



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:52 AM GMT

PDB ID : 3G8W
Title : Crystal structure of a probable acetyltransferase from Staphylococcus epidermidis ATCC 12228
Authors : Tan, K.; Sather, A.; Marshall, N.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-02-12
Resolution : 2.70 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

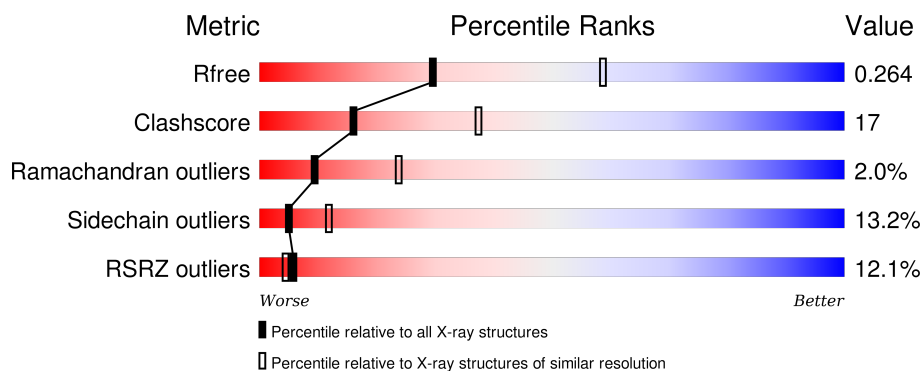
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	169	<div> <div>62%</div> <div>30%</div> <div>• •</div> </div>
1	B	169	<div> <div>11%</div> <div>63%</div> <div>28%</div> <div>7%</div> <div>•</div> </div>
1	C	169	<div> <div>3%</div> <div>55%</div> <div>35%</div> <div>6%</div> <div>•</div> </div>
1	D	169	<div> <div>31%</div> <div>57%</div> <div>32%</div> <div>6%</div> <div>5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NHE	A	167	-	-	-	X
2	NHE	A	168	-	-	-	X
2	NHE	A	169	-	-	-	X
2	NHE	B	168	-	-	-	X
2	NHE	B	169	-	-	-	X
2	NHE	C	167	-	-	-	X
2	NHE	C	169	-	-	-	X
2	NHE	C	170	-	-	-	X
2	NHE	C	171	-	-	X	X
3	FLC	C	172	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5447 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.

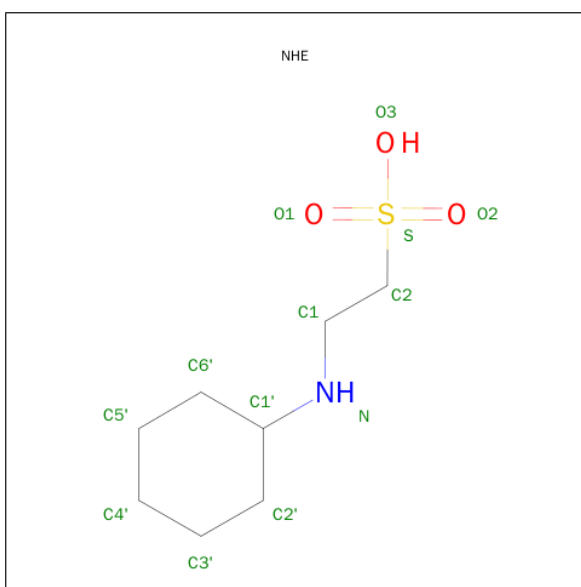
- Molecule 1 is a protein called Lactococcal prophage ps3 protein 05.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	Se	0	0	0
			1342	855	223	259	2	3			
1	B	164	Total	C	N	O	S	Se	0	0	0
			1348	859	225	259	2	3			
1	C	162	Total	C	N	O	S	Se	0	0	0
			1338	853	223	257	2	3			
1	D	161	Total	C	N	O	S	Se	0	0	0
			1229	777	211	236	2	3			

There are 12 discrepancies between the modelled and reference sequences:

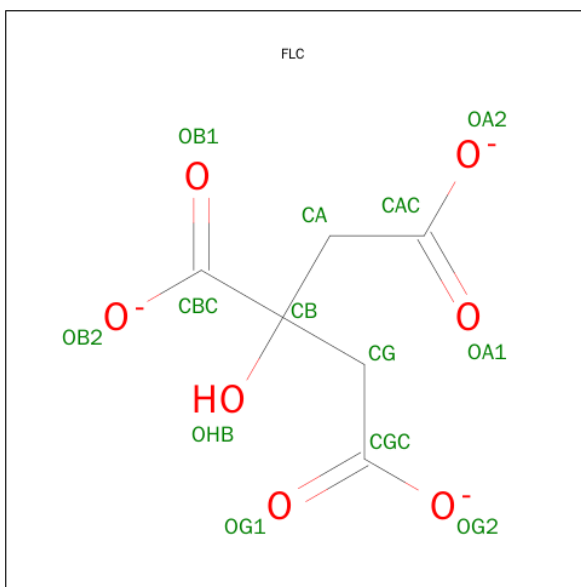
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8CPX3
A	-1	ASN	-	EXPRESSION TAG	UNP Q8CPX3
A	0	ALA	-	EXPRESSION TAG	UNP Q8CPX3
B	-2	SER	-	EXPRESSION TAG	UNP Q8CPX3
B	-1	ASN	-	EXPRESSION TAG	UNP Q8CPX3
B	0	ALA	-	EXPRESSION TAG	UNP Q8CPX3
C	-2	SER	-	EXPRESSION TAG	UNP Q8CPX3
C	-1	ASN	-	EXPRESSION TAG	UNP Q8CPX3
C	0	ALA	-	EXPRESSION TAG	UNP Q8CPX3
D	-2	SER	-	EXPRESSION TAG	UNP Q8CPX3
D	-1	ASN	-	EXPRESSION TAG	UNP Q8CPX3
D	0	ALA	-	EXPRESSION TAG	UNP Q8CPX3

