A	196	SER	N-CA-C	5.34	117.11	111.28
1	C	89	GLN	N-CA-C	5.24	116.68	111.07
1	D	83	VAL	N-CA-C	-5.07	105.77	110.53
1	A	207	GLY	N-CA-C	5.02	120.17	111.14

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	2298	0	2312	40	0
1	B	2300	0	2315	41	0
1	C	2271	0	2279	33	0
1	D	2297	0	2309	39	0
2	B	1	0	0	0	0
3	B	23	0	28	7	0
3	C	7	0	6	2	0
4	A	172	0	0	3	0
4	B	195	0	0	3	0
4	C	188	0	0	4	0
4	D	203	0	0	3	0
All	All	9955	0	9249	142	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 8.

All (142) 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:33:PHE:CD2	1:A:264:VAL:HG13	2.05	0.91
1:D:97:ARG:NH2	4:D:2094:HOH:O	2.12	0.82
1:C:79:HIS:HE1	1:C:106:VAL:H	1.27	0.80
1:A:179:ARG:HD3	1:C:237:THR:HG23	1.67	0.77
1:D:0:HIS:O	1:D:3:THR:HG22	1.84	0.76
1:A:0:HIS:O	1:A:3:THR:HG22	1.85	0.76
1:D:194:PHE:CE2	1:D:198:LEU:HD11	2.20	0.76
1:B:139:ILE:HD12	1:B:167:THR:HG21	1.68	0.76
1:B:79:HIS:HE1	1:B:106:VAL:H	1.33	0.74
1:D:213[B]:MET:HE1	1:D:242:VAL:HG21	1.69	0.74
1:D:135:VAL:HG22	1:D:163:ALA:HB3	1.70	0.74
1:C:171:LEU:H	3:C:1297:1PE:C24	2.01	0.73
1:B:237:THR:HG23	1:D:179:ARG:HD3	1.70	0.73
1:A:33:PHE:CE2	1:A:264:VAL:HG22	2.24	0.72
1:D:253:ARG:HG3	1:D:277:VAL:HG22	1.72	0.71
1:B:170:ASP:OD2	3:B:1299:1PE:OH7	2.07	0.70
1:A:33:PHE:CE2	1:A:264:VAL:HG13	2.27	0.70
1:B:236:GLN:HE21	1:B:240:ASN:HD21	1.39	0.70
1:B:170:ASP:HB3	3:B:1299:1PE:H261	1.75	0.68
1:C:173:GLN:HA	1:C:176:GLN:HE21	1.60	0.67
1:A:171:LEU:HD12	1:C:171:LEU:HD12	1.77	0.66
1:B:173:GLN:HA	1:B:176:GLN:HE21	1.62	0.64
1:A:169:GLY:HA3	3:C:1297:1PE:H131	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLN:NE2	4:C:2008:HOH:O	2.31	0.63
1:C:108:PRO:HD2	1:C:118:HIS:HD2	1.64	0.62
1:A:33:PHE:CZ	1:A:264:VAL:HG22	2.34	0.62
1:B:170:ASP:CB	3:B:1299:1PE:H261	2.30	0.61
1:D:236:GLN:HE21	1:D:240:ASN:ND2	1.98	0.61
1:A:79:HIS:HE1	1:A:106:VAL:H	1.47	0.61
1:B:199:LEU:HD22	1:D:199:LEU:HD22	1.81	0.60
1:A:179:ARG:HD2	4:A:2130:HOH:O	2.00	0.60
1:A:156:VAL:HA	1:A:161:VAL:HG11	1.83	0.60
1:A:33:PHE:CD2	1:A:264:VAL:CG1	2.81	0.60
1:B:36:GLN:NE2	4:B:2027:HOH:O	2.34	0.60
1:D:79:HIS:HE1	1:D:106:VAL:H	1.51	0.59
1:D:10:ALA:HB3	1:D:42:LEU:HD23	1.85	0.59
