



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:14 PM GMT

PDB ID : 4BWL
Title : Structure of the Y137A mutant of E. coli N-acetylneuraminic acid lyase in complex with pyruvate, N-acetyl-D-mannosamine and N- acetylneuraminic acid
Authors : Campeotto, I.; Phillips, S.E.V.; Pearson, A.R.; Nelson, A.; Berry, A.
Deposited on : 2013-07-03
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

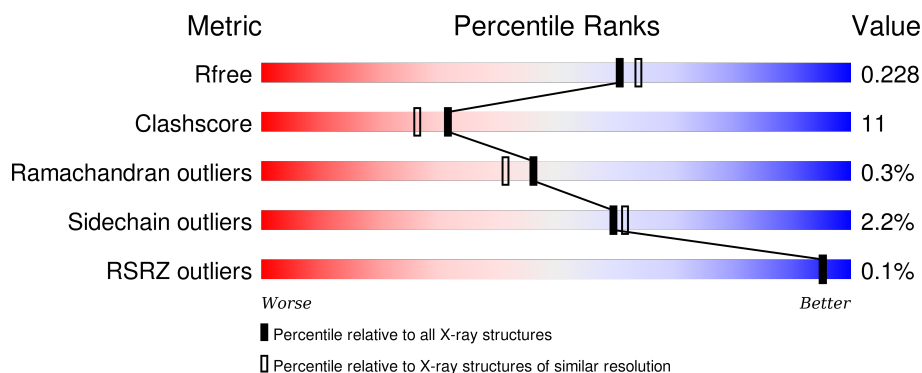
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 ≥ 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>73%</div> <div>25%</div> <div>..</div> </div>
1	B	304	<div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	D	304	<div> <div>76%</div> <div>21%</div> <div>..</div> </div>
2	C	304	<div> <div>73%</div> <div>24%</div> <div>..</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	KPI	C	165	-	-	X	-
3	SI3	A	1165	X	-	-	-
3	SI3	B	1165	X	-	-	-
3	SI3	D	1165	X	-	-	-
4	1PE	B	1297	-	-	-	X
5	MN9	C	1297	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9360 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	299	Total	C	N	O	S	0	0	0
			2306	1466	396	434	10			
1	B	295	Total	C	N	O	S	0	0	0
			2272	1446	386	430	10			
1	D	298	Total	C	N	O	S	0	0	0
			2301	1464	394	433	10			

There are 27 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	ALA	TYR	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	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	0	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	1	HIS	-	EXPRESSION TAG	UNP P0A6L4
D	137	ALA	TYR	ENGINEERED MUTATION	UNP P0A6L4

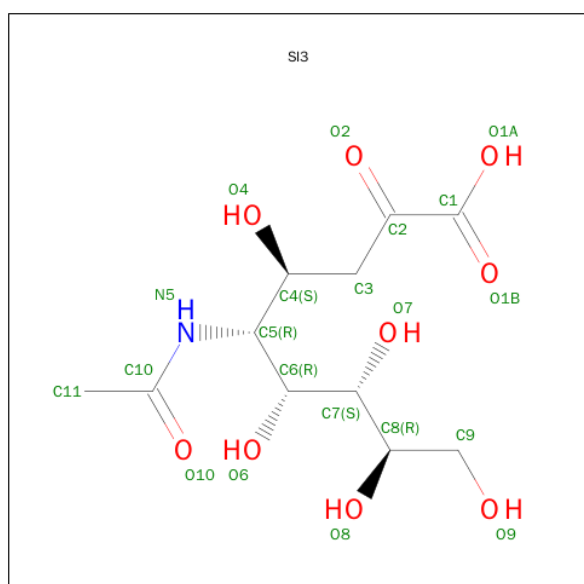
- Molecule 2 is a protein called N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	296	Total	C	N	O	S	0	0	0
			2287	1455	389	433	10			

There are 9 discrepancies between the modelled and reference sequences:

