W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 12:28 PM EST

PDB ID	:	2P5T
Title	:	Molecular and structural characterization of the PezAT chromosomal toxin-antitoxin system of the human pathogen Streptococcus pneumoniae
Authors	:	Loll, B.; Meinhart, A.
Deposited on	:	2007-03-16
Resolution	:	3.20 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

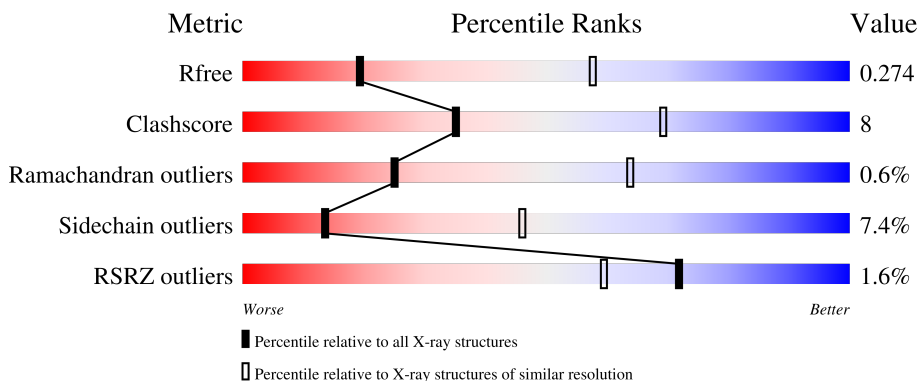|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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.
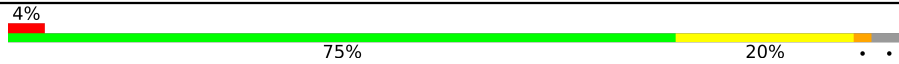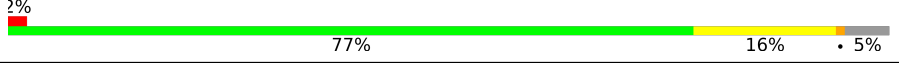

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	X	33	100%
2	A	158	44% 13% • 42%
2	C	158	42% 16% • 41%
2	E	158	43% 15% • 40%
2	G	158	43% 14% • 41%

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Mol	Chain	Length	Quality of chain
3	B	253	4% 75% 20%
3	D	253	% 74% 20%
3	F	253	2% 77% 16% 5%
3	H	253	% 70% 23%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11093 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 fragment of PezA helix-turn-helix motif.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	X	33	Total 132	C 66	N 33	O 33	0	0	0

- Molecule 2 is a protein called Putative transcriptional regulator PezA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	92	Total 759	C 478	N 122	O 156	S 3	0	0	0
2	C	93	Total 767	C 483	N 123	O 157	S 4	0	0	0
2	E	95	Total 784	C 493	N 126	O 161	S 4	0	0	0
2	G	93	Total 767	C 483	N 123	O 157	S 4	0	0	0

- Molecule 3 is a protein called PezT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	244	Total 1979	C 1253	N 342	O 381	S 3	0	0	0
3	D	247	Total 2002	C 1268	N 345	O 385	S 4	0	0	0
3	F	240	Total 1944	C 1232	N 332	O 377	S 3	0	0	0
3	H	242	Total 1959	C 1242	N 334	O 379	S 4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	GLY	ARG	conflict	UNP Q97QZ1
B	228	PHE	LEU	conflict	UNP Q97QZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	109	GLY	ARG	conflict	UNP Q97QZ1
D	228	PHE	LEU	conflict	UNP Q97QZ1
F	109	GLY	ARG	conflict	UNP Q97QZ1
F	228	PHE	LEU	conflict	UNP Q97QZ1
H	109	GLY	ARG	conflict	UNP Q97QZ1
H	228	PHE	LEU	conflict	UNP Q97QZ1

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: fragment of PezA helix-turn-helix motif

Chain X: 100%

There are no outlier residues recorded for this chain.