1:A:29:ARG:HB3	1:A:33:PHE:CE2	2.38	0.59
1:B:237:THR:CG2	1:D:179:ARG:HD3	2.33	0.58
1:B:140:PRO:HG2	3:B:1299:1PE:H251	1.85	0.58
1:B:236:GLN:HE21	1:B:240:ASN:ND2	2.00	0.58
1:A:29:ARG:HB3	1:A:33:PHE:HE2	1.69	0.57
1:A:96:LYS:HD3	1:A:132:LEU:HD13	1.86	0.57
1:C:12:LEU:HD13	1:C:42:LEU:HD13	1.88	0.56
1:D:218:GLN:HE21	1:D:218:GLN:HA	1.70	0.56
1:C:166:GLN:HE21	1:C:166:GLN:HA	1.71	0.55
1:B:80:VAL:HG11	1:B:92:ALA:HA	1.88	0.55
1:D:213[B]:MET:HE2	1:D:292:LEU:HD11	1.88	0.55
1:D:120:ASP:OD1	1:D:123:ARG:NH1	2.39	0.55
1:C:238:GLU:HG2	4:C:2164:HOH:O	2.07	0.55
1:C:240:ASN:HD22	1:C:243:ILE:HD12	1.73	0.54
1:C:267:VAL:CG1	1:C:269:LEU:HD12	2.37	0.53
1:B:168:SER:HA	3:B:1299:1PE:H242	1.91	0.53
1:D:290:GLN:HA	1:D:293:MET:HE3	1.91	0.53
1:C:192:GLU:HA	1:C:240:ASN:HD21	1.73	0.52
1:A:48:THR:HA	1:A:252:PHE:CZ	2.44	0.52
1:A:234:LYS:O	1:A:238:GLU:HG2	2.10	0.52
1:C:245:LEU:HD23	1:C:288:LEU:HD22	1.93	0.51
1:B:229:ILE:HD13	1:D:224:LEU:HD22	1.93	0.51
1:D:118:HIS:O	1:D:121:HIS:HB3	2.10	0.51
1:A:33:PHE:CD2	1:A:264:VAL:HG22	2.45	0.51
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.76	0.50
1:A:265:VAL:HG13	4:A:2012:HOH:O	2.12	0.50
1:B:262[B]:MET:HG3	1:B:289:ALA:HB1	1.92	0.50
1:D:236:GLN:HE21	1:D:240:ASN:HD21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:LEU:HA	1:D:202:ALA:HB3	1.94	0.50
1:B:218:GLN:HE21	1:B:218:GLN:HA	1.76	0.50
1:C:213:MET:HE1	1:C:242:VAL:HB	1.94	0.50
1:D:165:KPI:HA	1:D:187:TYR:HB2	1.94	0.49
1:A:267:VAL:HG12	1:A:269:LEU:HG	1.95	0.49
1:A:44:VAL:HG21	1:A:66:VAL:HG11	1.93	0.49
1:D:108:PRO:HD2	1:D:118:HIS:HD2	1.77	0.48
1:C:33:PHE:CD1	1:C:264:VAL:HG21	2.48	0.48
1:A:209:THR:HG22	1:A:246:LEU:CD1	2.44	0.48
1:A:135:VAL:HG22	1:A:163:ALA:HB3	1.95	0.48
1:C:12:LEU:HD13	1:C:42:LEU:HD22	1.96	0.48
1:C:108:PRO:HD2	1:C:118:HIS:CD2	2.46	0.48
1:B:229:ILE:HD12	1:D:224:LEU:O	2.13	0.47
1:A:213[B]:MET:HE1	1:A:242:VAL:HB	1.96	0.47
1:C:79:HIS:CE1	1:C:106:VAL:H	2.19	0.47
1:D:194:PHE:CZ	1:D:198:LEU:HD11	2.48	0.47
1:A:45:GLY:O	1:A:51:ALA:HB2	2.14	0.47
1:B:159:PRO:O	4:B:2122:HOH:O	2.20	0.47
1:A:253:ARG:NH2	1:D:117:GLU:OE2	2.46	0.47
1:D:37:GLN:NE2	4:D:2034:HOH:O	2.47	0.47