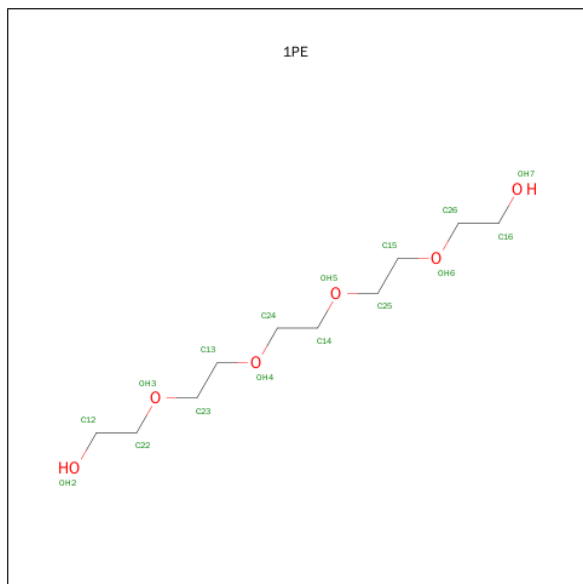
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	EXPRESSION TAG	UNP P0A6L4
C	-5	GLU	-	EXPRESSION TAG	UNP P0A6L4
C	-4	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-3	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-2	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	-1	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	0	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	1	HIS	-	EXPRESSION TAG	UNP P0A6L4
C	137	ALA	TYR	ENGINEERED MUTATION	UNP P0A6L4

- Molecule 3 is SUGAR (5-(ACETYLAMINO)-3,5-DIDEOXY-D-GLYCERO-D-GALACTO-NON-2-ULOSONIC ACID) (three-letter code: SI3) (formula: C₁₁H₁₉NO₉).



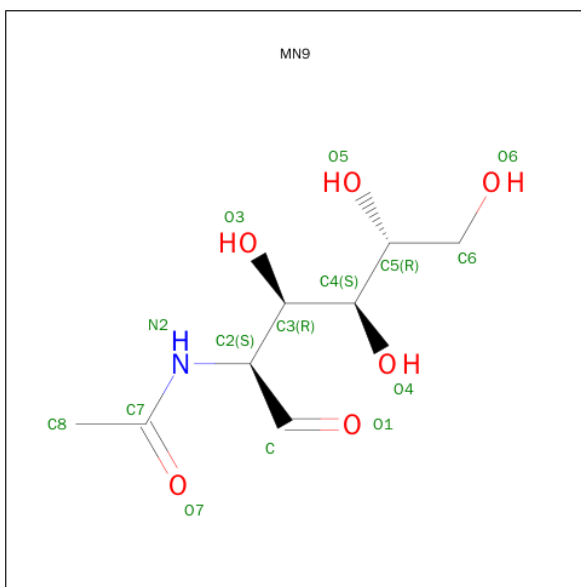
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	11	1	8		
3	B	1	Total	C	N	O	0	0
			20	11	1	8		
3	D	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			9	6	3		
4	C	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is 2-(ACETYLAMINO)-2-DEOXY-D-MANNOSE (three-letter code: MN9) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			15	8	1	6		

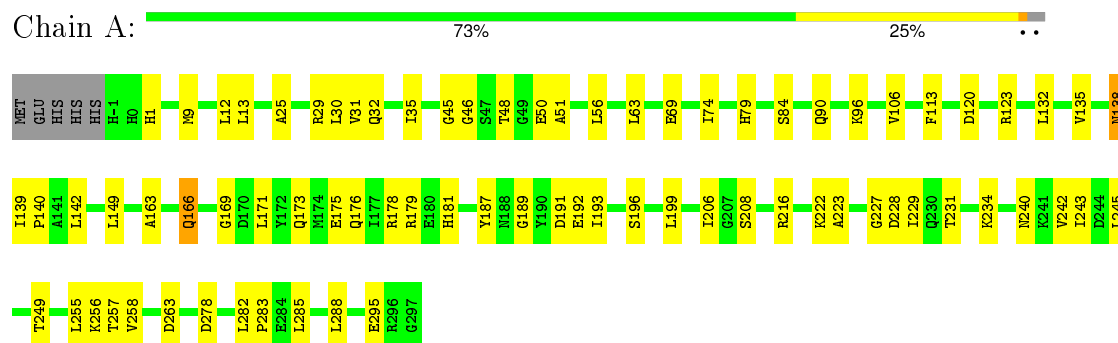
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total	O	0	0
			34	34		
6	B	22	Total	O	0	0
			22	22		
6	C	22	Total	O	0	0
			22	22		
6	D	24	Total	O	0	0
			24	24		

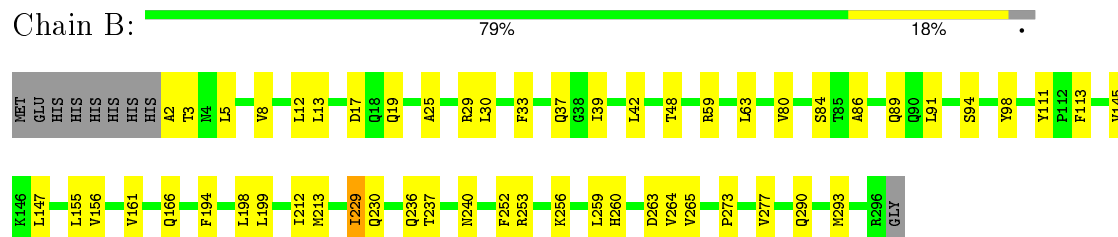
3 Residue-property plots

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.