• Molecule 2: Putative transcriptional regulator PezA

Chain A: 44% 13% • 42%

• Molecule 2: Putative transcriptional regulator PezA

Chain C: 42% 16% • 41%

• Molecule 2: Putative transcriptional regulator PezA

Chain E: % 43% 15% • 40%

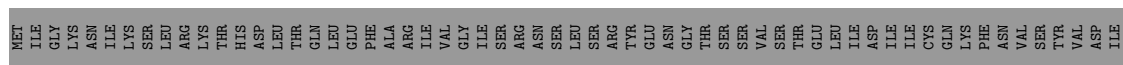• Molecule 2: Putative transcriptional regulator PezA

Chain G: % 43% 14% • 41%

MET ILE GLY LYS ASN ILE LYS SER LEU ARG LYS THR HIS ASP LEU THR GLN LEU GLU PHE ALA ARG ILE VAL GLY ILE LEU SER ARG ASN SER LEU SER ARG TYR GLU ASN GLY THR SER SER VAL SER THR GLU LEU ILE ASP ILE ILE CYS GLN LYS PHE ASN VAL SER TYR VAL ASP ILE

VAL GLY GLU ASP LYS M66 L67 N68 Y73 K78 I79 K83 G86 D98 S103 I104 P110 W111 M114 S115 D116 L121 I122 I126 Y127 D133 E134 I135 E136 R137 Y141 I145 I151 S152 R155 M156 V157 A158

• Molecule 3: PezT

Chain B:

MET GLU I3 Q4 R20 S21 L22 T23 R24 P32 I33 Q40 K45 T46 Q53 G58 I62 R69 S70 Q71 H72 Q79 Q80 E81 Y82 G83 K84 D85 S86 V87 E88 Y89 F93 N111 L112 L113 L118 R119 T120 V121 L131 Y136 I143 A144 T145

S153 R157 E160 L161 I164 N165 P166 N167 Q168 ALA ARG ALA THR PRO LYS GLU H176 H177 D178 F179 I180 L191 I196 F197 E198 R199 Q204 R205 D206 R207 S208 Y211 D212 S213 K214 E215 N216 V223 L227 E238 N248 E249 L250 L251 E252 K253

• Molecule 3: PezT

Chain D:

M1 T7 R17 R24 G25 K26 I35 L36 L37 T46 I51 K52 Q53 G58 N59 I60 V61 I62 I63 D64 G65 D66 R69 S70 Q71 H72 P73 H74 Y75 Q79 V87 E88 Y89 T90 K91 G95 E99 S100 L108 L113 I114 E115 G116 T117 L118 R119

T120 V121 L131 Y136 L140 A141 L142 P147 Y151 R157 N165 P166 N167 Q168 ALA ARG ALA THR P173 K174 E175 H176 H177 I200 Q201 I202 Y203 Q204 V210 Y211 T218 S219 D222 V223 F229 L251 GLU LYS

• Molecule 3: PezT

Chain F:

MET E2 I3 T7 D8 K12 L19 T23 R24 K27 S28 S41 T46 H49 N59 I60 S70 Q79 G83 K84 D85 N111 L112 L113 T117 L118 R119 T120 V121 D122 V123 P124 A144 S150 E160 L161 Y162 I163 I164 N165 PRO ASN GLN

ALA ARG ALA THR PRO LYS GLU HIS HIS D178 F179 I180 V185 D212 E215 D222 Q225 F228 S233 E236 K245 E249 K253

• Molecule 3: PezT

Chain H:

M1 T7 D8 S9 H13 A14 R17 N18 S21 R24 G25 K26 P32 I35 L36 L37 Q40 S41 G42 A43 A94 R50 I51 K54 G58 I62 S70 Q79 G83 K84 A94 V98 S106 L113 L118 R119 T120 V121 D122 K125

Q129 Y136 Q139 T145 E148 L152 S153 T154 L155 I156 R157 Y158 E159 I164 N165 P166 ASN GLN ALA ARG ALA THR PRO LYS GLU HIS HIS D178 N182 H183 I196 R199 Q204 R205 D206 R207 N216 T217 A221 L224 W232 L240 Q241

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.52Å 102.86Å 254.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 3.20 47.68 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-3.20) 98.5 (47.68-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.277 0.211 , 0.274	Depositor DCC
R_{free} test set	1726 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	90.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 84.5	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11093	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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
2	A	0.38	0/770	0.54	0/1039
2	C	0.39	0/778	0.55	0/1049
2	E	0.44	0/795	0.56	0/1071
2	G	0.41	0/778	0.55	0/1049
3	B	0.38	0/2010	0.52	0/2703
3	D	0.39	0/2034	0.55	0/2736
3	F	0.38	0/1972	0.54	0/2650
3	H	0.43	0/1988	0.57	0/2672
All	All	0.40	0/11125	0.55	0/14969