1:D:56:LEU:HD11	1:D:87:GLU:HG2	1.95	0.47
1:C:179:ARG:HB2	4:C:2132:HOH:O	2.14	0.47
3:B:1298:1PE:H222	4:B:2109:HOH:O	2.14	0.47
1:A:139:ILE:HD12	1:A:167:THR:HG21	1.95	0.47
1:B:224:LEU:HD22	1:D:229:ILE:HD11	1.97	0.46
1:C:34:ASN:HA	1:C:37:GLN:HG2	1.97	0.46
1:A:209:THR:HB	1:A:213[B]:MET:HE2	1.96	0.46
1:A:213[A]:MET:HE3	1:A:217:TYR:CE2	2.51	0.46
1:C:260:HIS:HA	1:C:265:VAL:O	2.16	0.46
1:B:37[B]:GLN:HE21	1:B:39:ILE:HB	1.80	0.46
1:D:115:PHE:CE1	1:D:151:GLN:HB3	2.51	0.46
1:D:164:LEU:HD23	1:D:186:LEU:CD1	2.46	0.46
1:A:209:THR:HG22	1:A:246:LEU:HD13	1.97	0.45
1:B:45:GLY:O	1:B:79:HIS:HD2	1.99	0.45
1:C:253:ARG:HG3	1:C:277:VAL:HG22	1.98	0.45
1:C:56:LEU:HD21	1:C:87:GLU:HB3	1.97	0.45
1:C:165:KPI:H1A	1:C:206:ILE:HG22	1.98	0.45
1:B:144:GLY:HA2	3:B:1298:1PE:H132	1.98	0.45
1:B:10:ALA:HB3	1:B:42:LEU:HD23	1.99	0.45
1:C:27:LEU:O	1:C:31:VAL:HG23	2.17	0.45
1:D:192:GLU:HA	1:D:240:ASN:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ASN:HA	1:C:37:GLN:CG	2.47	0.45
1:C:135:VAL:HG22	1:C:163:ALA:HB3	1.97	0.45
1:A:24:LYS:NZ	4:A:2014:HOH:O	2.51	0.44
1:A:261:TYR:OH	1:A:282:LEU:HD22	2.16	0.44
1:B:253:ARG:NH2	1:C:117:GLU:OE2	2.48	0.44
1:B:34:ASN:O	1:B:37[B]:GLN:HG2	2.17	0.44
1:D:213[B]:MET:HE2	1:D:213[B]:MET:HB3	1.93	0.44
1:D:45:GLY:O	1:D:79:HIS:HD2	2.01	0.43
1:A:249:THR:HG22	1:A:281:TYR:CG	2.54	0.43
1:A:222:LYS:O	1:A:225:LYS:HG2	2.18	0.43
1:B:33:PHE:HZ	1:B:262[B]:MET:HE2	1.83	0.43
1:B:153:ASN:OD1	1:B:181:HIS:HE1	2.02	0.43
1:D:213[B]:MET:CE	1:D:292:LEU:HD11	2.48	0.43
1:B:23:ASP:OD1	1:B:23:ASP:C	2.62	0.43
1:A:108:PRO:HD2	1:A:118:HIS:HD2	1.83	0.42
1:C:286:LYS:NZ	4:C:2187:HOH:O	2.52	0.42
1:D:194:PHE:CE2	1:D:198:LEU:CD1	2.97	0.42
1:B:42:LEU:HG	1:B:74:ILE:HD11	2.01	0.42
1:A:165:KPI:HA	1:A:187:TYR:HB2	2.01	0.42
1:B:115:PHE:CE1	1:B:151:GLN:HB3	2.54	0.42
1:B:96:LYS:HD3	1:B:132:LEU:HD13	2.02	0.42
1:A:43:TYR:CD1	1:A:206:ILE:HD13	2.54	0.42
1:B:224:LEU:HD22	1:D:229:ILE:CD1	2.50	0.42
1:B:56:LEU:HD11	1:B:87:GLU:HG2	2.02	0.42
1:B:80:VAL:HB	1:B:91:LEU:HB2	2.01	0.42
1:D:146:LYS:NZ	4:D:2119:HOH:O	2.52	0.42
1:A:33:PHE:HD2	1:A:264:VAL:HG13	1.70	0.42
1:C:267:VAL:HG11	1:C:269:LEU:HD12	2.01	0.42