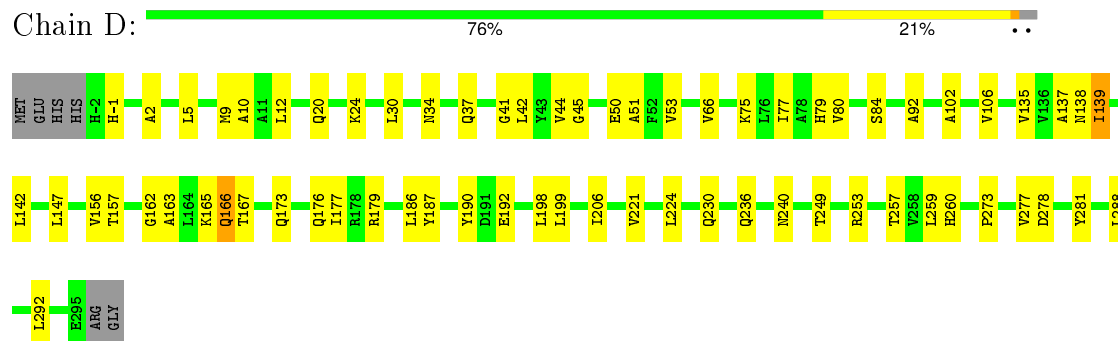
• Molecule 1: N-ACETYLNEURAMINATE LYASE



• Molecule 1: N-ACETYLNEURAMINATE LYASE

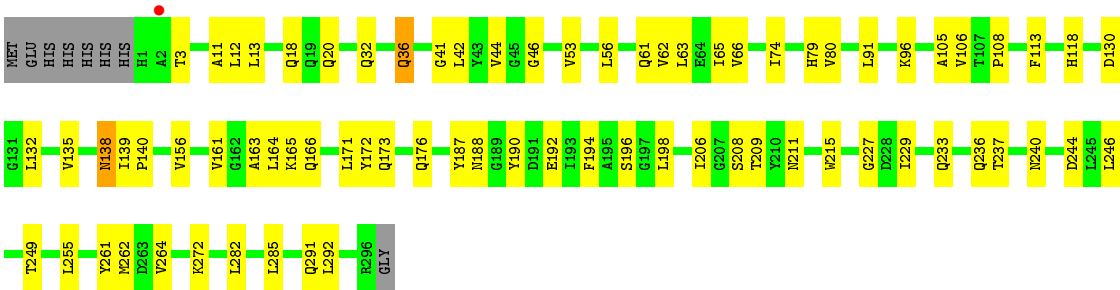


• Molecule 1: N-ACETYLNEURAMINATE LYASE



• Molecule 2: 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	55.97Å 143.22Å 83.41Å 90.00° 109.51° 90.00°	Depositor
Resolution (Å)	49.46 – 2.00 49.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.46-2.00) 99.4 (49.50-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0097	Depositor
R, R_{free}	0.180 , 0.235 0.186 , 0.228	Depositor DCC
R_{free} test set	4143 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.9	EDS
Estimated twinning fraction	0.512 for H, K, L 0.488 for -H, -K, H+L 0.107 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.512 for H, K, L 0.488 for -H, -K, H+L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 83318 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9360	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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, 0.375 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: SI3, MN9, 1PE, 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	0.53	0/2348	0.65	0/3178
1	B	0.56	0/2311	0.66	0/3128
1	D	0.58	0/2344	0.67	0/3174
2	C	0.57	0/2312	0.68	0/3129
All	All	0.56	0/9315	0.67	0/12609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2306	0	2320	57	0
1	B	2272	0	2293	35	0
1	D	2301	0	2312	51	0
2	C	2287	0	2305	66	0
3	A	20	0	18	2	0
3	B	20	0	18	0	0
3	D	20	0	18	1	0
4	B	9	0	10	0	0
4	C	8	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	15	0	15	8	0
6	A	34	0	0	0	0
6	B	22	0	0	1	0
6	C	22	0	0	1	0
6	D	24	0	0	2	0
All	All	9360	0	9318	199	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 11.