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 ⓘ

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	X	132	0	2	0	0
2	A	759	0	740	20	0
2	C	767	0	749	22	0
2	E	784	0	766	18	0
2	G	767	0	749	24	0
3	B	1979	0	1997	31	0
3	D	2002	0	2023	37	0
3	F	1944	0	1968	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1959	0	1987	42	0
All	All	11093	0	10981	180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (180) 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:G:104:ILE:HD11	3:H:17:ARG:HB2	1.51	0.89
3:D:147:PRO:HB2	3:H:148:GLU:HG2	1.58	0.85
2:G:79:ILE:HD13	3:H:50:ARG:HD2	1.61	0.80
3:H:40:GLN:HB2	3:H:43:ALA:HB2	1.65	0.79
2:C:131:THR:HG23	2:C:134:GLU:HB2	1.66	0.77
3:B:204:GLN:HE21	3:B:227:LEU:HD21	1.48	0.76
2:G:116:ASP:HB3	3:H:24:ARG:NH1	2.02	0.75
3:H:204:GLN:HA	3:H:204:GLN:HE21	1.53	0.73
3:B:45:LYS:HG3	3:B:143:ILE:HG21	1.69	0.72
3:B:204:GLN:NE2	3:B:227:LEU:HD21	2.08	0.68
3:H:240:LEU:O	3:H:244:GLU:HB2	1.94	0.67
3:D:118:LEU:HD11	3:D:140:LEU:HD11	1.78	0.66
2:A:121:LEU:HD23	2:A:125:ASN:HD22	1.61	0.66
3:H:26:LYS:NZ	3:H:58:GLY:O	2.29	0.65
2:C:120:ASP:OD1	3:D:24:ARG:HD3	1.97	0.65
3:F:24:ARG:HH11	3:F:24:ARG:HG3	1.62	0.65
2:E:129:VAL:HG11	2:E:135:ILE:HG12	1.79	0.64
2:G:104:ILE:HD12	3:H:13:HIS:CE1	2.32	0.64
3:D:69:ARG:HE	3:D:90:THR:HG23	1.61	0.63
3:D:95:GLY:O	3:D:99:GLU:HG2	1.98	0.63
3:F:185:VAL:HG11	3:F:225:GLN:HG3	1.80	0.63
3:F:117:THR:HB	3:F:180:ILE:HD11	1.79	0.63
3:D:72:HIS:HD2	3:D:74:HIS:H	1.45	0.62
3:B:204:GLN:HE21	3:B:227:LEU:CD2	2.12	0.62
2:A:140:GLY:CA	2:C:137:ARG:HG2	2.30	0.62
3:D:62:ILE:HD12	3:D:113:LEU:HD23	1.81	0.61
3:B:160:GLU:HG3	3:B:250:LEU:HD21	1.82	0.61
2:G:73:TYR:CE1	3:H:205:ARG:HG2	2.36	0.60
3:H:159:GLU:HB3	3:H:250:LEU:HD23	1.82	0.60
2:C:131:THR:CG2	2:C:134:GLU:HB2	2.30	0.60
3:B:45:LYS:HG3	3:B:143:ILE:CG2	2.32	0.59
3:B:81:GLU:HG3	3:B:82:TYR:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:250:LEU:HD12	3:H:253:LYS:HD2	1.83	0.59
2:C:121:LEU:HA	2:C:125:ASN:HB2	1.85	0.58
3:B:33:ILE:H	3:B:111:ASN:HD22	1.51	0.58
3:B:69:ARG:HH21	3:B:87:VAL:HG13	1.68	0.57
2:A:75:LEU:O	2:A:79:ILE:HG12	2.03	0.57
3:B:4:GLN:HG3	3:B:89:TYR:HD1	1.69	0.57
2:A:79:ILE:HD13	2:A:135:ILE:HD11	1.87	0.56
3:B:165:ASN:HB3	3:B:168:GLN:HG3	1.88	0.56
2:G:104:ILE:CD1	3:H:17:ARG:HB2	2.28	0.56
3:D:219:SER:HB2	3:D:222:ASP:H	1.71	0.56
