



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 PM UTC

PDB ID : 1GVM / pdb_00001gvm
Title : CHOLINE BINDING DOMAIN OF THE MAJOR AUTOLYSIN (C-LYTA)
FROM STREPTOCOCCUS PNEUMONIAE
Authors : Fernandez-Tornero, C.; Lopez, R.; Garcia, E.; Gimenez-Gallego, G.; Romero,
A.
Deposited on : 2002-02-15
Resolution : 2.80 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

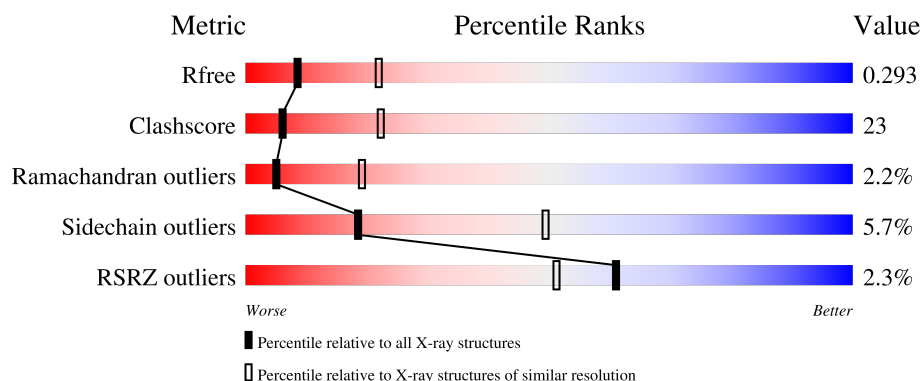
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	136	
1	B	136	
1	C	136	
1	D	136	
1	E	136	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	136	% 59% 37% ..

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
4	TRS	F	1319	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6651 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.

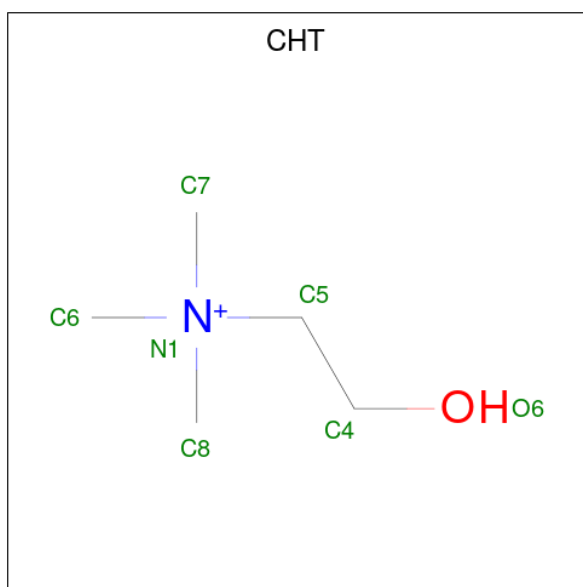
- Molecule 1 is a protein called AUTOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1061	692	166	199	4			
1	B	133	Total	C	N	O	S	0	0	0
			1104	718	174	208	4			
1	C	127	Total	C	N	O	S	0	0	0
			1061	692	166	199	4			
1	D	125	Total	C	N	O	S	0	0	0
			1044	681	164	195	4			
1	E	123	Total	C	N	O	S	0	0	0
			1032	673	162	193	4			
1	F	134	Total	C	N	O	S	0	0	0
			1108	720	175	209	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	ARG	LYS	variant	UNP P06653
B	304	ARG	LYS	variant	UNP P06653
C	304	ARG	LYS	variant	UNP P06653
D	304	ARG	LYS	variant	UNP P06653
E	304	ARG	LYS	variant	UNP P06653
F	304	ARG	LYS	variant	UNP P06653

- Molecule 2 is CHOLINE ION (CCD ID: CHT) (formula: C₅H₁₄NO).



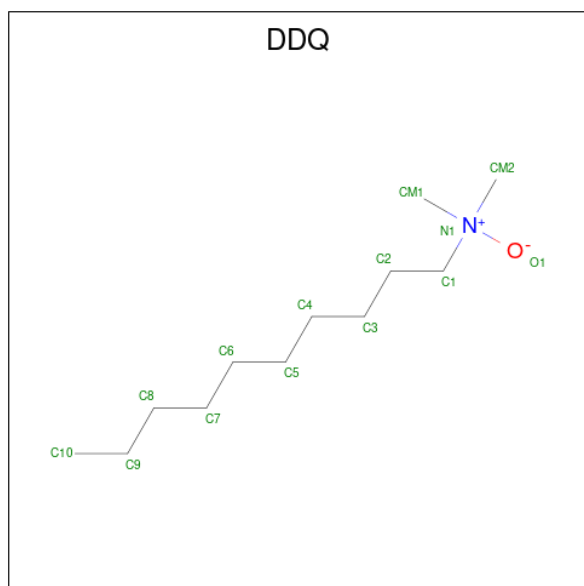
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		
2	C	1	Total	C	N	O	0	0
			7	5	1	1		
2	C	1	Total	C	N	O	0	0
			7	5	1	1		
2	C	1	Total	C	N	O	0	0
			7	5	1	1		
2	D	1	Total	C	N	O	0	0
			7	5	1	1		
2	D	1	Total	C	N	O	0	0
			7	5	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			7	5	1	1		
2	E	1	Total	C	N	O	0	0
			7	5	1	1		
2	F	1	Total	C	N	O	0	0
			7	5	1	1		
2	F	1	Total	C	N	O	0	0
			7	5	1	1		
2	F	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	14	Total	O	0	0
			14	14		
5	C	25	Total	O	0	0
			25	25		
5	D	11	Total	O	0	0
			11	11		
5	F	16	Total	O	0	0
			16	16		

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.