1:B:236:GLN:NE2	1:B:240:ASN:HD21	2.12	0.41
1:C:45:GLY:O	1:C:51:ALA:HB2	2.21	0.41
1:A:260:HIS:HA	1:A:265:VAL:O	2.20	0.41
1:B:12:LEU:CD2	1:B:66:VAL:HG21	2.50	0.41
1:B:224:LEU:CD2	1:D:229:ILE:HD11	2.51	0.41
1:A:173:GLN:HA	1:A:176:GLN:HE21	1.84	0.41
1:B:213:MET:HE1	1:B:242:VAL:HB	2.03	0.41
1:C:290:GLN:HA	1:C:293:MET:HE3	2.01	0.41
1:B:37[B]:GLN:NE2	1:B:39:ILE:HD13	2.36	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	295/303 (97%)	290 (98%)	5 (2%)	0	100	100
1	B	297/303 (98%)	287 (97%)	9 (3%)	1 (0%)	36	21
1	C	292/303 (96%)	286 (98%)	6 (2%)	0	100	100
1	D	296/303 (98%)	290 (98%)	6 (2%)	0	100	100
All	All	1180/1212 (97%)	1153 (98%)	26 (2%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	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	243/250 (97%)	239 (98%)	4 (2%)	55	34
1	B	245/250 (98%)	239 (98%)	6 (2%)	43	20
1	C	239/250 (96%)	235 (98%)	4 (2%)	53	32
1	D	243/250 (97%)	238 (98%)	5 (2%)	47	24
All	All	970/1000 (97%)	951 (98%)	19 (2%)	50	26

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	213[A]	MET
1	A	213[B]	MET
1	A	229	ILE
1	B	22	LEU
1	B	69	GLU
1	B	166	GLN
1	B	210	TYR
1	B	218	GLN
1	B	258	VAL
1	C	166	GLN
1	C	210	TYR
1	C	221	VAL
1	C	263	ASP
1	D	37	GLN
1	D	158	LEU
1	D	166	GLN
1	D	210	TYR
1	D	218	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	37	GLN
1	A	61	GLN
1	A	79	HIS
1	A	90	GLN
1	A	118	HIS
1	A	138	ASN
1	A	166	GLN
1	A	176	GLN
1	A	181	HIS
1	A	230	GLN
1	A	240	ASN
1	A	291	GLN
1	B	19	GLN
1	B	79	HIS
1	B	118	HIS
1	B	138	ASN
1	B	166	GLN
1	B	176	GLN
1	B	181	HIS

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Mol	Chain	Res	Type
1	B	218	GLN
1	B	240	ASN
1	B	291	GLN
1	C	20	GLN
1	C	34	ASN
1	C	79	HIS
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	34	ASN
1	D	54	GLN
1	D	79	HIS
1	D	118	HIS
1	D	138	ASN
1	D	166	GLN
1	D	176	GLN
1	D	211	ASN
1	D	218	GLN
1	D	230	GLN
1	D	240	ASN
1	D	260	HIS

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	1.17	1 (9%)	9,15,17	2.11	2 (22%)
1	KPI	D	165	1	11,13,14	0.77	0	9,15,17	2.07	2 (22%)
1	KPI	B	165	1	11,13,14	1.22	2 (18%)	9,15,17	1.91	2 (22%)