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		

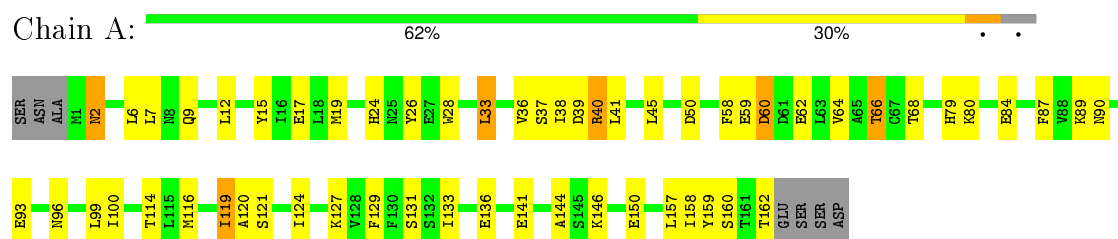
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	5	Total	O	0	0
			5	5		
4	C	8	Total	O	0	0
			8	8		
4	D	1	Total	O	0	0
			1	1		

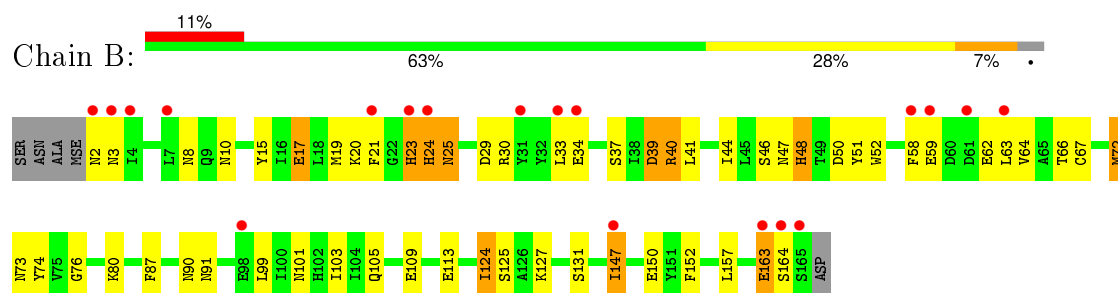
3 Residue-property plots

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.

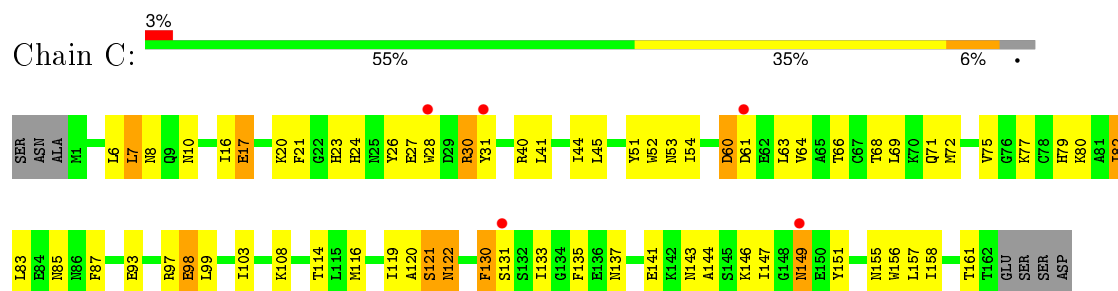
- Molecule 1: Lactococcal prophage ps3 protein 05



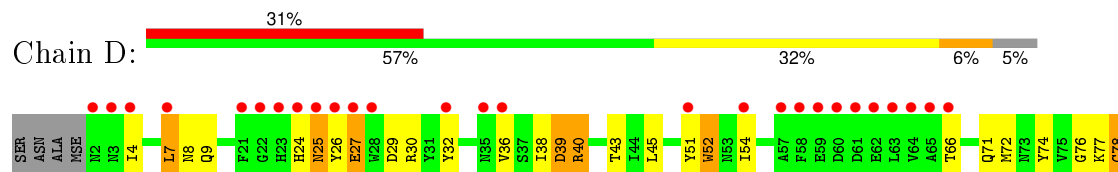
- Molecule 1: Lactococcal prophage ps3 protein 05