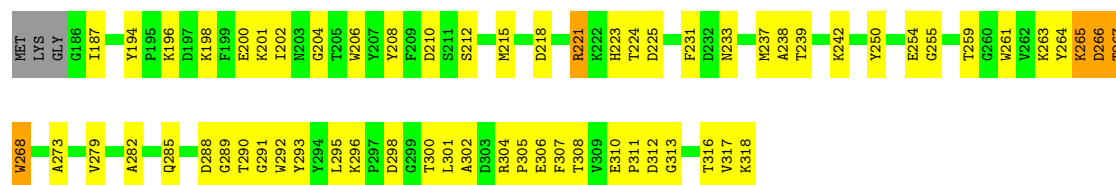
• Molecule 1: AUTOLYSIN

Chain A: 



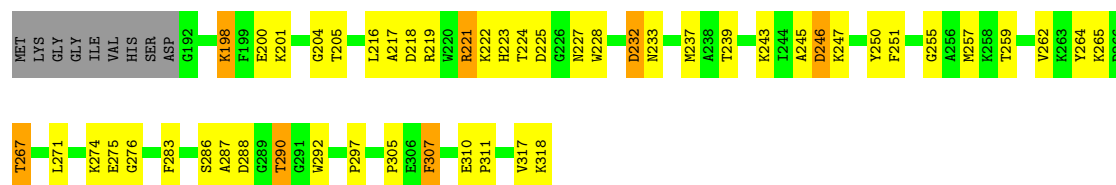
• Molecule 1: AUTOLYSIN

Chain B: 



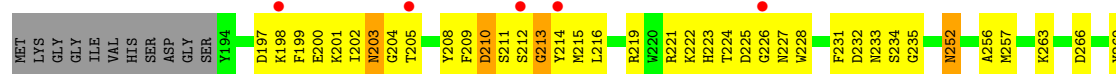
• Molecule 1: AUTOLYSIN

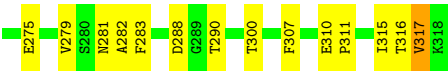
Chain C: 



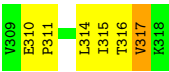
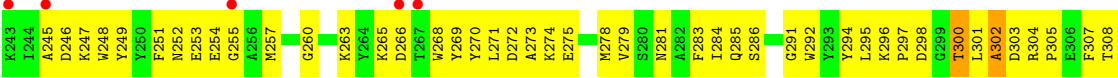
• Molecule 1: AUTOLYSIN

Chain D: 

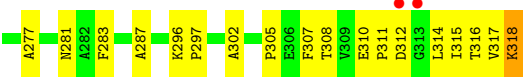
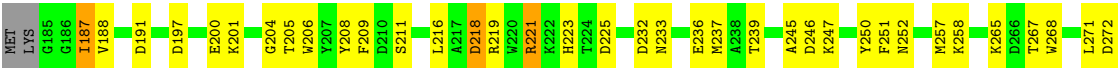




● Molecule 1: AUTOLYSIN



● Molecule 1: AUTOLYSIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	56.72Å 85.39Å 204.14Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (8.00-2.80) 94.1 (8.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.294 0.225 , 0.293	Depositor DCC
R_{free} test set	1994 reflections (7.86%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6651	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHT, DDQ, TRS

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	0.50	0/1101	0.90	4/1492 (0.3%)
1	B	0.47	0/1145	0.91	4/1552 (0.3%)
1	C	0.52	0/1101	0.89	2/1492 (0.1%)
1	D	0.42	0/1083	0.80	1/1468 (0.1%)
1	E	0.35	0/1070	0.71	1/1449 (0.1%)
1	F	0.49	0/1149	0.86	2/1557 (0.1%)
All	All	0.46	0/6649	0.85	14/9010 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLY	N-CA-C	7.64	123.78	114.69
1	B	265	LYS	N-CA-C	-6.88	101.72	111.56
1	A	220	TRP	N-CA-C	-6.82	101.34	110.55
1	B	268	TRP	N-CA-C	6.66	120.34	110.48
1	A	216	LEU	N-CA-C	-6.30	101.16	110.48
1	F	187	ILE	N-CA-C	6.20	118.58	108.97
1	A	199	PHE	N-CA-C	-5.94	102.53	110.55
1	C	307	PHE	N-CA-C	5.65	118.69	109.59
1	E	317	VAL	N-CA-C	5.61	116.02	108.17
1	D	213	GLY	N-CA-C	-5.50	106.91	114.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	VAL	N-CA-C	5.38	116.73	108.71
1	C	275	GLU	N-CA-C	5.08	119.19	113.15
1	F	268	TRP	N-CA-C	5.06	118.37	110.32
1	A	213	GLY	N-CA-C	-5.02	108.14	115.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	TYR	Sidechain

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	1061	0	970	38	0
1	B	1104	0	1009	43	0
1	C	1061	0	970	38	0
1	D	1044	0	955	48	0
1	E	1032	0	946	89	0
1	F	1108	0	1012	47	0
2	A	28	0	56	2	0
2	B	28	0	56	0	0
2	C	28	0	56	0	0
2	D	21	0	42	0	0
2	E	7	0	14	0	0
2	F	28	0	56	0	0
3	F	14	0	27	0	0
4	F	8	0	12	0	0
5	A	13	0	0	0	0
5	B	14	0	0	0	0
5	C	25	0	0	1	0
5	D	11	0	0	1	0
5	F	16	0	0	1	0
All	All	6651	0	6181	288	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 23.