All (199) 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:C:165:KPI:C1	5:C:1297:MN9:H	1.74	1.16
1:B:2:ALA:HB1	1:B:5:LEU:HD12	1.36	1.07
1:D:139:ILE:HD11	1:D:142:LEU:HD12	1.37	1.05
2:C:165:KPI:H1B	5:C:1297:MN9:H	1.36	1.03
2:C:165:KPI:H1A	2:C:206:ILE:HG22	1.42	0.97
1:A:173:GLN:HA	1:A:176:GLN:HE21	1.30	0.94
1:B:2:ALA:HB1	1:B:5:LEU:CD1	1.98	0.94
1:D:139:ILE:CD1	1:D:142:LEU:HD12	2.00	0.90
1:D:139:ILE:HD11	1:D:142:LEU:CD1	2.03	0.88
2:C:165:KPI:H1B	5:C:1297:MN9:C	2.06	0.86
2:C:139:ILE:HG23	2:C:139:ILE:O	1.77	0.84
2:C:194:PHE:CE2	2:C:198:LEU:HD11	2.15	0.82
1:B:156:VAL:HA	1:B:161:VAL:HG11	1.61	0.82
2:C:165:KPI:HG	2:C:206:ILE:HD12	1.60	0.82
1:A:173:GLN:HA	1:A:176:GLN:NE2	1.98	0.79
1:B:253:ARG:HG3	1:B:277:VAL:HG22	1.66	0.77
2:C:36:GLN:HE21	2:C:36:GLN:HA	1.50	0.77
1:D:135:VAL:HG22	1:D:163:ALA:HB3	1.67	0.76
1:A:135:VAL:HG22	1:A:163:ALA:HB3	1.68	0.75
2:C:135:VAL:HG22	2:C:163:ALA:HB3	1.67	0.75
1:B:2:ALA:CB	1:B:5:LEU:HD12	2.17	0.72
1:A:192:GLU:HA	1:A:240:ASN:HD21	1.55	0.71
1:D:173:GLN:HA	1:D:176:GLN:HE21	1.56	0.70
1:B:12:LEU:HD13	1:B:42:LEU:HD13	1.72	0.70
1:A:138:ASN:ND2	1:A:140:PRO:HD3	2.06	0.70
1:A:242:VAL:HG13	1:A:288:LEU:HD21	1.71	0.70
1:A:223:ALA:HB1	1:A:231:THR:HG23	1.73	0.70
1:D:249:THR:HG22	1:D:281:TYR:CG	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:CB	1:A:231:THR:HG23	2.22	0.69
1:D:192:GLU:HA	1:D:240:ASN:HD21	1.57	0.68
1:B:8:VAL:HG12	1:B:39:ILE:HD11	1.76	0.67
2:C:96:LYS:NZ	2:C:130:ASP:O	2.24	0.66
1:A:227:GLY:HA2	2:C:229:ILE:HD12	1.76	0.65
1:B:199:LEU:HD22	1:D:199:LEU:HD13	1.79	0.65
1:D:79:HIS:HE1	1:D:106:VAL:H	1.43	0.64
2:C:165:KPI:H1	5:C:1297:MN9:H	1.75	0.64
2:C:20:GLN:HE22	2:C:272:LYS:HG2	1.62	0.64
2:C:165:KPI:CX1	5:C:1297:MN9:H	2.28	0.63
2:C:79:HIS:HE1	2:C:106:VAL:H	1.47	0.63
2:C:165:KPI:H1A	2:C:206:ILE:CG2	2.25	0.61
2:C:139:ILE:HD11	5:C:1297:MN9:O7	2.02	0.59
2:C:18:GLN:HB2	6:C:2005:HOH:O	2.02	0.58
1:A:171:LEU:HD12	2:C:171:LEU:HD12	1.86	0.58
2:C:12:LEU:HD13	2:C:42:LEU:HD22	1.86	0.57
1:D:44:VAL:HG21	1:D:66:VAL:HG11	1.86	0.57
1:A:187:TYR:CD2	1:A:206:ILE:HD11	2.39	0.57
2:C:80:VAL:HB	2:C:91:LEU:HB2	1.87	0.56
1:B:8:VAL:HG12	1:B:39:ILE:CD1	2.36	0.56
1:B:30:LEU:HA	1:B:264:VAL:HG11	1.86	0.56
2:C:261:TYR:OH	2:C:282:LEU:HD22	2.06	0.56