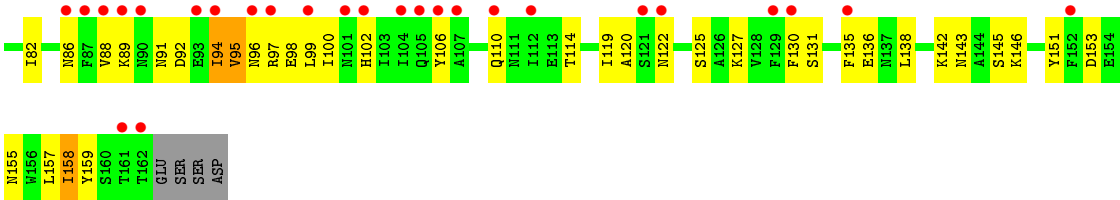


- Molecule 1: Lactococcal prophage ps3 protein 05



- Molecule 1: Lactococcal prophage ps3 protein 05





M155
M156
L157
I158
Y159
S160
T161
T162
GLU
SER
SER
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.96Å 110.41Å 220.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.70 49.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.39-2.70) 98.9 (49.36-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.213 , 0.256 0.219 , 0.264	Depositor DCC
R_{free} test set	1639 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 32409 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5447	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: NHE, FLC

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	0.89	0/1367	0.86	0/1845
1	B	0.69	0/1373	0.72	0/1853
1	C	0.84	2/1363 (0.1%)	0.82	0/1840
1	D	0.54	0/1249	0.67	0/1695
All	All	0.75	2/5352 (0.0%)	0.77	0/7233

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	GLU	CG-CD	5.16	1.59	1.51
1	C	130	PHE	CE2-CZ	5.08	1.47	1.37

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	1342	0	1283	38	0
1	B	1348	0	1286	44	0
1	C	1338	0	1279	48	0
1	D	1229	0	1099	50	0
2	A	39	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	51	3	0
2	C	65	0	85	18	0
2	D	13	0	17	2	0
3	C	13	0	5	3	0
4	A	7	0	0	0	0
4	B	5	0	0	2	0
4	C	8	0	0	1	0
4	D	1	0	0	0	0
All	All	5447	0	5155	179	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 17.