All (288) 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:E:219:ARG:HB2	1:E:219:ARG:HH11	1.16	1.06
1:A:219:ARG:HH11	1:A:219:ARG:HB3	1.17	1.05
1:A:219:ARG:HB3	1:A:219:ARG:NH1	1.75	1.02
1:F:216:LEU:HD22	1:F:219:ARG:HE	1.25	1.00
1:A:310:GLU:HB3	1:A:311:PRO:HD2	1.41	0.99
1:A:219:ARG:HH11	1:A:219:ARG:CB	1.80	0.94
1:D:310:GLU:HB3	1:D:311:PRO:HD2	1.55	0.89
1:D:252:ASN:HD21	1:D:256:ALA:H	1.19	0.89
1:B:201:LYS:HE2	1:B:204:GLY:HA2	1.58	0.86
1:E:219:ARG:HB2	1:E:219:ARG:NH1	1.90	0.84
1:D:263:LYS:HE2	1:D:266:ASP:HA	1.60	0.83
1:D:209:PHE:HA	1:D:215:MET:HA	1.60	0.83
1:A:265:LYS:O	1:A:267:THR:HG22	1.80	0.82
1:E:286:SER:HB3	1:F:314:LEU:HD11	1.66	0.78
1:A:315:ILE:HD13	1:B:307:PHE:HZ	1.50	0.77
1:B:308:THR:O	1:B:316:THR:HG22	1.84	0.76
1:C:307:PHE:HZ	1:D:315:ILE:HD13	1.51	0.75
1:B:198:LYS:HE2	1:B:200:GLU:OE1	1.85	0.75
1:D:223:HIS:HB3	1:D:225:ASP:OD1	1.86	0.75
1:D:199:PHE:O	1:D:200:GLU:HG3	1.87	0.74
1:C:201:LYS:NZ	1:C:204:GLY:HA2	2.02	0.74
1:D:222:LYS:HD3	1:D:228:TRP:CE2	2.23	0.74
1:E:247:LYS:HB3	1:E:249:TYR:HE1	1.53	0.74
1:E:222:LYS:HE3	1:E:228:TRP:HE1	1.52	0.73
1:B:265:LYS:O	1:B:267:THR:HG23	1.88	0.73
1:E:271:LEU:HD23	1:E:278:MET:HA	1.71	0.72
1:D:209:PHE:CD1	1:D:215:MET:HB3	2.24	0.72
1:B:308:THR:HB	1:B:316:THR:HG23	1.70	0.71
1:D:252:ASN:ND2	1:D:256:ALA:H	1.89	0.71
1:E:198:LYS:HD2	1:E:199:PHE:H	1.55	0.70
1:E:201:LYS:HG3	1:E:205:THR:C	2.17	0.69
1:A:264:TYR:O	1:A:267:THR:HG23	1.94	0.68
1:A:274:LYS:HG3	1:A:275:GLU:OE2	1.93	0.68
1:E:206:TRP:HB2	1:E:237:MET:HB2	1.76	0.67
1:F:221:ARG:HG2	1:F:221:ARG:HH11	1.60	0.67
1:E:237:MET:HA	1:E:237:MET:HE3	1.75	0.67
1:F:310:GLU:HB2	1:F:312:ASP:OD2	1.95	0.66
1:D:215:MET:HE3	1:D:235:GLY:HA3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:THR:HB	1:B:316:THR:CG2	2.25	0.65
1:E:307:PHE:HZ	1:F:315:ILE:HD13	1.60	0.65
1:E:310:GLU:HB3	1:E:311:PRO:HD2	1.78	0.65
1:C:243:LYS:NZ	1:C:246:ASP:HA	2.13	0.64
1:F:310:GLU:HB3	1:F:311:PRO:HD2	1.79	0.64
1:A:223:HIS:CG	1:A:224:THR:H	2.15	0.64
1:D:252:ASN:HD21	1:D:256:ALA:N	1.95	0.63
1:F:250:TYR:CE2	1:F:258:LYS:HD3	2.33	0.63
1:B:187:ILE:HD11	1:B:202:ILE:CD1	2.29	0.63
1:C:317:VAL:HG12	1:C:318:LYS:N	2.14	0.63
1:D:222:LYS:HD3	1:D:228:TRP:CZ2	2.34	0.62
1:E:201:LYS:O	1:E:202:ILE:HD13	1.99	0.62
1:C:297:PRO:HD2	5:C:2023:HOH:O	1.99	0.62
1:E:252:ASN:OD1	1:E:254:GLU:HB2	1.99	0.62
1:B:223:HIS:CE1	1:B:224:THR:HG22	2.34	0.62
1:C:217:ALA:O	1:C:219:ARG:HG2	2.00	0.62
1:E:221:ARG:HE	1:E:222:LYS:N	1.98	0.61
1:E:196:LYS:HB2	1:E:213:GLY:HA2	1.83	0.61
1:A:288:ASP:OD2	1:A:290:THR:HB	2.01	0.60
1:F:245:ALA:O	1:F:246:ASP:HB2	2.01	0.60
1:C:317:VAL:HG12	1:C:318:LYS:H	1.65	0.60
1:B:223:HIS:HB3	1:B:225:ASP:OD1	2.02	0.60
1:E:201:LYS:HG3	1:E:205:THR:O	2.01	0.59
1:F:302:ALA:CB	1:F:305:PRO:HG3	2.31	0.59
1:E:221:ARG:HA	1:E:221:ARG:NE	2.17	0.59
1:B:261:TRP:CH2	1:B:295:LEU:HD21	2.38	0.59
1:B:259:THR:HB	1:B:273:ALA:HA	1.85	0.59
1:C:201:LYS:HZ3	1:C:204:GLY:HA2	1.68	0.59
1:D:209:PHE:CE1	1:D:215:MET:HB3	2.39	0.58
1:F:216:LEU:CD2	1:F:219:ARG:HE	2.10	0.58
1:E:208:TYR:HD2	1:E:209:PHE:H	1.51	0.58
1:E:239:THR:HG23	1:E:252:ASN:O	2.03	0.58
1:F:216:LEU:HD22	1:F:219:ARG:NE	2.09	0.58
1:E:304:ARG:NH2	1:F:311:PRO:HA	2.19	0.58
1:E:281:ASN:HA	1:E:295:LEU:O	2.03	0.58
1:D:252:ASN:C	1:D:252:ASN:HD22	2.10	0.57
1:E:298:ASP:HB3	1:E:300:THR:HG22	1.85	0.57
1:F:318:LYS:HA	1:F:318:LYS:HE3	1.86	0.57
1:A:206:TRP:HB2	1:A:237:MET:HE2	1.86	0.57
1:A:310:GLU:HB3	1:A:311:PRO:CD	2.25	0.57
1:E:294:TYR:C	1:E:295:LEU:HD12	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:LYS:CE	1:E:228:TRP:HE1	2.17	0.57
1:D:252:ASN:ND2	1:D:256:ALA:N	2.52	0.57
1:E:265:LYS:O	1:E:266:ASP:HB2	2.04	0.57
1:E:247:LYS:HB3	1:E:249:TYR:CE1	2.38	0.57
1:E:265:LYS:O	1:E:265:LYS:HG2	2.03	0.57
1:F:223:HIS:HB3	1:F:225:ASP:OD1	2.05	0.57
1:D:307:PHE:CE2	1:D:317:VAL:HG13	2.39	0.56
1:E:209:PHE:HB3	1:E:213:GLY:O	2.06	0.56
1:E:296:LYS:HG3	1:E:302:ALA:HB2	1.87	0.56
1:E:208:TYR:HD2	1:E:209:PHE:N	2.03	0.56
1:E:209:PHE:HA	1:E:215:MET:HA	1.87	0.56
1:B:310:GLU:HB3	1:B:311:PRO:HD2	1.86	0.56
1:C:259:THR:HA	1:C:271:LEU:HB2	1.87	0.56
1:A:270:TYR:HB3	1:A:295:LEU:HD11	1.87	0.56
1:C:310:GLU:HB3	1:C:311:PRO:HD2	1.88	0.56
1:B:208:TYR:O	1:B:215:MET:HA	2.06	0.56
1:D:224:THR:C	1:D:226:GLY:H	2.14	0.55
1:F:250:TYR:HE2	1:F:258:LYS:HD3	1.70	0.55
1:F:187:ILE:HD12	1:F:200:GLU:HG2	1.89	0.55
1:F:283:PHE:HZ	1:F:317:VAL:HG21	1.71	0.55
1:E:238:ALA:O	1:E:255:GLY:HA2	2.06	0.55