1	KPI	A	165	1	11,13,14	0.99	0	9,15,17	2.20	2 (22%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	KPI	O1-CX2	-2.27	1.24	1.30
1	B	165	KPI	C1-CX1	2.20	1.54	1.49
1	C	165	KPI	C1-CX1	2.03	1.53	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	KPI	O2-CX2-CX1	-4.39	115.98	121.35
1	D	165	KPI	O2-CX2-CX1	-4.39	115.98	121.35
1	A	165	KPI	O2-CX2-CX1	-4.30	116.10	121.35
1	A	165	KPI	C1-CX1-CX2	4.20	122.08	118.11
1	B	165	KPI	C1-CX1-CX2	4.14	122.02	118.11
1	D	165	KPI	C1-CX1-CX2	3.61	121.52	118.11
1	C	165	KPI	C1-CX1-CX2	3.59	121.50	118.11
1	B	165	KPI	O2-CX2-CX1	-3.26	117.36	121.35

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

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Mol	Chain	Res	Type	Atoms
1	A	165	KPI	CX2-CX1-NZ-CE
1	B	165	KPI	C1-CX1-NZ-CE
1	B	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	C	165	KPI	1	0
1	D	165	KPI	1	0
1	A	165	KPI	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	1PE	C	1297	-	6,6,15	0.68	0	5,5,14	0.66	0
3	1PE	B	1298	-	6,6,15	0.58	0	5,5,14	0.41	0
3	1PE	B	1299	-	15,15,15	0.85	0	14,14,14	0.94	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	1PE	C	1297	-	-	3/4/4/13	-
3	1PE	B	1298	-	-	2/4/4/13	-
3	1PE	B	1299	-	-	8/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1297	1PE	OH4-C13-C23-OH3
3	B	1299	1PE	OH5-C14-C24-OH4
3	B	1298	1PE	OH4-C13-C23-OH3
3	C	1297	1PE	C12-C22-OH3-C23
3	B	1299	1PE	OH2-C12-C22-OH3
3	B	1299	1PE	OH4-C13-C23-OH3
3	B	1299	1PE	C25-C15-OH6-C26
3	B	1299	1PE	OH7-C16-C26-OH6
3	C	1297	1PE	C13-C23-OH3-C22
3	B	1299	1PE	C23-C13-OH4-C24
3	B	1299	1PE	C24-C14-OH5-C25
3	B	1298	1PE	C12-C22-OH3-C23
3	B	1299	1PE	OH6-C15-C25-OH5

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1297	1PE	2	0
3	B	1298	1PE	2	0
3	B	1299	1PE	5	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	295/303 (97%)	1.87	124 (42%) 0 0	11, 25, 37, 44	2 (0%)
1	B	294/303 (97%)	1.53	94 (31%) 1 1	9, 22, 33, 40	5 (1%)
1	C	294/303 (97%)	1.31	73 (24%) 2 2	9, 21, 33, 47	0
1	D	296/303 (97%)	1.21	58 (19%) 3 3	11, 21, 32, 47	2 (0%)
All	All	1179/1212 (97%)	1.48	349 (29%) 1 1	9, 22, 36, 47	9 (0%)

All (349) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	PHE	8.2
1	A	268	PRO	7.2