All (179) 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:116:MSE:HE1	2:B:168:NHE:HC11	1.33	1.05
1:A:19:MSE:HE2	1:A:87:PHE:CE2	1.94	1.01
1:B:23:HIS:HB2	1:B:87:PHE:HD1	1.28	0.99
1:B:23:HIS:HB2	1:B:87:PHE:CD1	2.08	0.88
1:A:89:LYS:O	1:A:90:ASN:HB2	1.70	0.88
1:D:32:TYR:O	1:D:36:VAL:HG12	1.73	0.86
1:D:127:LYS:HE2	1:D:155:ASN:HD22	1.45	0.81
1:A:19:MSE:CE	1:A:87:PHE:CE2	2.63	0.79
1:A:19:MSE:HB3	1:A:33:LEU:HD12	1.67	0.77
1:C:51:TYR:N	1:C:51:TYR:CD2	2.58	0.72
1:B:23:HIS:NE2	4:B:188:HOH:O	2.22	0.72
1:D:72:MSE:O	1:D:78:CYS:HB3	1.88	0.72
1:D:9:GLN:HA	1:D:45:LEU:HD13	1.72	0.72
1:A:59:GLU:O	1:A:60:ASP:HB2	1.91	0.71
1:C:141:GLU:HB3	1:C:144:ALA:HB2	1.71	0.70
1:C:75:VAL:HG22	2:C:171:NHE:H2'2	1.73	0.70
1:D:127:LYS:HE2	1:D:155:ASN:ND2	2.06	0.70
1:C:120:ALA:HB2	2:C:170:NHE:H5'2	1.75	0.69
1:B:15:TYR:CE2	1:B:19:MSE:HE3	2.27	0.68
1:A:68:THR:HB	1:A:84:GLU:HG3	1.76	0.67
1:D:40:ARG:O	1:D:43:THR:HB	1.96	0.66
1:B:72:MSE:HE2	1:B:80:LYS:HE2	1.77	0.66
1:D:66:THR:O	1:D:86:ASN:HA	1.96	0.66
1:B:76:GLY:N	2:B:169:NHE:O3	2.29	0.66
1:B:46:SER:HB3	1:B:48:HIS:HD2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:171:NHE:C2	1:D:40:ARG:HD3	2.28	0.64
1:B:163:GLU:HG2	1:B:163:GLU:O	1.99	0.63
1:C:143:ASN:HD22	1:C:151:TYR:HB3	1.64	0.63
1:B:46:SER:HB3	1:B:48:HIS:CD2	2.34	0.62
1:C:121:SER:HA	1:C:155:ASN:HD22	1.63	0.62
1:D:146:LYS:HD2	1:D:151:TYR:CE1	2.35	0.62
1:B:23:HIS:CB	1:B:87:PHE:HD1	2.09	0.61
1:A:89:LYS:O	1:A:90:ASN:CB	2.44	0.61
1:C:40:ARG:HD2	2:C:168:NHE:O2	2.02	0.60
1:D:138:LEU:HD22	1:D:158:ILE:HG21	1.83	0.60
1:D:76:GLY:H	2:D:167:NHE:H6'2	1.66	0.60
1:A:19:MSE:HE2	1:A:87:PHE:HE2	1.64	0.59
1:C:72:MSE:HB2	1:C:77:LYS:O	2.02	0.59
1:B:124:ILE:CD1	1:B:124:ILE:H	2.14	0.59
1:B:40:ARG:O	1:B:44:ILE:HG13	2.03	0.59
1:A:119:ILE:HD13	1:A:157:LEU:HD22	1.85	0.58
1:B:124:ILE:N	1:B:124:ILE:CD1	2.67	0.58
1:D:4:ILE:HD13	1:D:102:HIS:HB2	1.86	0.57
2:C:171:NHE:HC21	1:D:40:ARG:HH21	1.68	0.57
1:C:63:LEU:HD11	1:C:66:THR:HG22	1.85	0.57
1:C:24:HIS:HD2	1:C:26:TYR:H	1.52	0.57
1:B:124:ILE:HD12	1:B:124:ILE:H	1.70	0.56
1:C:28:TRP:CZ2	2:C:170:NHE:HC22	2.41	0.56
1:C:8:ASN:OD1	1:C:10:ASN:HB2	2.06	0.56
1:C:16:ILE:HG22	1:C:20:LYS:HE2	1.87	0.55
1:A:2:ASN:HA	1:A:58:PHE:O	2.06	0.55
1:C:24:HIS:CD2	1:C:26:TYR:H	2.23	0.55
1:D:136:GLU:HA	1:D:136:GLU:OE1	2.06	0.55
1:A:160:SER:HB3	1:A:162:THR:HG23	1.88	0.55
1:A:24:HIS:HD2	1:A:26:TYR:H	1.55	0.55
1:D:25:ASN:C	1:D:27:GLU:H	2.09	0.54
1:D:119:ILE:HD13	1:D:157:LEU:HD13	1.89	0.54
1:C:75:VAL:H	2:C:171:NHE:HC12	1.73	0.54
1:B:51:TYR:CD2	1:B:51:TYR:N	2.75	0.54
1:A:28:TRP:CE3	2:A:169:NHE:H6'1	2.43	0.54
1:B:163:GLU:CG	1:B:163:GLU:O	2.55	0.54
1:D:30:ARG:HD2	1:D:30:ARG:H	1.73	0.54
1:C:133:ILE:HG22	1:C:133:ILE:O	2.07	0.53
1:A:19:MSE:CE	1:A:87:PHE:HE2	2.18	0.53
1:A:141:GLU:HB3	1:A:144:ALA:HB2	1.90	0.53
1:D:158:ILE:HG12	1:D:159:TYR:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:HE1	1:A:66:THR:HG21	1.74	0.53
1:C:75:VAL:HG23	2:C:171:NHE:HC12	1.89	0.53
2:C:168:NHE:HC22	1:D:74:TYR:CD1	2.44	0.52
1:C:72:MSE:HE3	1:C:82:ILE:HG23	1.90	0.52
1:D:127:LYS:O	1:D:131:SER:HB2	2.10	0.52
1:C:28:TRP:CE2	2:C:170:NHE:HC22	2.44	0.52
1:C:93:GLU:OE1	2:C:169:NHE:H5'1	2.09	0.52
1:B:127:LYS:O	1:B:131:SER:CB	2.58	0.52
1:B:23:HIS:O	1:B:29:ASP:CB	2.58	0.51
1:B:124:ILE:HD13	1:B:125:SER:H	1.75	0.51
1:A:36:VAL:HG22	1:A:37:SER:N	2.26	0.51
1:D:120:ALA:HA	1:D:153:ASP:O	2.11	0.51
1:C:97:ARG:HH22	2:C:169:NHE:HC22	1.76	0.51
1:D:51:TYR:HB3	1:D:71:GLN:HB3	1.93	0.51
1:A:58:PHE:HA	1:A:62:GLU:O	2.11	0.50
1:B:127:LYS:O	1:B:131:SER:HB3	2.11	0.50
1:D:143:ASN:N	1:D:143:ASN:HD22	2.09	0.50
1:A:24:HIS:CD2	1:A:26:TYR:H	2.29	0.50
1:D:94:ILE:HG22	1:D:95:VAL:N	2.26	0.50
1:B:59:GLU:HB2	1:B:64:VAL:HG21	1.92	0.50
2:C:168:NHE:HC22	1:D:74:TYR:HD1	1.77	0.49
1:B:105:GLN:HG3	1:B:109:GLU:OE2	2.13	0.49
1:C:7:LEU:HD22	1:C:54:ILE:HG22	1.95	0.49
1:A:127:LYS:O	1:A:131:SER:HB3	2.13	0.49
1:A:158:ILE:HG12	1:A:159:TYR:N	2.27	0.49
1:C:121:SER:HA	1:C:155:ASN:ND2	2.28	0.48
1:B:157:LEU:N	1:B:157:LEU:HD12	2.27	0.48
1:A:59:GLU:O	1:A:60:ASP:CB	2.58	0.48