1:F:206:TRP:HB2	1:F:237:MET:HE2	1.88	0.55
1:C:237:MET:SD	1:C:255:GLY:HA3	2.46	0.54
1:D:222:LYS:O	1:D:222:LYS:HG3	2.07	0.54
1:E:203:ASN:C	1:E:203:ASN:HD22	2.15	0.54
1:C:216:LEU:HD11	1:C:221:ARG:HG3	1.89	0.54
1:B:304:ARG:N	1:B:305:PRO:CD	2.70	0.54
1:A:270:TYR:HB3	1:A:295:LEU:CD1	2.38	0.54
1:A:310:GLU:CD	1:A:314:LEU:HD23	2.33	0.54
1:C:288:ASP:OD2	1:C:290:THR:HB	2.08	0.54
1:C:223:HIS:CE1	1:C:224:THR:HG22	2.43	0.53
1:D:221:ARG:HB3	1:D:231:PHE:HE1	1.73	0.53
1:E:223:HIS:HB3	1:E:225:ASP:OD1	2.06	0.53
1:B:288:ASP:O	1:B:290:THR:N	2.42	0.53
1:C:198:LYS:HE3	1:C:200:GLU:OE1	2.08	0.53
1:F:296:LYS:HB3	1:F:297:PRO:CD	2.39	0.53
1:E:294:TYR:O	1:E:295:LEU:HD12	2.09	0.53
1:E:285:GLN:HB2	1:E:292:TRP:CZ3	2.43	0.53
1:F:302:ALA:HB1	1:F:305:PRO:HG3	1.90	0.52
1:A:250:TYR:HB3	1:A:271:LEU:HD11	1.91	0.52
1:C:201:LYS:HZ1	1:C:204:GLY:HA2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:TYR:CE2	1:C:265:LYS:HE2	2.44	0.52
1:E:270:TYR:HB3	1:E:295:LEU:HD21	1.91	0.52
1:B:264:TYR:O	1:B:265:LYS:HB2	2.10	0.52
1:C:245:ALA:O	1:C:246:ASP:CG	2.53	0.52
1:A:223:HIS:CG	1:A:224:THR:N	2.75	0.52
1:E:198:LYS:CD	1:E:199:PHE:H	2.20	0.51
1:E:208:TYR:O	1:E:216:LEU:HD13	2.10	0.51
1:E:231:PHE:HB3	1:E:235:GLY:HA2	1.93	0.51
1:A:221:ARG:HD3	1:A:221:ARG:C	2.35	0.51
1:B:221:ARG:O	1:B:221:ARG:HG3	2.10	0.51
1:B:288:ASP:C	1:B:290:THR:H	2.18	0.51
1:B:295:LEU:HD23	1:B:301:LEU:HA	1.93	0.51
1:F:197:ASP:HA	1:F:209:PHE:O	2.11	0.51
1:D:227:ASN:N	1:D:227:ASN:HD22	2.07	0.51
1:D:288:ASP:OD2	1:D:290:THR:HB	2.11	0.51
1:E:202:ILE:O	1:E:203:ASN:HB3	2.11	0.51
1:B:254:GLU:HA	1:B:254:GLU:OE2	2.12	0.50
1:C:218:ASP:OD2	1:C:233:ASN:HA	2.12	0.50
1:C:221:ARG:NH1	1:C:223:HIS:ND1	2.60	0.50
1:A:243:LYS:HE3	1:A:246:ASP:HA	1.94	0.50
1:E:218:ASP:OD2	1:E:233:ASN:HA	2.11	0.50
1:E:310:GLU:HB2	1:E:314:LEU:HB3	1.93	0.49
1:F:221:ARG:HH11	1:F:221:ARG:CG	2.25	0.49
1:D:252:ASN:ND2	1:D:252:ASN:C	2.69	0.49
1:B:263:LYS:HG2	1:B:266:ASP:HA	1.95	0.49
1:E:198:LYS:N	1:E:208:TYR:CE2	2.80	0.49
1:E:232:ASP:OD1	1:E:236:GLU:HB2	2.12	0.49
1:F:265:LYS:HB2	5:F:2013:HOH:O	2.12	0.49
1:E:279:VAL:HG11	1:E:284:ILE:HD11	1.94	0.49
1:E:241:TRP:O	1:E:242:LYS:HD3	2.13	0.49
1:D:269:TYR:CE2	1:D:300:THR:HG22	2.48	0.49
1:F:271:LEU:O	1:F:272:ASP:C	2.56	0.49
1:D:203:ASN:O	1:D:205:THR:N	2.46	0.49
1:D:211:SER:C	1:D:213:GLY:H	2.20	0.49
1:B:285:GLN:HG3	1:B:291:GLY:O	2.13	0.48
1:D:201:LYS:O	1:D:203:ASN:N	2.45	0.48
1:D:212:SER:C	1:D:214:TYR:H	2.20	0.48
1:E:302:ALA:O	1:E:305:PRO:HD3	2.12	0.48
1:F:252:ASN:OD1	1:F:252:ASN:C	2.55	0.48
1:E:221:ARG:NE	1:E:221:ARG:CA	2.76	0.48
1:E:198:LYS:N	1:E:208:TYR:HE2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:TRP:N	1:E:220:TRP:CD1	2.82	0.48
1:E:304:ARG:HH21	1:F:311:PRO:HA	1.76	0.48
1:B:298:ASP:OD2	1:B:300:THR:OG1	2.30	0.48
1:B:285:GLN:HB2	1:B:292:TRP:CZ3	2.48	0.48
1:E:208:TYR:CD2	1:E:209:PHE:N	2.82	0.48
1:A:219:ARG:NH1	1:A:219:ARG:CB	2.55	0.47
1:D:198:LYS:HD2	1:D:200:GLU:OE1	2.13	0.47
1:B:194:TYR:CE2	1:B:196:LYS:HD3	2.48	0.47
1:B:296:LYS:HG2	1:B:302:ALA:HB2	1.96	0.47
1:B:265:LYS:O	1:B:267:THR:CG2	2.62	0.47
1:F:302:ALA:HB3	1:F:305:PRO:HG3	1.97	0.46
1:B:304:ARG:HG2	1:B:304:ARG:HH11	1.81	0.46
1:C:283:PHE:CZ	1:C:317:VAL:HG21	2.49	0.46
1:D:208:TYR:HD2	1:D:216:LEU:HD12	1.81	0.46
1:E:210:ASP:O	1:E:211:SER:C	2.58	0.46
1:E:216:LEU:CD1	1:E:216:LEU:N	2.78	0.46
1:E:221:ARG:HE	1:E:221:ARG:CA	2.29	0.46
1:D:216:LEU:HD22	1:D:219:ARG:HD2	1.97	0.46
1:C:264:TYR:O	1:C:267:THR:HG23	2.15	0.46
1:B:206:TRP:HB2	1:B:237:MET:HE2	1.97	0.46
1:E:274:LYS:HE3	1:E:275:GLU:OE2	2.15	0.46
1:E:301:LEU:O	1:E:303:ASP:N	2.49	0.46
1:A:283:PHE:CZ	1:A:317:VAL:HG21	2.51	0.45
1:E:283:PHE:HZ	1:E:317:VAL:HG21	1.80	0.45
1:B:312:ASP:C	1:B:312:ASP:OD2	2.59	0.45
1:C:227:ASN:HD22	1:C:227:ASN:N	2.14	0.45
1:F:307:PHE:CD1	1:F:307:PHE:N	2.84	0.45
1:D:283:PHE:HZ	1:D:317:VAL:HG21	1.81	0.45
1:C:259:THR:HG22	1:C:276:GLY:HA2	1.99	0.45
1:E:221:ARG:HE	1:E:221:ARG:C	2.23	0.45
1:C:201:LYS:HA	1:C:205:THR:O	2.17	0.45
1:E:308:THR:HB	1:E:316:THR:OG1	2.17	0.45
1:A:294:TYR:CD2	1:A:317:VAL:HG11	2.52	0.45
1:C:223:HIS:HB3	1:C:225:ASP:OD1	2.16	0.45
1:E:247:LYS:O	1:E:249:TYR:HD1	2.00	0.45
1:C:307:PHE:CZ	1:D:315:ILE:HD13	2.40	0.45
1:A:254:GLU:O	2:A:401:CHT:H81	2.17	0.45
1:B:218:ASP:OD2	1:B:233:ASN:OD1	2.35	0.45
1:A:241:TRP:HB3	1:A:248:TRP:CZ3	2.52	0.44
1:B:238:ALA:HB1	1:B:242:LYS:HG3	1.99	0.44
1:D:199:PHE:C	1:D:200:GLU:HG3	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LYS:HD2	1:F:206:TRP:NE1	2.32	0.44