1:D:166:GLN:HA	1:D:166:GLN:HE21	1.71	0.56
1:A:45:GLY:O	1:A:51:ALA:HB2	2.06	0.56
2:C:20:GLN:NE2	2:C:272:LYS:HG2	2.20	0.56
1:D:20:GLN:OE1	6:D:2005:HOH:O	2.18	0.55
1:D:139:ILE:HD11	1:D:142:LEU:CG	2.37	0.55
1:A:31:VAL:HG11	1:A:69:GLU:HB2	1.89	0.55
1:B:86:ALA:HA	1:B:89:GLN:HE21	1.72	0.55
1:A:228:ASP:O	1:A:231:THR:HG22	2.07	0.54
2:C:139:ILE:CG2	2:C:139:ILE:O	2.49	0.54
1:A:50:GLU:OE2	1:A:256:LYS:NZ	2.40	0.54
1:B:273:PRO:HG2	2:C:113:PHE:CZ	2.43	0.54
1:B:212:ILE:HG13	1:B:213:MET:HG2	1.90	0.53
1:A:245:LEU:O	1:A:249:THR:HG23	2.07	0.53
1:A:228:ASP:CG	1:A:231:THR:HG22	2.28	0.53
1:D:10:ALA:HB3	1:D:42:LEU:HD23	1.90	0.53
1:A:191:ASP:HB2	1:A:243:ILE:HD11	1.90	0.53
2:C:41:GLY:HA2	2:C:74:ILE:HB	1.90	0.53
2:C:56:LEU:HD22	2:C:91:LEU:HD21	1.91	0.53
2:C:138:ASN:ND2	2:C:140:PRO:HD3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HA	1:A:166:GLN:HE21	1.72	0.53
1:B:80:VAL:HB	1:B:91:LEU:HB2	1.91	0.53
1:B:30:LEU:HD12	1:B:264:VAL:HG11	1.91	0.52
2:C:215:TRP:CH2	2:C:292:LEU:HD22	2.44	0.52
1:A:12:LEU:CD1	1:A:30:LEU:HD23	2.39	0.52
1:A:12:LEU:HD11	1:A:30:LEU:HD23	1.92	0.52
1:D:106:VAL:HA	1:D:137:ALA:HB3	1.91	0.52
2:C:36:GLN:NE2	2:C:36:GLN:HA	2.22	0.52
5:C:1297:MN9:H83C	5:C:1297:MN9:O4	2.10	0.51
1:A:199:LEU:HD12	2:C:233:GLN:HE21	1.74	0.51
1:A:173:GLN:CA	1:A:176:GLN:HE21	2.12	0.51
1:D:173:GLN:HA	1:D:176:GLN:NE2	2.24	0.51
2:C:236:GLN:HE21	2:C:240:ASN:HD21	1.59	0.51
1:A:96:LYS:HD3	1:A:132:LEU:HD13	1.92	0.51
1:A:35:ILE:HG22	1:A:74:ILE:HD13	1.92	0.51
1:D:30:LEU:HD13	1:D:259:LEU:HD13	1.92	0.51
1:B:237:THR:HG23	1:D:179:ARG:HD3	1.92	0.51
1:D:198:LEU:HD11	1:D:221:VAL:HG22	1.91	0.51
2:C:11:ALA:O	2:C:211:ASN:ND2	2.43	0.51
1:A:227:GLY:HA2	2:C:229:ILE:CD1	2.39	0.51
1:B:236:GLN:HE21	1:B:240:ASN:ND2	2.08	0.50
1:D:138:ASN:ND2	1:D:147:LEU:HD12	2.26	0.50
2:C:156:VAL:HA	2:C:161:VAL:HG11	1.93	0.50
1:B:229:ILE:HG23	1:B:230:GLN:N	2.27	0.49
1:A:192:GLU:HA	1:A:240:ASN:ND2	2.23	0.49
2:C:215:TRP:CZ2	2:C:292:LEU:HD22	2.47	0.49
1:A:79:HIS:HE1	1:A:106:VAL:H	1.61	0.49
1:D:5:LEU:O	1:D:187:TYR:OH	2.25	0.49
1:D:9:MET:HB2	1:D:206:ILE:HG12	1.93	0.49
1:B:25:ALA:HB1	1:B:29:ARG:HH12	1.76	0.49
2:C:44:VAL:CG1	2:C:63:LEU:HD23	2.43	0.49
1:D:34:ASN:HA	1:D:37:GLN:HE21	1.78	0.49
1:A:178:ARG:NH1	1:A:181:HIS:O	2.45	0.49
2:C:164:LEU:HD21	2:C:166:GLN:NE2	2.28	0.48