1:D:71:GLN:HG2	1:D:72:MSE:N	2.29	0.48
1:C:21:PHE:HB3	1:C:23:HIS:CD2	2.48	0.48
2:C:171:NHE:HC21	1:D:40:ARG:NH2	2.27	0.48
2:A:168:NHE:HC11	1:B:74:TYR:CD1	2.48	0.48
1:B:23:HIS:CE1	4:B:188:HOH:O	2.64	0.48
1:C:83:LEU:HD21	1:C:103:ILE:HG21	1.96	0.47
1:C:108:LYS:HG2	1:C:161:THR:HG23	1.95	0.47
1:C:85:ASN:HB3	1:C:87:PHE:CE2	2.49	0.47
2:C:171:NHE:HC22	1:D:40:ARG:HD3	1.96	0.47
1:A:36:VAL:HG22	1:A:37:SER:H	1.80	0.47
1:B:90:ASN:O	1:B:91:ASN:CB	2.62	0.47
1:D:96:ASN:O	1:D:100:ILE:HD12	2.14	0.47
1:B:37:SER:HB2	1:B:39:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD11	1:C:53:ASN:HB3	1.97	0.47
1:D:36:VAL:HG13	1:D:36:VAL:O	2.15	0.47
1:A:120:ALA:HB2	2:A:169:NHE:H2'2	1.95	0.47
1:A:127:LYS:O	1:A:131:SER:CB	2.63	0.47
1:C:156:TRP:CZ2	3:C:172:FLC:OB2	2.68	0.47
2:C:171:NHE:N	1:D:40:ARG:HD3	2.30	0.47
1:C:27:GLU:OE1	1:C:30:ARG:NH2	2.48	0.46
1:C:52:TRP:O	4:C:177:HOH:O	2.20	0.46
1:C:156:TRP:CE2	3:C:172:FLC:OB2	2.69	0.46
1:B:124:ILE:N	1:B:124:ILE:HD13	2.31	0.46
1:C:8:ASN:HA	1:C:45:LEU:O	2.15	0.46
1:C:146:LYS:HE3	1:C:149:ASN:HA	1.98	0.46
1:B:23:HIS:CB	1:B:87:PHE:CD1	2.90	0.46
1:D:7:LEU:HB2	1:D:54:ILE:O	2.16	0.45
1:D:7:LEU:HD22	1:D:54:ILE:HG21	1.98	0.45
1:C:116:MSE:HE1	3:C:172:FLC:HG1	1.99	0.45
1:D:38:ILE:O	1:D:39:ASP:C	2.54	0.45
1:B:147:ILE:HB	1:B:152:PHE:HE2	1.81	0.45
1:B:58:PHE:CZ	1:B:63:LEU:HD13	2.52	0.45
1:D:72:MSE:C	1:D:78:CYS:HB3	2.37	0.45
1:D:52:TRP:CE3	1:D:52:TRP:N	2.85	0.45
1:D:130:PHE:O	1:D:135:PHE:HB2	2.17	0.44
1:C:60:ASP:HB3	1:C:61:ASP:H	1.67	0.44
1:A:133:ILE:O	1:A:133:ILE:HG22	2.17	0.44
1:A:19:MSE:CB	1:A:33:LEU:HD12	2.44	0.44
1:D:138:LEU:HD22	1:D:158:ILE:CG2	2.46	0.44
1:C:98:GLU:HG2	1:C:98:GLU:H	1.59	0.44
1:D:4:ILE:HB	1:D:102:HIS:CD2	2.53	0.44
1:C:51:TYR:HB2	1:C:71:GLN:HB3	1.99	0.44
1:D:71:GLN:CG	1:D:72:MSE:H	2.31	0.44
1:D:106:TYR:O	1:D:110:GLN:HG2	2.18	0.44
1:B:8:ASN:HD21	1:B:10:ASN:HB2	1.83	0.44
1:B:52:TRP:HZ2	2:B:167:NHE:HC11	1.83	0.43
1:D:71:GLN:CG	1:D:72:MSE:N	2.81	0.43
1:A:146:LYS:HA	1:A:150:GLU:O	2.17	0.43
1:D:135:PHE:CE1	1:D:159:TYR:HB2	2.54	0.43
1:A:79:HIS:CD2	1:A:80:LYS:HG3	2.53	0.43
1:C:122:ASN:N	1:C:122:ASN:OD1	2.49	0.43
1:A:158:ILE:CG1	1:A:159:TYR:N	2.81	0.43
1:D:138:LEU:HB2	1:D:158:ILE:HG23	2.01	0.42
1:C:130:PHE:HB3	1:C:135:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:HIS:CD2	1:B:30:ARG:HG3	2.54	0.42
1:B:2:ASN:O	1:B:3:ASN:HB2	2.19	0.42
1:B:23:HIS:O	1:B:25:ASN:N	2.43	0.42
1:D:7:LEU:HD22	1:D:54:ILE:CG2	2.50	0.42
1:D:71:GLN:HG2	1:D:72:MSE:H	1.85	0.42
1:A:146:LYS:O	1:B:76:GLY:HA2	2.18	0.42
1:B:46:SER:CB	1:B:48:HIS:HD2	2.30	0.42
2:C:168:NHE:H5'2	1:D:77:LYS:HE2	2.01	0.42
1:D:94:ILE:O	1:D:97:ARG:HB3	2.20	0.42
1:C:108:LYS:HG2	1:C:161:THR:CG2	2.50	0.42
1:A:19:MSE:HE2	1:A:87:PHE:CZ	2.50	0.41
1:B:90:ASN:O	1:B:91:ASN:HB3	2.20	0.41
1:A:40:ARG:HB2	1:A:40:ARG:HE	1.71	0.41
1:B:67:CYS:HB3	1:B:103:ILE:CD1	2.50	0.41
1:B:17:GLU:OE2	1:B:21:PHE:CE1	2.73	0.41
1:B:157:LEU:N	1:B:157:LEU:CD1	2.84	0.41
1:C:44:ILE:HG12	1:C:52:TRP:CE2	2.55	0.41
1:C:75:VAL:HG23	2:C:171:NHE:C1	2.51	0.41
1:D:25:ASN:C	1:D:27:GLU:N	2.74	0.41
1:C:79:HIS:CD2	1:C:80:LYS:HG3	2.56	0.41
1:A:12:LEU:HD13	1:A:45:LEU:CD1	2.50	0.41
1:B:20:LYS:NZ	1:B:33:LEU:HD21	2.36	0.41
1:B:46:SER:CB	1:B:48:HIS:CD2	3.04	0.41
1:C:68:THR:HG22	1:C:69:LEU:N	2.35	0.41
1:C:26:TYR:CD2	1:C:26:TYR:N	2.89	0.41
1:A:93:GLU:HG2	1:A:129:PHE:CE1	2.56	0.40
1:C:28:TRP:O	1:C:28:TRP:CG	2.73	0.40
1:D:78:CYS:SG	2:D:167:NHE:H6'1	2.62	0.40
1:A:40:ARG:O	1:A:40:ARG:HG3	2.18	0.40
1:C:31:TYR:HD1	1:C:147:ILE:HG21	1.86	0.40
1:A:96:ASN:O	1:A:100:ILE:HD12	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	160/169 (95%)	154 (96%)	5 (3%)	1 (1%)	30	59
1	B	162/169 (96%)	144 (89%)	14 (9%)	4 (2%)	7	18
1	C	160/169 (95%)	149 (93%)	11 (7%)	0	100	100
1	D	159/169 (94%)	135 (85%)	16 (10%)	8 (5%)	3	5
All	All	641/676 (95%)	582 (91%)	46 (7%)	13 (2%)	9	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	HIS
1	B	164	SER
1	D	39	ASP
1	D	89	LYS
1	B	163	GLU
1	D	24	HIS
1	D	91	ASN
1	D	94	ILE
1	B	50	ASP
1	D	78	CYS
1	A	60	ASP
1	D	26	TYR
1	D	27	GLU