1:D:216:LEU:O	1:D:235:GLY:HA2	2.18	0.44
1:E:216:LEU:N	1:E:216:LEU:HD12	2.33	0.44
1:F:208:TYR:CZ	1:F:221:ARG:NH1	2.85	0.44
1:D:215:MET:HE1	1:D:234:SER:O	2.18	0.44
1:E:201:LYS:HD3	1:E:206:TRP:NE1	2.32	0.44
1:A:205:THR:CG2	1:A:236:GLU:HG3	2.48	0.44
1:A:272:ASP:OD1	1:A:274:LYS:HB3	2.18	0.44
1:C:305:PRO:HG3	1:D:315:ILE:HD11	1.99	0.44
1:B:279:VAL:CG1	1:B:282:ALA:HB3	2.48	0.44
1:D:281:ASN:C	1:D:281:ASN:HD22	2.25	0.44
1:E:304:ARG:NH2	1:F:310:GLU:C	2.76	0.44
1:C:250:TYR:HB3	1:C:271:LEU:HD11	2.00	0.44
1:E:294:TYR:HE2	1:E:296:LYS:HG2	1.83	0.44
1:F:247:LYS:HD3	1:F:277:ALA:CB	2.48	0.44
1:A:248:TRP:CE2	2:A:403:CHT:HC42	2.52	0.43
1:D:224:THR:C	1:D:226:GLY:N	2.77	0.43
1:E:205:THR:HB	1:E:207:TYR:CE1	2.53	0.43
1:A:252:ASN:ND2	1:A:256:ALA:HB3	2.34	0.43
1:F:221:ARG:CG	1:F:221:ARG:NH1	2.82	0.43
1:E:269:TYR:HE2	1:E:300:THR:HA	1.84	0.43
1:E:296:LYS:HB3	1:E:297:PRO:HD2	2.01	0.43
1:E:315:ILE:HD13	1:F:307:PHE:HZ	1.82	0.43
1:F:206:TRP:CB	1:F:237:MET:HE2	2.48	0.43
1:D:210:ASP:N	1:D:214:TYR:O	2.51	0.43
1:D:211:SER:C	1:D:213:GLY:N	2.77	0.43
1:A:210:ASP:HB3	1:A:216:LEU:HD21	2.00	0.43
1:B:261:TRP:HB3	1:B:268:TRP:CE3	2.53	0.43
1:C:232:ASP:OD2	1:C:232:ASP:C	2.61	0.43
1:C:286:SER:O	1:C:287:ALA:C	2.62	0.43
1:D:203:ASN:C	1:D:205:THR:H	2.26	0.42
1:C:317:VAL:CG1	1:C:318:LYS:N	2.82	0.42
1:A:303:ASP:HA	1:B:313:GLY:HA3	2.00	0.42
1:E:304:ARG:NH2	1:F:311:PRO:CA	2.83	0.42
1:F:251:PHE:CE1	1:F:257:MET:HB2	2.54	0.42
1:B:298:ASP:OD2	1:B:298:ASP:C	2.62	0.42
1:C:305:PRO:HA	1:C:318:LYS:OXT	2.19	0.42
1:F:201:LYS:HE2	1:F:204:GLY:HA2	2.01	0.42
1:A:260:GLY:HA2	1:A:270:TYR:CE1	2.55	0.42
1:E:283:PHE:CZ	1:E:317:VAL:HG21	2.55	0.42
1:B:218:ASP:N	1:B:231:PHE:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:TYR:CZ	1:D:300:THR:HG22	2.55	0.42
1:B:210:ASP:C	1:B:212:SER:H	2.28	0.42
1:B:296:LYS:CG	1:B:302:ALA:HB2	2.49	0.42
1:B:306:GLU:OE1	1:B:318:LYS:HD2	2.20	0.42
1:D:221:ARG:HD3	1:D:221:ARG:C	2.45	0.42
1:E:224:THR:C	1:E:226:GLY:H	2.27	0.42
1:E:230:TRP:CZ3	1:E:232:ASP:HA	2.55	0.42
1:F:250:TYR:CD2	1:F:258:LYS:HD3	2.55	0.42
1:F:308:THR:HB	1:F:316:THR:OG1	2.19	0.42
1:D:279:VAL:CG1	1:D:282:ALA:HB3	2.49	0.41
1:E:263:LYS:HE3	1:E:268:TRP:CZ2	2.55	0.41
1:F:283:PHE:CZ	1:F:317:VAL:HG21	2.52	0.41
1:A:215:MET:HE3	1:A:215:MET:HB2	1.81	0.41
1:E:203:ASN:C	1:E:203:ASN:ND2	2.75	0.41
1:A:252:ASN:C	1:A:254:GLU:H	2.28	0.41
5:D:2008:HOH:O	1:F:287:ALA:HB1	2.20	0.41
1:E:210:ASP:O	1:E:213:GLY:N	2.54	0.41
1:E:221:ARG:HE	1:E:221:ARG:HA	1.84	0.41
1:E:291:GLY:HA3	1:F:314:LEU:HG	2.02	0.41
1:F:218:ASP:OD1	1:F:233:ASN:HA	2.20	0.41
1:F:187:ILE:HG22	1:F:188:VAL:N	2.35	0.41
1:A:274:LYS:HE3	1:A:275:GLU:OE2	2.20	0.41
1:C:251:PHE:CE1	1:C:257:MET:HB2	2.55	0.41
1:E:204:GLY:O	1:E:205:THR:HG23	2.20	0.41
1:F:191:ASP:OD1	1:F:191:ASP:C	2.64	0.41
1:C:246:ASP:OD1	1:C:247:LYS:HG3	2.20	0.41
1:C:250:TYR:HB3	1:C:271:LEU:CD1	2.51	0.41
1:E:202:ILE:O	1:E:203:ASN:CB	2.69	0.41
1:E:268:TRP:O	1:E:269:TYR:HD2	2.03	0.41
1:A:196:LYS:O	1:A:197:ASP:C	2.64	0.41
1:B:288:ASP:C	1:B:290:THR:N	2.79	0.41
1:C:222:LYS:HE2	1:C:228:TRP:CE2	2.56	0.41
1:D:221:ARG:HD2	1:D:223:HIS:ND1	2.36	0.41
1:E:198:LYS:CG	1:E:199:PHE:N	2.84	0.41
1:F:281:ASN:HB2	1:F:297:PRO:HA	2.02	0.41
1:D:257:MET:HE1	1:D:275:GLU:O	2.21	0.40
1:E:272:ASP:C	1:E:274:LYS:N	2.79	0.40
1:A:314:LEU:HB2	1:B:293:TYR:CE2	2.57	0.40
1:C:292:TRP:HZ2	1:D:281:ASN:ND2	2.20	0.40
1:E:251:PHE:CE1	1:E:257:MET:HB2	2.56	0.40
1:A:210:ASP:OD1	1:A:210:ASP:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:LYS:HE3	1:E:275:GLU:OE1	2.21	0.40
1:A:252:ASN:HD21	1:A:256:ALA:HB3	1.87	0.40
1:E:218:ASP:HA	1:E:230:TRP:CZ2	2.56	0.40
1:E:245:ALA:O	1:E:246:ASP:HB2	2.21	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	125/136 (92%)	115 (92%)	10 (8%)	0	100	100
1	B	131/136 (96%)	120 (92%)	9 (7%)	2 (2%)	8	28
1	C	125/136 (92%)	116 (93%)	7 (6%)	2 (2%)	7	27
1	D	123/136 (90%)	106 (86%)	11 (9%)	6 (5%)	1	6
1	E	121/136 (89%)	96 (79%)	19 (16%)	6 (5%)	1	5
1	F	132/136 (97%)	115 (87%)	16 (12%)	1 (1%)	16	44
All	All	757/816 (93%)	668 (88%)	72 (10%)	17 (2%)	5	19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	232	ASP
1	B	289	GLY
1	C	232	ASP
1	D	204	GLY
1	E	302	ALA
1	B	266	ASP
1	C	274	LYS
1	D	202	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	210	ASP
1	D	232	ASP
1	E	203	ASN
1	E	211	SER
1	D	197	ASP
1	D	203	ASN
1	E	260	GLY
1	E	273	ALA
1	F	232	ASP