1	A	285	LEU	6.7
1	D	2	ALA	5.3
1	A	22	LEU	5.3
1	A	292	LEU	5.0
1	B	3	THR	4.9
1	A	229	ILE	4.9
1	D	0	HIS	4.9
1	D	1	HIS	4.9
1	D	-1	HIS	4.8
1	A	265	VAL	4.8
1	B	2	ALA	4.8
1	A	264	VAL	4.8
1	A	255	LEU	4.7
1	B	292	LEU	4.7
1	C	212	ILE	4.7
1	B	67	ALA	4.7
1	C	289	ALA	4.7
1	D	3	THR	4.6
1	B	215	TRP	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	258	VAL	4.6
1	A	287	ALA	4.5
1	C	231	THR	4.5
1	C	36	GLN	4.5
1	A	8	VAL	4.5
1	A	25	ALA	4.4
1	B	229	ILE	4.4
1	A	232	ALA	4.4
1	A	289	ALA	4.4
1	D	18	GLN	4.4
1	A	258	VAL	4.4
1	A	259	LEU	4.4
1	A	223	ALA	4.3
1	A	261	TYR	4.3
1	C	3	THR	4.3
1	D	124	ALA	4.3
1	D	157	THR	4.3
1	B	288	LEU	4.3
1	A	282	LEU	4.2
1	A	279	GLU	4.2
1	B	31	VAL	4.2
1	C	283	PRO	4.2
1	A	35	ILE	4.2
1	A	31	VAL	4.1
1	A	288	LEU	4.1
1	B	289	ALA	4.0
1	A	293	MET	4.0
1	A	257	THR	4.0
1	B	35	ILE	4.0
1	A	219	GLY	4.0
1	C	288	LEU	4.0
1	A	215	TRP	4.0
1	B	25	ALA	3.9
1	D	289	ALA	3.9
1	C	265	VAL	3.9
1	A	290	GLN	3.9
1	A	275	GLY	3.9
1	D	177	ILE	3.9
1	A	27	LEU	3.9
1	C	292	LEU	3.9
1	C	2	ALA	3.9
1	A	212	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	258	VAL	3.8
1	C	33	PHE	3.8
1	C	294	GLN	3.8
1	C	296	ARG	3.8
1	B	225	LYS	3.7
1	A	242	VAL	3.6
1	A	30	LEU	3.6
1	A	254	GLY	3.6
1	D	225	LYS	3.6
1	B	282	LEU	3.6
1	A	286	LYS	3.6
1	A	74	ILE	3.6
1	A	243	ILE	3.6
1	B	227	GLY	3.6
1	D	149	LEU	3.6
1	D	152	ILE	3.5
1	C	223	ALA	3.5
1	D	127	ASP	3.5
1	A	245	LEU	3.5
1	A	227	GLY	3.5
1	A	235	LEU	3.4
1	B	66	VAL	3.4
1	D	161	VAL	3.4
1	A	231	THR	3.4
1	A	283	PRO	3.4
1	A	220	ILE	3.4
1	B	39	ILE	3.4
1	A	0	HIS	3.4
1	C	37	GLN	3.4
1	A	222	LYS	3.4
1	A	224	LEU	3.4
1	B	285	LEU	3.4
1	B	290	GLN	3.4
1	C	293	MET	3.4
1	C	235	LEU	3.3
1	B	221	VAL	3.3
1	C	264	VAL	3.3
1	D	185	VAL	3.3
1	A	70	ALA	3.3
1	C	232	ALA	3.3
1	B	30	LEU	3.3
1	B	235	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	283	PRO	3.3
1	B	242	VAL	3.3
1	B	268	PRO	3.3
1	A	221	VAL	3.3
1	B	263	ASP	3.2
1	C	224	LEU	3.2
1	B	65	ILE	3.2
1	C	263	ASP	3.2
1	B	231	THR	3.2
1	D	159	PRO	3.2
1	A	39	ILE	3.2
1	A	269	LEU	3.2
1	D	158	LEU	3.2
1	B	223	ALA	3.2
1	B	277	VAL	3.2
1	A	207	GLY	3.1
1	A	214	GLY	3.1
1	A	263	ASP	3.1
1	C	219	GLY	3.1
1	C	227	GLY	3.1
1	B	264	VAL	3.1