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	147/150 (98%)	128 (87%)	19 (13%)	5	12
1	B	147/150 (98%)	128 (87%)	19 (13%)	5	12
1	C	146/150 (97%)	128 (88%)	18 (12%)	6	14
1	D	120/150 (80%)	102 (85%)	18 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	560/600 (93%)	486 (87%)	74 (13%)	5 12

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	6	LEU
1	A	7	LEU
1	A	9	GLN
1	A	17	GLU
1	A	33	LEU
1	A	38	ILE
1	A	39	ASP
1	A	40	ARG
1	A	41	LEU
1	A	50	ASP
1	A	64	VAL
1	A	66	THR
1	A	99	LEU
1	A	114	THR
1	A	119	ILE
1	A	121	SER
1	A	124	ILE
1	A	136	GLU
1	B	17	GLU
1	B	23	HIS
1	B	25	ASN
1	B	34	GLU
1	B	39	ASP
1	B	40	ARG
1	B	41	LEU
1	B	47	ASN
1	B	48	HIS
1	B	62	GLU
1	B	66	THR
1	B	72	MSE
1	B	73	ASN
1	B	99	LEU
1	B	101	ASN
1	B	113	GLU
1	B	124	ILE
1	B	147	ILE

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Mol	Chain	Res	Type
1	B	150	GLU
1	C	7	LEU
1	C	17	GLU
1	C	30	ARG
1	C	41	LEU
1	C	60	ASP
1	C	64	VAL
1	C	82	ILE
1	C	98	GLU
1	C	99	LEU
1	C	114	THR
1	C	119	ILE
1	C	121	SER
1	C	122	ASN
1	C	131	SER
1	C	137	ASN
1	C	149	ASN
1	C	157	LEU
1	C	158	ILE
1	D	7	LEU
1	D	8	ASN
1	D	25	ASN
1	D	29	ASP
1	D	40	ARG
1	D	52	TRP
1	D	82	ILE
1	D	88	VAL
1	D	92	ASP
1	D	95	VAL
1	D	98	GLU
1	D	99	LEU
1	D	114	THR
1	D	122	ASN
1	D	125	SER
1	D	142	LYS
1	D	145	SER
1	D	158	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN