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	105/112 (94%)	97 (92%)	8 (8%)	12	36
1	B	110/112 (98%)	107 (97%)	3 (3%)	39	74
1	C	105/112 (94%)	98 (93%)	7 (7%)	15	42
1	D	103/112 (92%)	99 (96%)	4 (4%)	28	64
1	E	102/112 (91%)	96 (94%)	6 (6%)	18	48
1	F	110/112 (98%)	102 (93%)	8 (7%)	13	38
All	All	635/672 (94%)	599 (94%)	36 (6%)	18	49

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	ARG
1	A	224	THR
1	A	239	THR
1	A	253	GLU
1	A	267	THR
1	A	290	THR
1	A	308	THR
1	A	316	THR
1	B	221	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	239	THR
1	B	267	THR
1	C	198	LYS
1	C	221	ARG
1	C	239	THR
1	C	246	ASP
1	C	262	VAL
1	C	267	THR
1	C	290	THR
1	D	233	ASN
1	D	252	ASN
1	D	316	THR
1	D	317	VAL
1	E	199	PHE
1	E	209	PHE
1	E	219	ARG
1	E	248	TRP
1	E	253	GLU
1	E	300	THR
1	F	205	THR
1	F	211	SER
1	F	218	ASP
1	F	221	ARG
1	F	236	GLU
1	F	239	THR
1	F	267	THR
1	F	318	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	227	ASN
1	B	203	ASN
1	B	227	ASN
1	B	281	ASN
1	C	227	ASN
1	C	281	ASN
1	D	227	ASN
1	D	233	ASN
1	D	252	ASN
1	D	281	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	203	ASN
1	E	223	HIS
1	F	203	ASN
1	F	227	ASN
1	F	233	ASN
1	F	281	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	CHT	A	404	-	6,6,6	0.94	0	8,8,8	0.54	0
2	CHT	D	402	-	6,6,6	1.04	1 (16%)	8,8,8	0.52	0
2	CHT	F	401	-	6,6,6	1.09	1 (16%)	8,8,8	0.50	0
2	CHT	C	401	-	6,6,6	0.93	0	8,8,8	0.55	0
2	CHT	A	402	-	6,6,6	0.92	0	8,8,8	0.57	0
2	CHT	A	403	-	6,6,6	0.88	0	8,8,8	0.48	0
2	CHT	B	402	-	6,6,6	0.90	0	8,8,8	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHT	B	404	-	6,6,6	1.15	1 (16%)	8,8,8	0.50	0
2	CHT	B	403	-	6,6,6	1.01	0	8,8,8	0.57	0
2	CHT	F	402	-	6,6,6	1.24	1 (16%)	8,8,8	0.47	0
3	DDQ	F	404	-	11,13,13	2.58	1 (9%)	12,15,15	1.51	3 (25%)
2	CHT	C	404	-	6,6,6	1.09	1 (16%)	8,8,8	0.47	0
2	CHT	D	403	-	6,6,6	1.13	1 (16%)	8,8,8	0.50	0
4	TRS	F	1319	-	7,7,7	0.47	0	9,9,9	4.07	4 (44%)
2	CHT	B	401	-	6,6,6	1.03	0	8,8,8	0.52	0
2	CHT	D	404	-	6,6,6	1.11	1 (16%)	8,8,8	0.51	0
2	CHT	F	403	-	6,6,6	0.93	0	8,8,8	0.52	0
2	CHT	E	414	-	6,6,6	1.09	1 (16%)	8,8,8	0.52	0
2	CHT	A	401	-	6,6,6	0.91	0	8,8,8	0.52	0
2	CHT	F	400	-	6,6,6	1.08	1 (16%)	8,8,8	0.54	0
2	CHT	C	403	-	6,6,6	1.13	1 (16%)	8,8,8	0.50	0
2	CHT	C	402	-	6,6,6	1.01	0	8,8,8	0.55	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	CHT	A	404	-	-	3/4/4/4	-
2	CHT	D	402	-	-	3/4/4/4	-
2	CHT	F	401	-	-	4/4/4/4	-
2	CHT	C	401	-	-	3/4/4/4	-
2	CHT	A	402	-	-	3/4/4/4	-
2	CHT	A	403	-	-	3/4/4/4	-
2	CHT	B	402	-	-	4/4/4/4	-
2	CHT	B	404	-	-	4/4/4/4	-
2	CHT	B	403	-	-	4/4/4/4	-
2	CHT	F	402	-	-	3/4/4/4	-
3	DDQ	F	404	-	-	3/11/11/11	-
2	CHT	C	404	-	-	4/4/4/4	-
2	CHT	D	403	-	-	3/4/4/4	-
4	TRS	F	1319	-	-	8/9/9/9	-
2	CHT	B	401	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHT	D	404	-	-	3/4/4/4	-
2	CHT	F	403	-	-	4/4/4/4	-
2	CHT	E	414	-	-	4/4/4/4	-
2	CHT	A	401	-	-	4/4/4/4	-
2	CHT	F	400	-	-	4/4/4/4	-
2	CHT	C	403	-	-	4/4/4/4	-
2	CHT	C	402	-	-	3/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	404	DDQ	O1-N1	-8.08	1.22	1.42
2	F	402	CHT	C5-C4	2.47	1.61	1.51
2	D	404	CHT	C5-C4	2.24	1.60	1.51
2	B	404	CHT	C5-C4	2.22	1.60	1.51
2	F	401	CHT	C5-C4	2.21	1.60	1.51
2	D	403	CHT	C5-C4	2.20	1.60	1.51
2	C	403	CHT	C5-C4	2.17	1.59	1.51
2	C	404	CHT	C5-C4	2.10	1.59	1.51
2	E	414	CHT	C5-C4	2.08	1.59	1.51
2	D	402	CHT	C5-C4	2.05	1.59	1.51
2	F	400	CHT	C5-C4	2.01	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1319	TRS	O2-C2-C	7.80	132.61	110.88
4	F	1319	TRS	C2-C-C1	7.01	129.34	110.66
4	F	1319	TRS	C3-C-C1	-4.33	99.13	110.66
4	F	1319	TRS	C2-C-N	-3.19	100.04	108.17
3	F	404	DDQ	CM2-N1-C1	2.85	116.22	110.23
3	F	404	DDQ	CM1-N1-C1	-2.16	105.70	110.23
3	F	404	DDQ	C6-C5-C4	-2.09	103.78	114.37