1	A	247	ILE	3.1
1	B	224	LEU	3.1
1	C	222	LYS	3.1
1	B	6	ARG	3.1
1	A	3	THR	3.1
1	C	215	TRP	3.0
1	C	277	VAL	3.0
1	B	214	GLY	3.0
1	B	27	LEU	3.0
1	C	259	LEU	3.0
1	A	67	ALA	3.0
1	A	20	GLN	3.0
1	C	267	VAL	3.0
1	B	279	GLU	3.0
1	A	38	GLY	3.0
1	A	260	HIS	3.0
1	A	9	MET	3.0
1	A	291	GLN	3.0
1	B	126	ILE	3.0
1	C	282	LEU	3.0
1	A	16	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	277	VAL	2.9
1	D	36	GLN	2.9
1	A	-2	HIS	2.9
1	A	234	LYS	2.9
1	A	21	ALA	2.9
1	C	287	ALA	2.9
1	C	229	ILE	2.9
1	B	228	ASP	2.9
1	B	259	LEU	2.9
1	A	99	GLY	2.9
1	B	71	LYS	2.9
1	A	267	VAL	2.9
1	A	210	TYR	2.9
1	B	294	GLN	2.9
1	C	18	GLN	2.9
1	A	76	LEU	2.9
1	A	66	VAL	2.8
1	B	265	VAL	2.8
1	B	100	PHE	2.8
1	C	228	ASP	2.8
1	A	7	GLY	2.8
1	B	124	ALA	2.8
1	D	103	VAL	2.8
1	A	199	LEU	2.8
1	A	19	GLN	2.8
1	A	262	MET	2.8
1	B	260	HIS	2.8
1	B	287	ALA	2.8
1	B	5	LEU	2.8
1	C	225	LYS	2.8
1	A	28	ARG	2.7
1	A	36	GLN	2.7
1	B	211	ASN	2.7
1	A	251	VAL	2.7
1	D	126	ILE	2.7
1	D	229	ILE	2.7
1	D	154	THR	2.7
1	A	-1	HIS	2.7
1	A	270	CYS	2.7
1	D	155	LEU	2.7
1	D	125	ILE	2.7
1	B	296	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	2.7
1	C	198	LEU	2.7
1	D	221	VAL	2.7
1	A	281	TYR	2.7
1	B	92	ALA	2.7
1	A	274	PHE	2.6
1	B	38	GLY	2.6
1	C	30	LEU	2.6
1	A	44	VAL	2.6
1	B	243	ILE	2.6
1	A	256	LYS	2.6
1	B	185	VAL	2.6
1	A	18	GLN	2.6
1	C	220	ILE	2.6
1	C	234	LYS	2.6
1	C	4	ASN	2.6
1	B	97	ARG	2.6
1	A	68	GLU	2.6
1	C	291	GLN	2.6
1	C	255	LEU	2.6
1	D	119	CYS	2.6
1	A	1	HIS	2.6
1	D	156	VAL	2.6
1	D	37	GLN	2.5
1	A	252	PHE	2.5
1	B	33	PHE	2.5
1	A	211	ASN	2.5
1	A	32	GLN	2.5
1	C	230	GLN	2.5
1	C	290	GLN	2.5
1	A	205	GLY	2.5
1	D	160	GLY	2.5
1	B	26	SER	2.5
1	C	184	LEU	2.5
1	A	2	ALA	2.5
1	D	264	VAL	2.5
1	C	247	ILE	2.5
1	D	181	HIS	2.5
1	B	68	GLU	2.5
1	D	147	LEU	2.5
1	D	224	LEU	2.5
1	D	235	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	261	TYR	2.5
1	C	161	VAL	2.5
1	A	69	GLU	2.5
1	A	284	GLU	2.5
1	B	293	MET	2.5
1	A	40	ASP	2.4
1	D	130	ASP	2.4
1	A	239	CYS	2.4
1	A	42	LEU	2.4
1	D	132	LEU	2.4
1	C	261	TYR	2.4
1	B	69	GLU	2.4
1	C	226	GLU	2.4
1	B	63	LEU	2.4
1	B	219	GLY	2.4
1	C	199	LEU	2.4
1	C	35	ILE	2.4
1	C	177	ILE	2.4
1	A	208	SER	2.4
1	A	230	GLN	2.4