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Mol	Chain	Res	Type
1	A	24	HIS
1	A	25	ASN
1	A	90	ASN
1	A	137	ASN
1	A	143	ASN
1	A	155	ASN
1	B	9	GLN
1	B	24	HIS
1	B	35	ASN
1	B	48	HIS
1	B	90	ASN
1	B	101	ASN
1	C	9	GLN
1	C	10	ASN
1	C	24	HIS
1	C	25	ASN
1	C	48	HIS
1	C	71	GLN
1	C	86	ASN
1	C	96	ASN
1	C	101	ASN
1	C	137	ASN
1	C	143	ASN
1	C	155	ASN
1	D	85	ASN
1	D	86	ASN
1	D	91	ASN
1	D	96	ASN
1	D	102	HIS
1	D	111	ASN
1	D	143	ASN
1	D	149	ASN
1	D	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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	NHE	A	167	-	12,13,13	0.84	0	15,17,17	3.34	8 (53%)
2	NHE	A	168	-	12,13,13	0.76	0	15,17,17	1.69	2 (13%)
2	NHE	A	169	-	12,13,13	0.70	0	15,17,17	2.28	4 (26%)
2	NHE	B	167	-	12,13,13	0.70	0	15,17,17	1.58	2 (13%)
2	NHE	B	168	-	12,13,13	0.81	0	15,17,17	2.07	3 (20%)
2	NHE	B	169	-	12,13,13	0.80	0	15,17,17	1.83	3 (20%)
2	NHE	C	167	-	12,13,13	0.89	0	15,17,17	2.63	6 (40%)
2	NHE	C	168	-	12,13,13	0.79	0	15,17,17	1.38	2 (13%)
2	NHE	C	169	-	12,13,13	0.73	0	15,17,17	3.22	5 (33%)
2	NHE	C	170	-	12,13,13	0.97	0	15,17,17	2.44	3 (20%)
2	NHE	C	171	-	12,13,13	0.65	0	15,17,17	1.54	3 (20%)
3	FLC	C	172	-	3,12,12	0.59	0	3,17,17	0.44	0
2	NHE	D	167	-	12,13,13	0.73	0	15,17,17	1.73	2 (13%)