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	403	CHT	O6-C4-C5-N1
4	F	1319	TRS	C2-C-C1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	1319	TRS	C3-C-C1-O1
4	F	1319	TRS	C1-C-C2-O2
4	F	1319	TRS	C3-C-C2-O2
4	F	1319	TRS	N-C-C2-O2
2	A	401	CHT	C4-C5-N1-C7
2	B	403	CHT	C4-C5-N1-C7
2	B	404	CHT	C4-C5-N1-C7
2	D	402	CHT	C4-C5-N1-C7
2	D	403	CHT	C4-C5-N1-C7
2	F	400	CHT	C4-C5-N1-C7
2	F	403	CHT	C4-C5-N1-C7
2	A	401	CHT	O6-C4-C5-N1
2	B	403	CHT	O6-C4-C5-N1
2	B	404	CHT	O6-C4-C5-N1
2	C	403	CHT	O6-C4-C5-N1
2	C	404	CHT	O6-C4-C5-N1
2	E	414	CHT	O6-C4-C5-N1
2	A	402	CHT	C4-C5-N1-C7
2	A	403	CHT	C4-C5-N1-C7
2	A	404	CHT	C4-C5-N1-C7
2	B	401	CHT	C4-C5-N1-C7
2	B	401	CHT	C4-C5-N1-C8
2	B	402	CHT	C4-C5-N1-C7
2	C	401	CHT	C4-C5-N1-C7
2	C	402	CHT	C4-C5-N1-C7
2	C	403	CHT	C4-C5-N1-C7
2	C	404	CHT	C4-C5-N1-C7
2	D	404	CHT	C4-C5-N1-C7
2	E	414	CHT	C4-C5-N1-C7
2	F	401	CHT	C4-C5-N1-C7
2	F	402	CHT	C4-C5-N1-C7
2	A	401	CHT	C4-C5-N1-C6
2	A	402	CHT	C4-C5-N1-C6
2	A	402	CHT	C4-C5-N1-C8
2	A	404	CHT	C4-C5-N1-C6
2	A	404	CHT	C4-C5-N1-C8
2	B	401	CHT	C4-C5-N1-C6
2	B	404	CHT	C4-C5-N1-C6
2	C	401	CHT	C4-C5-N1-C6
2	D	402	CHT	C4-C5-N1-C6
2	D	402	CHT	C4-C5-N1-C8
2	D	403	CHT	C4-C5-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	404	CHT	C4-C5-N1-C6
2	D	404	CHT	C4-C5-N1-C8
2	F	400	CHT	C4-C5-N1-C6
2	F	401	CHT	C4-C5-N1-C6
3	F	404	DDQ	C6-C7-C8-C9
3	F	404	DDQ	C2-C3-C4-C5
2	A	401	CHT	C4-C5-N1-C8
2	A	403	CHT	C4-C5-N1-C6
2	A	403	CHT	C4-C5-N1-C8
2	B	402	CHT	C4-C5-N1-C6
2	B	402	CHT	C4-C5-N1-C8
2	B	403	CHT	C4-C5-N1-C6
2	B	403	CHT	C4-C5-N1-C8
2	B	404	CHT	C4-C5-N1-C8
2	C	401	CHT	C4-C5-N1-C8
2	C	402	CHT	C4-C5-N1-C6
2	C	402	CHT	C4-C5-N1-C8
2	C	403	CHT	C4-C5-N1-C6
2	C	403	CHT	C4-C5-N1-C8
2	C	404	CHT	C4-C5-N1-C6
2	C	404	CHT	C4-C5-N1-C8
2	D	403	CHT	C4-C5-N1-C8
2	E	414	CHT	C4-C5-N1-C6
2	E	414	CHT	C4-C5-N1-C8
2	F	400	CHT	C4-C5-N1-C8
2	F	401	CHT	C4-C5-N1-C8
2	F	402	CHT	C4-C5-N1-C6
2	F	402	CHT	C4-C5-N1-C8
2	F	403	CHT	C4-C5-N1-C6
2	F	403	CHT	C4-C5-N1-C8
2	B	401	CHT	O6-C4-C5-N1
2	F	400	CHT	O6-C4-C5-N1
2	B	402	CHT	O6-C4-C5-N1
4	F	1319	TRS	C1-C-C3-O3
4	F	1319	TRS	N-C-C3-O3
2	F	401	CHT	O6-C4-C5-N1
4	F	1319	TRS	N-C-C1-O1
3	F	404	DDQ	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	CHT	1	0
2	A	401	CHT	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