1:B:13:LEU:HD22	1:B:256:LYS:HG3	1.95	0.48
2:C:192:GLU:HA	2:C:240:ASN:HD21	1.78	0.48
2:C:173:GLN:HA	2:C:176:GLN:HE21	1.79	0.48
2:C:249:THR:HG21	2:C:285:LEU:HD11	1.96	0.48
1:B:290:GLN:HA	1:B:293:MET:HE3	1.96	0.47
1:B:236:GLN:HE21	1:B:240:ASN:HD21	1.61	0.47
1:D:34:ASN:HA	1:D:37:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD23	1:A:48:THR:HG22	1.96	0.47
2:C:187:TYR:CD2	2:C:206:ILE:HD11	2.50	0.47
1:B:155:LEU:O	1:B:161:VAL:HG21	2.15	0.46
1:B:111:TYR:HB2	1:B:113:PHE:CZ	2.50	0.46
2:C:79:HIS:CE1	2:C:105:ALA:HA	2.50	0.46
2:C:13:LEU:HD11	2:C:255:LEU:HB3	1.96	0.46
1:B:59:ARG:O	1:B:63:LEU:HG	2.16	0.46
1:A:216:ARG:NH2	1:A:295:GLU:OE2	2.48	0.46
1:D:45:GLY:O	1:D:79:HIS:HD2	1.99	0.46
2:C:165:KPI:C1	5:C:1297:MN9:C	2.66	0.46
1:D:167:THR:HG22	1:D:190:TYR:CE2	2.51	0.45
1:D:288:LEU:HD11	1:D:292:LEU:HD11	1.97	0.45
1:B:229:ILE:HD12	1:D:224:LEU:O	2.16	0.45
1:A:229:ILE:HD13	2:C:227:GLY:HA2	1.97	0.45
2:C:236:GLN:HE21	2:C:240:ASN:ND2	2.14	0.45
1:D:135:VAL:HG22	1:D:163:ALA:CB	2.43	0.45
1:B:59:ARG:HB3	6:B:2007:HOH:O	2.16	0.45
1:A:25:ALA:HB1	1:A:29:ARG:NH2	2.32	0.45
1:A:223:ALA:HB2	1:A:231:THR:HG23	1.95	0.44
1:A:196:SER:HB3	2:C:196:SER:HB3	2.00	0.44
2:C:62:VAL:O	2:C:66:VAL:HG23	2.17	0.44
1:A:149:LEU:HD22	1:A:176:GLN:OE1	2.17	0.44
2:C:96:LYS:HD3	2:C:132:LEU:HD13	1.99	0.44
2:C:32:GLN:O	2:C:36:GLN:HG2	2.17	0.44
1:B:48:THR:HA	1:B:252:PHE:CE1	2.52	0.44
1:D:-1:HIS:NE2	1:D:156:VAL:O	2.42	0.44
1:A:208:SER:O	1:A:255:LEU:HD13	2.18	0.44
1:A:46:GLY:HA2	1:A:79:HIS:CD2	2.53	0.44
1:A:175:GLU:OE2	2:C:237:THR:HG23	2.18	0.44
2:C:36:GLN:HE21	2:C:36:GLN:CA	2.19	0.44
1:D:257:THR:O	1:D:260:HIS:HB3	2.18	0.44
1:A:9:MET:O	1:A:206:ILE:HA	2.17	0.43
1:D:253:ARG:HG3	1:D:277:VAL:CG2	2.47	0.43
1:A:120:ASP:OD1	1:A:123:ARG:NH1	2.50	0.43
1:A:113:PHE:CE2	1:D:273:PRO:HG2	2.53	0.43
1:D:12:LEU:HD13	1:D:42:LEU:HD13	1.99	0.43
1:A:223:ALA:HB1	1:A:231:THR:CG2	2.47	0.43
2:C:11:ALA:HB2	2:C:165:KPI:C1	2.48	0.43
2:C:192:GLU:HA	2:C:240:ASN:ND2	2.32	0.43
1:D:2:ALA:HB3	1:D:162:GLY:HA3	2.00	0.43
3:D:1165:SI3:H10	3:D:1165:SI3:O7	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:THR:HG22	1:D:281:TYR:CD1	2.52	0.43
1:A:32:GLN:O	1:A:35:ILE:HG13	2.18	0.43
1:B:17:ASP:OD1	1:B:19:GLN:N	2.51	0.43
1:A:189:GLY:O	3:A:1165:SI3:O4	2.36	0.43