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	NHE	A	167	-	-	0/7/15/15	0/1/1/1
2	NHE	A	168	-	-	0/7/15/15	0/1/1/1
2	NHE	A	169	-	-	0/7/15/15	0/1/1/1
2	NHE	B	167	-	-	0/7/15/15	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NHE	B	168	-	-	0/7/15/15	0/1/1/1
2	NHE	B	169	-	-	0/7/15/15	0/1/1/1
2	NHE	C	167	-	-	0/7/15/15	0/1/1/1
2	NHE	C	168	-	-	0/7/15/15	0/1/1/1
2	NHE	C	169	-	-	0/7/15/15	0/1/1/1
2	NHE	C	170	-	-	0/7/15/15	0/1/1/1
2	NHE	C	171	-	-	0/7/15/15	0/1/1/1
3	FLC	C	172	-	-	0/6/16/16	0/0/0/0
2	NHE	D	167	-	-	0/7/15/15	0/1/1/1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	170	NHE	O1-S-C2	-5.80	101.95	106.91
2	A	167	NHE	C6'-C1'-C2'	-3.60	104.69	110.82
2	A	167	NHE	O3-S-O2	-3.52	103.43	111.61
2	B	169	NHE	O3-S-O1	-3.08	104.44	111.61
2	A	167	NHE	O2-S-O1	-2.72	103.56	113.48
2	C	171	NHE	C6'-C1'-C2'	-2.49	106.57	110.82
2	C	169	NHE	O3-S-O1	-2.46	105.88	111.61
2	C	167	NHE	O3-S-O2	-2.46	105.89	111.61
2	A	169	NHE	O3-S-O1	-2.42	105.98	111.61
2	C	168	NHE	O3-S-O2	-2.39	106.04	111.61
2	C	169	NHE	O2-S-O1	-2.35	104.91	113.48
2	C	170	NHE	C1-C2-S	-2.31	107.50	113.73
2	C	167	NHE	C2-C1-N	2.02	117.28	111.32
2	C	169	NHE	C3'-C2'-C1'	2.20	114.54	111.13
2	A	169	NHE	C4'-C3'-C2'	2.25	116.15	111.44
2	C	167	NHE	C4'-C5'-C6'	2.30	116.27	111.44
2	A	167	NHE	C2-C1-N	2.32	118.16	111.32
2	B	168	NHE	C3'-C2'-C1'	2.44	114.91	111.13
2	A	168	NHE	O2-S-C2	2.47	109.01	106.91
2	D	167	NHE	O1-S-C2	2.59	109.12	106.91
2	C	167	NHE	C5'-C6'-C1'	2.67	115.26	111.13
2	A	167	NHE	C1-C2-S	2.77	121.20	113.73
2	B	168	NHE	C5'-C6'-C1'	2.80	115.46	111.13
2	C	169	NHE	O1-S-C2	2.92	109.40	106.91
2	B	167	NHE	O1-S-C2	2.93	109.40	106.91
2	A	169	NHE	C3'-C2'-C1'	2.94	115.68	111.13
2	B	169	NHE	O2-S-C2	3.05	109.51	106.91
2	C	171	NHE	O2-S-C2	3.18	109.62	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	171	NHE	O1-S-C2	3.36	109.77	106.91
2	C	168	NHE	O1-S-C2	3.64	110.01	106.91
2	C	167	NHE	O2-S-C2	3.77	110.12	106.91
2	B	167	NHE	O2-S-C2	3.90	110.23	106.91
2	A	167	NHE	O1-S-C2	4.66	110.88	106.91
2	A	167	NHE	C5'-C6'-C1'	4.73	118.44	111.13
2	B	169	NHE	O1-S-C2	5.17	111.31	106.91
2	A	168	NHE	O1-S-C2	5.36	111.48	106.91
2	D	167	NHE	O2-S-C2	5.42	111.53	106.91
2	C	170	NHE	O2-S-C2	6.47	112.43	106.91
2	B	168	NHE	O2-S-C2	6.53	112.48	106.91
2	A	169	NHE	O1-S-C2	6.94	112.82	106.91
2	C	167	NHE	O1-S-C2	7.72	113.50	106.91
2	A	167	NHE	O2-S-C2	8.31	114.00	106.91
2	C	169	NHE	O2-S-C2	11.04	116.33	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	168	NHE	1	0
2	A	169	NHE	2	0
2	B	167	NHE	1	0
2	B	168	NHE	1	0
2	B	169	NHE	1	0
2	C	168	NHE	4	0
2	C	169	NHE	2	0
2	C	170	NHE	3	0
2	C	171	NHE	9	0
3	C	172	FLC	3	0
2	D	167	NHE	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	158/169 (93%)	0.12	0 100 100	24, 42, 55, 67	0
1	B	161/169 (95%)	0.57	19 (11%) 6 5	37, 49, 74, 87	0
1	C	158/169 (93%)	0.43	5 (3%) 51 51	24, 38, 49, 54	0
1	D	158/169 (93%)	1.56	53 (33%) 0 0	17, 31, 64, 67	0
All	All	635/676 (93%)	0.67	77 (12%) 6 4	17, 41, 64, 87	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	TYR	10.5
1	D	64	VAL	7.9
1	D	65	ALA	7.9
1	D	28	TRP	6.9
1	D	23	HIS	6.8
1	D	4	ILE	6.6
1	D	25	ASN	6.0
1	D	89	LYS	5.7
1	D	90	ASN	5.4
1	B	23	HIS	5.3
1	D	135	PHE	5.2
1	C	149	ASN	5.0
1	D	112	ILE	5.0
1	D	7	LEU	4.9
1	D	22	GLY	4.8
1	B	24	HIS	4.7
1	D	87	PHE	4.7
1	B	164	SER	4.5
1	D	63	LEU	4.4
1	B	31	TYR	4.2
1	D	93	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	165	SER	4.1
1	D	96	ASN	3.9
1	D	99	LEU	3.8
1	D	24	HIS	3.7
1	B	163	GLU	3.6
1	B	21	PHE	3.6
1	D	36	VAL	3.6
1	D	35	ASN	3.6
1	C	61	ASP	3.6
1	D	106	TYR	3.5
1	D	130	PHE	3.5
1	D	2	ASN	3.5
1	D	58	PHE	3.5
1	D	59	GLU	3.5
1	D	121	SER	3.4
1	C	31	TYR	3.4
1	D	3	ASN	3.3
1	D	21	PHE	3.1
1	D	129	PHE	3.1
1	D	94	ILE	3.1
1	D	97	ARG	2.9
1	D	60	ASP	2.9
1	D	66	THR	2.9
1	B	4	ILE	2.9
1	B	33	LEU	2.8
1	D	102	HIS	2.8
1	B	59	GLU	2.8
1	B	7	LEU	2.8
1	D	32	TYR	2.8
1	D	51	TYR	2.8
1	B	2	ASN	2.7
1	D	107	ALA	2.7
1	D	152	PHE	2.6
1	D	54	ILE	2.6
1	D	57	ALA	2.6
1	D	162	THR	2.6
1	B	147	ILE	2.6
1	B	34	GLU	2.5
1	D	122	ASN	2.5
1	B	3	ASN	2.5
1	D	161	THR	2.4
1	D	101	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	27	GLU	2.4
1	D	62	GLU	2.4
1	D	88	VAL	2.4
1	D	104	ILE	2.3
1	D	86	ASN	2.2
1	B	58	PHE	2.2
1	C	131	SER	2.2
1	D	105	GLN	2.2
1	C	28	TRP	2.1
1	B	61	ASP	2.1
1	D	61	ASP	2.1
1	D	110	GLN	2.1
1	B	63	LEU	2.0
1	B	98	GLU	2.0

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 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
3	FLC	C	172	13/13	0.59	0.62	10.32	92,94,94,94	13
2	NHE	C	169	13/13	0.88	0.36	5.66	82,83,85,86	13
2	NHE	A	169	13/13	0.89	0.35	4.18	85,87,88,89	13
2	NHE	A	167	13/13	0.89	0.28	3.75	66,67,78,78	13
2	NHE	A	168	13/13	0.96	0.25	3.56	77,79,82,83	13
2	NHE	B	168	13/13	0.90	0.32	3.51	84,86,92,92	13
2	NHE	B	169	13/13	0.88	0.27	2.84	85,86,91,91	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NHE	C	167	13/13	0.87	0.29	2.65	75,76,85,85	13
2	NHE	C	170	13/13	0.80	0.37	2.39	79,80,83,83	13
2	NHE	C	171	13/13	0.68	0.50	2.19	86,87,88,88	13
2	NHE	B	167	13/13	0.91	0.28	1.16	121,121,122,122	13
2	NHE	D	167	13/13	0.79	0.27	1.06	104,105,108,108	13
2	NHE	C	168	13/13	0.92	0.23	0.37	89,90,91,91	13

6.5 Other polymers [i](#)

There are no such residues in this entry.