1	D	182	PRO	2.4
1	C	70	ALA	2.4
1	D	129	ALA	2.4
1	B	234	LYS	2.4
1	C	221	VAL	2.4
1	C	7	GLY	2.3
1	B	40	ASP	2.3
1	D	183	ASP	2.3
1	C	242	VAL	2.3
1	B	4	ASN	2.3
1	B	7	GLY	2.3
1	B	99	GLY	2.3
1	B	275	GLY	2.3
1	A	228	ASP	2.3
1	D	231	THR	2.3
1	B	70	ALA	2.3
1	B	262[A]	MET	2.3
1	A	13	LEU	2.3
1	A	194	PHE	2.3
1	B	29	ARG	2.3
1	A	41	GLY	2.3
1	B	213	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	37	GLN	2.3
1	A	63	LEU	2.3
1	B	22	LEU	2.3
1	B	246	LEU	2.3
1	D	5	LEU	2.3
1	D	285	LEU	2.3
1	A	187	TYR	2.3
1	C	281	TYR	2.3
1	C	23	ASP	2.3
1	C	39	ILE	2.3
1	C	31	VAL	2.3
1	B	36	GLN	2.2
1	B	291	GLN	2.2
1	B	232	ALA	2.2
1	D	92	ALA	2.2
1	A	4	ASN	2.2
1	A	278	ASP	2.2
1	C	194	PHE	2.2
1	A	65	ILE	2.2
1	B	125	ILE	2.2
1	B	220	ILE	2.2
1	D	290	GLN	2.2
1	B	267	VAL	2.2
1	A	15	PRO	2.2
1	C	200	ALA	2.2
1	A	266	SER	2.2
1	B	146	LYS	2.2
1	D	35	ILE	2.2
1	B	15	PRO	2.2
1	C	266	SER	2.2
1	C	183	ASP	2.2
1	D	232	ALA	2.2
1	B	37[A]	GLN	2.2
1	A	12	LEU	2.2
1	C	29	ARG	2.2
1	D	122	TYR	2.2
1	A	185	VAL	2.1
1	B	161	VAL	2.1
1	B	21	ALA	2.1
1	C	202	ALA	2.1
1	D	121	HIS	2.1
1	A	5	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	34	ASN	2.1
1	B	286	LYS	2.1
1	B	276	PRO	2.1
1	D	230	GLN	2.1
1	D	261	TYR	2.1
1	D	281	TYR	2.1
1	A	62	VAL	2.1
1	A	198	LEU	2.1
1	C	285	LEU	2.1
1	C	213	MET	2.1
1	A	26	SER	2.1
1	D	33	PHE	2.1
1	B	210	TYR	2.1
1	B	8	VAL	2.1
1	B	239	CYS	2.1
1	B	233	GLN	2.1
1	C	257	THR	2.1
1	C	260	HIS	2.1
1	A	98	TYR	2.1
1	C	217	TYR	2.1
1	B	72	GLY	2.0
1	D	72	GLY	2.0
1	A	10	ALA	2.0
1	B	156	VAL	2.0
1	C	22	LEU	2.0
1	D	116	GLU	2.0
1	C	38	GLY	2.0
1	D	215	TRP	2.0
1	A	193	ILE	2.0
1	B	28	ARG	2.0
1	D	115	PHE	2.0
1	A	11	ALA	2.0
1	A	53	VAL	2.0
1	D	8	VAL	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	D	165	14/15	0.92	0.08	11,16,17,17	0
1	KPI	A	165	14/15	0.93	0.09	16,18,20,20	0
1	KPI	B	165	14/15	0.94	0.08	13,15,17,17	0
1	KPI	C	165	14/15	0.95	0.06	11,13,15,15	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
3	1PE	B	1299	16/16	0.71	0.20	22,34,39,40	0
3	1PE	C	1297	7/16	0.77	0.16	11,25,28,29	0
3	1PE	B	1298	7/16	0.84	0.17	34,35,37,37	0
2	NA	B	1297	1/1	0.88	0.23	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.