1:D:165:LYS:HA	1:D:187:TYR:HB2	2.00	0.43
1:D:177:ILE:HG21	1:D:186:LEU:HD13	2.00	0.43
2:C:11:ALA:HB2	2:C:165:KPI:H1	2.01	0.43
1:B:145:VAL:HG12	1:B:147:LEU:CD2	2.49	0.43
1:A:169:GLY:HA2	1:A:193:ILE:CD1	2.48	0.43
2:C:172:TYR:O	2:C:176:GLN:HG3	2.19	0.42
1:D:77:ILE:HG12	1:D:102:ALA:HB3	2.01	0.42
2:C:208:SER:O	2:C:255:LEU:HD13	2.18	0.42
1:A:258:VAL:HG23	1:A:285:LEU:HD22	2.01	0.42
1:D:253:ARG:HG3	1:D:277:VAL:HG23	2.01	0.42
1:B:94:SER:O	1:B:98:TYR:CD2	2.72	0.42
1:A:282:LEU:N	1:A:283:PRO:CD	2.83	0.42
2:C:188:ASN:ND2	2:C:190:TYR:O	2.52	0.42
1:A:139:ILE:HG21	1:A:142:LEU:HD12	2.02	0.42
2:C:262:MET:O	2:C:264:VAL:HG23	2.19	0.42
1:A:179:ARG:NH1	2:C:244:ASP:OD2	2.45	0.42
2:C:61:GLN:O	2:C:65:ILE:HD12	2.20	0.42
1:D:80:VAL:HG11	1:D:92:ALA:HA	2.02	0.41
1:B:33:PHE:CG	1:B:264:VAL:HG21	2.55	0.41
1:A:245:LEU:HD23	1:A:288:LEU:HD22	2.02	0.41
1:A:223:ALA:CB	1:A:231:THR:CG2	2.95	0.41
2:C:108:PRO:HD2	2:C:118:HIS:HD2	1.85	0.41
1:D:50:GLU:O	1:D:53:VAL:HG22	2.21	0.41
1:A:257:THR:HG21	1:A:285:LEU:HD13	2.03	0.41
1:B:260:HIS:HD2	1:B:265:VAL:O	2.03	0.41
1:D:139:ILE:HG12	1:D:139:ILE:O	2.21	0.41
1:D:277:VAL:CG1	1:D:278:ASP:N	2.84	0.41
3:A:1165:SI3:C10	3:A:1165:SI3:H14	2.32	0.41
2:C:108:PRO:HG2	2:C:118:HIS:CD2	2.56	0.41
2:C:209:THR:HG22	2:C:246:LEU:HD13	2.01	0.41
1:B:194:PHE:CZ	1:B:198:LEU:HD11	2.56	0.41
1:A:63:LEU:HA	1:A:63:LEU:HD23	1.87	0.41
1:D:24:LYS:HG3	6:D:2006:HOH:O	2.20	0.41
1:B:212:ILE:HG22	1:B:259:LEU:HD21	2.03	0.41
1:A:242:VAL:HG22	1:A:288:LEU:HD11	2.03	0.40
1:A:45:GLY:O	1:A:79:HIS:HD2	2.04	0.40
1:D:277:VAL:HG12	1:D:278:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ILE:HG21	1:D:186:LEU:CD1	2.51	0.40
1:D:236:GLN:HE21	1:D:240:ASN:ND2	2.19	0.40
1:A:56:LEU:HD23	1:A:90:GLN:NE2	2.36	0.40
1:D:41:GLY:CA	1:D:75:LYS:O	2.69	0.40
1:D:45:GLY:O	1:D:51:ALA:HB2	2.21	0.40
2:C:46:GLY:HA2	2:C:79:HIS:CG	2.56	0.40
1:D:41:GLY:HA2	1:D:75:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/304 (98%)	282 (95%)	13 (4%)	2 (1%)	26	19
1	B	293/304 (96%)	277 (94%)	15 (5%)	1 (0%)	46	41
1	D	296/304 (97%)	287 (97%)	9 (3%)	0	100	100
2	C	293/304 (96%)	279 (95%)	14 (5%)	0	100	100
All	All	1179/1216 (97%)	1125 (95%)	51 (4%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	B	37	GLN
1	A	1	HIS