2:G:79:ILE:CD1	3:H:50:ARG:HD2	2.35	0.55
3:D:131:LEU:O	3:D:136:TYR:HB2	2.06	0.55
3:D:211:TYR:CD2	3:D:223:VAL:HG21	2.41	0.55
2:E:68:ASN:HB2	2:E:71:GLU:HB2	1.88	0.55
3:B:62:ILE:HG12	3:B:113:LEU:HD23	1.89	0.55
3:B:212:ASP:H	3:B:216:ASN:HD22	1.54	0.55
3:H:14:ALA:O	3:H:18:ASN:ND2	2.40	0.55
2:A:116:ASP:HB3	3:B:24:ARG:NH2	2.22	0.54
3:D:51:ILE:HD13	3:D:203:TYR:CD1	2.43	0.54
2:A:80:GLU:HG3	3:B:46:THR:HG21	1.90	0.54
3:B:53:GLN:HE21	3:B:58:GLY:HA2	1.72	0.54
3:D:175:GLU:HG2	3:D:176:HIS:HD2	1.72	0.54
2:E:111:TRP:CE2	2:G:110:PRO:HG3	2.43	0.54
3:H:35:ILE:HB	3:H:113:LEU:HD12	1.90	0.54
2:E:121:LEU:HD11	2:E:138:TYR:CE1	2.43	0.54
3:H:50:ARG:NH2	3:H:207:ARG:HH11	2.05	0.54
2:A:143:ASP:CB	2:C:137:ARG:NH1	2.71	0.53
2:G:121:LEU:HD12	2:G:126:ILE:HG12	1.89	0.53
2:A:151:ILE:O	2:A:155:ARG:HG3	2.08	0.53
3:D:87:VAL:HA	3:D:90:THR:HG22	1.89	0.53
3:D:69:ARG:HE	3:D:90:THR:CG2	2.22	0.53
2:A:140:GLY:HA3	2:C:137:ARG:HG2	1.89	0.53
3:F:27:LYS:H	3:F:59:ASN:ND2	2.07	0.52
2:A:68:ASN:HB2	2:A:69:PRO:HD2	1.92	0.52
2:C:79:ILE:HG23	2:C:126:ILE:HG12	1.91	0.52
3:D:114:ILE:HG22	3:D:115:GLU:O	2.10	0.52
2:G:151:ILE:O	2:G:155:ARG:HG2	2.09	0.52
3:B:199:ARG:HD2	3:B:214:LYS:HD3	1.92	0.52
2:A:143:ASP:HB3	2:C:137:ARG:NH1	2.25	0.52
2:G:141:TYR:CE2	2:G:145:ILE:HD11	2.45	0.51
3:H:32:PRO:HB2	3:H:136:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:67:LEU:HD22	2:E:71:GLU:HB3	1.91	0.51
2:E:121:LEU:O	2:E:126:ILE:HG12	2.10	0.51
3:H:119:ARG:CG	3:H:183:HIS:HD2	2.24	0.51
3:H:50:ARG:O	3:H:54:LYS:HG3	2.11	0.51
3:H:121:VAL:O	3:H:125:LYS:HB2	2.10	0.51
2:C:150:GLU:O	2:C:154:LYS:HG3	2.11	0.51
2:E:121:LEU:HD21	2:E:138:TYR:CD1	2.46	0.50
3:H:62:ILE:HG12	3:H:113:LEU:HD23	1.92	0.50
3:D:204:GLN:CD	3:D:210:VAL:HG21	2.32	0.50
3:F:59:ASN:CG	3:F:59:ASN:O	2.49	0.50
2:C:80:GLU:OE1	3:D:157:ARG:NH2	2.44	0.50
3:D:70:SER:HA	3:D:75:TYR:CD1	2.45	0.50
2:G:73:TYR:CD1	3:H:205:ARG:HG2	2.47	0.50
3:B:40:GLN:NE2	3:B:178:ASP:O	2.34	0.49
3:D:229:PHE:HB3	3:H:232:TRP:HB2	1.94	0.49
3:B:32:PRO:HB2	3:B:136:TYR:CE1	2.48	0.49
2:E:148:MET:HE1	2:G:114:MET:HG3	1.94	0.49
2:C:104:ILE:HG12	3:D:17:ARG:HB3	1.95	0.49
3:D:69:ARG:NH2	3:D:91:LYS:HB3	2.28	0.49
2:A:110:PRO:HG3	2:C:111:TRP:CE2	2.48	0.49
2:A:121:LEU:O	2:A:126:ILE:HG12	2.13	0.48
2:A:113:LEU:HB3	2:C:148:MET:HG2	1.95	0.48
2:E:97:GLN:OE1	2:E:115:SER:OG	2.31	0.48
2:G:86:GLY:HA3	2:G:122:ILE:CD1	2.44	0.48