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(Å²)	Q<0.9	
1	A	127/136 (93%)	-0.54	0	100	100	8, 28, 45, 55	0
1	B	133/136 (97%)	-0.57	0	100	100	12, 26, 39, 53	0
1	C	127/136 (93%)	-0.75	0	100	100	7, 20, 35, 43	0
1	D	125/136 (91%)	-0.01	5 (4%)	42	33	11, 47, 92, 95	0
1	E	123/136 (90%)	0.78	11 (8%)	15	11	44, 91, 97, 98	0
1	F	134/136 (98%)	-0.56	2 (1%)	72	63	10, 23, 60, 74	0
All	All	769/816 (94%)	-0.29	18 (2%)	61	51	7, 29, 93, 98	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	312	ASP	3.9
1	D	198	LYS	3.0
1	E	209	PHE	2.7
1	E	245	ALA	2.6
1	E	224	THR	2.6
1	D	214	TYR	2.3
1	E	243	LYS	2.3
1	E	199	PHE	2.3
1	E	212	SER	2.3
1	E	214	TYR	2.3
1	E	266	ASP	2.3
1	D	212	SER	2.3
1	E	267	THR	2.2
1	D	205	THR	2.2
1	E	227	ASN	2.1
1	D	226	GLY	2.1
1	F	313	GLY	2.1
1	E	255	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CHT	E	414	7/7	0.72	0.16	91,91,92,92	0
2	CHT	F	402	7/7	0.76	0.19	37,38,46,48	0
2	CHT	F	401	7/7	0.80	0.18	49,51,56,57	0
2	CHT	D	402	7/7	0.81	0.12	66,67,68,69	0
2	CHT	A	403	7/7	0.81	0.16	83,83,84,86	0
2	CHT	D	404	7/7	0.82	0.11	42,43,47,48	0
4	TRS	F	1319	8/8	0.82	0.16	69,71,72,72	0
3	DDQ	F	404	14/14	0.83	0.15	54,59,61,61	0
2	CHT	D	403	7/7	0.83	0.14	67,67,68,69	0
2	CHT	A	402	7/7	0.86	0.13	45,46,50,52	0
2	CHT	C	401	7/7	0.89	0.13	51,52,53,54	0
2	CHT	C	402	7/7	0.90	0.14	55,56,59,60	0
2	CHT	C	403	7/7	0.90	0.10	37,38,40,41	0
2	CHT	B	402	7/7	0.90	0.12	42,42,45,47	0
2	CHT	B	404	7/7	0.90	0.10	36,37,37,38	0
2	CHT	A	401	7/7	0.90	0.11	32,33,39,41	0
2	CHT	A	404	7/7	0.91	0.08	32,33,34,37	0
2	CHT	F	400	7/7	0.92	0.10	70,71,71,71	0
2	CHT	B	401	7/7	0.94	0.08	35,37,39,40	0
2	CHT	C	404	7/7	0.95	0.11	24,28,32,34	0
2	CHT	F	403	7/7	0.95	0.09	21,22,26,30	0
2	CHT	B	403	7/7	0.96	0.07	29,30,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.