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	245/250 (98%)	239 (98%)	6 (2%)	57	58
1	B	242/250 (97%)	237 (98%)	5 (2%)	61	63
1	D	245/250 (98%)	240 (98%)	5 (2%)	63	65
2	C	242/249 (97%)	237 (98%)	5 (2%)	61	63
All	All	974/999 (98%)	953 (98%)	21 (2%)	60	62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	138	ASN
1	A	166	GLN
1	A	222	LYS
1	A	234	LYS
1	A	278	ASP
1	B	3	THR
1	B	84	SER
1	B	166	GLN
1	B	229	ILE
1	B	263	ASP
2	C	3	THR
2	C	36	GLN
2	C	53	VAL
2	C	138	ASN
2	C	291	GLN
1	D	84	SER
1	D	139	ILE
1	D	157	THR
1	D	166	GLN
1	D	230	GLN

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	20	GLN
1	A	36	GLN

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Mol	Chain	Res	Type
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	240	ASN
1	A	260	HIS
1	B	37	GLN
1	B	54	GLN
1	B	89	GLN
1	B	118	HIS
1	B	138	ASN
1	B	166	GLN
1	B	181	HIS
1	B	240	ASN
1	B	260	HIS
2	C	20	GLN
2	C	36	GLN
2	C	79	HIS
2	C	89	GLN
2	C	118	HIS
2	C	138	ASN
2	C	166	GLN
2	C	176	GLN
2	C	181	HIS
2	C	233	GLN
2	C	240	ASN
2	C	291	GLN
1	D	37	GLN
1	D	79	HIS
1	D	118	HIS
1	D	138	ASN
1	D	153	ASN
1	D	166	GLN
1	D	176	GLN
1	D	181	HIS
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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	KPI	C	165	2	10,13,14	1.02	1 (10%)	9,15,17	0.80	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	KPI	C	165	2	-	0/8/14/16	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	165	KPI	CX1-NZ	2.32	1.32	1.29

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	165	KPI	11	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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
3	SI3	A	1165	1	16,19,20	1.20	2 (12%)	18,25,27	1.01	2 (11%)
3	SI3	B	1165	1	16,19,20	0.91	1 (6%)	18,25,27	1.43	3 (16%)
4	1PE	B	1297	-	8,8,15	0.82	0	7,7,14	0.57	0
5	MN9	C	1297	-	13,14,14	0.66	0	13,18,18	1.05	1 (7%)
4	1PE	C	1298	-	7,7,15	0.72	0	6,6,14	0.44	0
3	SI3	D	1165	1	16,19,20	1.16	1 (6%)	18,25,27	1.34	3 (16%)

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	SI3	A	1165	1	1/1/7/9	0/25/27/30	0/0/0/0
3	SI3	B	1165	1	1/1/7/9	0/25/27/30	0/0/0/0
4	1PE	B	1297	-	-	0/6/6/13	0/0/0/0
5	MN9	C	1297	-	-	0/18/20/20	0/0/0/0
4	1PE	C	1298	-	-	0/5/5/13	0/0/0/0
3	SI3	D	1165	1	1/1/7/9	0/25/27/30	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1165	SI3	C8-C7	-2.15	1.49	1.53
3	A	1165	SI3	C10-N5	2.83	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1165	SI3	C10-N5	2.90	1.45	1.34
3	D	1165	SI3	C10-N5	3.24	1.46	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1165	SI3	C4-C5-N5	-2.75	104.42	110.03
3	B	1165	SI3	C4-C5-N5	-2.71	104.50	110.03
5	C	1297	MN9	C6-C5-C4	-2.41	106.81	112.48
3	A	1165	SI3	C4-C5-N5	-2.27	105.42	110.03
3	D	1165	SI3	O4-C4-C5	2.02	113.83	109.85
3	B	1165	SI3	O8-C8-C7	2.07	114.21	109.02
3	D	1165	SI3	C8-C7-C6	2.11	115.90	112.47
3	A	1165	SI3	C3-C2-C1	2.24	122.15	113.02
3	B	1165	SI3	C8-C7-C6	3.35	117.92	112.47

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1165	SI3	C4
3	A	1165	SI3	C4
3	D	1165	SI3	C4

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1165	SI3	2	0
5	C	1297	MN9	8	0
3	D	1165	SI3	1	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 [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(Å²)	Q<0.9	
1	A	299/304 (98%)	-0.51	0	100	100	18, 28, 44, 58	4 (1%)
1	B	295/304 (97%)	-0.51	0	100	100	17, 27, 36, 44	4 (1%)
1	D	298/304 (98%)	-0.62	0	100	100	16, 25, 35, 52	1 (0%)
2	C	295/304 (97%)	-0.44	1 (0%)	94	94	17, 25, 38, 46	0
All	All	1187/1216 (97%)	-0.52	1 (0%)	95	95	16, 26, 39, 58	9 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	2	ALA	2.1

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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	KPI	C	165	14/15	0.96	0.11	-	16,20,28,30	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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	1PE	B	1297	9/16	0.93	0.12	4.79	24,30,33,34	0
3	SI3	B	1165	20/21	0.95	0.09	0.53	19,26,31,33	0
3	SI3	D	1165	20/21	0.94	0.08	0.16	20,24,27,29	0
5	MN9	C	1297	15/15	0.97	0.09	0.14	13,25,28,31	0
3	SI3	A	1165	20/21	0.96	0.08	-0.01	20,25,31,31	0
4	1PE	C	1298	8/16	0.95	0.14	-	38,39,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.