3:D:66:ASP:HA	3:D:69:ARG:HG3	1.96	0.48
2:E:78:LYS:HB3	2:E:135:ILE:HG21	1.95	0.47
3:F:160:GLU:O	3:F:164:ILE:HG12	2.14	0.47
3:H:50:ARG:NH2	3:H:207:ARG:NH1	2.63	0.47
3:H:51:ILE:HD11	3:H:207:ARG:HA	1.96	0.47
3:H:139:GLN:HG2	3:H:199:ARG:HB3	1.97	0.47
3:F:122:ASP:N	3:F:122:ASP:OD1	2.47	0.46
3:H:125:LYS:HG3	3:H:196:ILE:HD13	1.97	0.46
3:D:72:HIS:HD2	3:D:74:HIS:N	2.12	0.46
2:G:133:ASP:OD1	2:G:133:ASP:N	2.45	0.46
2:A:91:SER:OG	3:B:70:SER:HB2	2.15	0.46
3:H:119:ARG:HG2	3:H:183:HIS:HD2	1.81	0.46
3:D:151:TYR:HD1	3:D:174:LYS:HE2	1.81	0.46
2:A:110:PRO:HG2	2:C:110:PRO:HB2	1.98	0.46
3:B:69:ARG:NH2	3:B:87:VAL:HG13	2.29	0.46
3:B:157:ARG:HG3	3:B:161:LEU:HD12	1.98	0.46
3:B:206:ASP:OD1	3:B:208:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:122:ILE:O	2:E:126:ILE:HD11	2.16	0.46
2:E:96:TYR:CE1	2:E:152:SER:HB3	2.51	0.45
3:H:152:LEU:O	3:H:156:ILE:HG12	2.16	0.45
3:F:24:ARG:HG3	3:F:24:ARG:NH1	2.28	0.45
2:E:82:VAL:HG21	2:E:135:ILE:HD12	1.99	0.45
2:C:138:TYR:O	2:C:141:TYR:HB3	2.17	0.45
3:D:35:ILE:HB	3:D:113:LEU:HD13	1.99	0.45
3:H:7:THR:HG22	3:H:9:SER:H	1.82	0.45
3:D:69:ARG:NH2	3:D:87:VAL:HG13	2.32	0.45
3:H:246:ARG:HH12	3:H:253:LYS:HE2	1.82	0.44
2:G:98:ASP:OD1	3:H:17:ARG:NH2	2.44	0.44
2:G:135:ILE:HD13	2:G:135:ILE:HA	1.85	0.44
3:H:159:GLU:HB3	3:H:250:LEU:CD2	2.46	0.44
2:A:110:PRO:HG3	2:C:111:TRP:NE1	2.32	0.44
3:F:233:SER:OG	3:F:236:GLU:HG3	2.16	0.44
3:B:131:LEU:O	3:B:136:TYR:HB2	2.18	0.44
2:C:132:PHE:O	2:C:135:ILE:HB	2.17	0.44
3:D:26:LYS:HE2	3:D:58:GLY:O	2.18	0.44
3:F:212:ASP:HB3	3:F:215:GLU:HB2	1.99	0.44
3:F:144:ALA:HB1	3:F:228:PHE:CE1	2.52	0.44
3:D:142:LEU:HB2	3:D:202:ILE:HG12	1.99	0.44
3:B:211:TYR:CD2	3:B:223:VAL:HG21	2.53	0.43
3:D:175:GLU:HG2	3:D:176:HIS:N	2.32	0.43
2:E:140:GLY:HA3	2:G:137:ARG:O	2.19	0.43
3:D:219:SER:O	3:D:223:VAL:HG23	2.18	0.43
3:F:8:ASP:O	3:F:12:LYS:HG2	2.19	0.43
2:E:125:ASN:HA	2:E:128:LEU:HD12	2.00	0.43
2:A:91:SER:HB3	2:A:95:ARG:NH2	2.34	0.42
3:D:37:LEU:HB2	3:D:115:GLU:HA	1.99	0.42
3:D:72:HIS:CD2	3:D:74:HIS:H	2.31	0.42
2:G:111:TRP:HZ2	2:G:152:SER:HG	1.63	0.42
3:F:60:ILE:HG13	3:F:111:ASN:HB3	2.01	0.42
2:G:141:TYR:CZ	2:G:145:ILE:HD11	2.55	0.42
2:C:92:ARG:HD3	2:C:149:LEU:HD13	2.01	0.42
2:A:83:LYS:NZ	3:B:46:THR:HG22	2.34	0.42
3:B:33:ILE:H	3:B:111:ASN:ND2	2.16	0.42
3:D:202:ILE:HB	3:D:211:TYR:HB3	2.01	0.42
3:D:53:GLN:NE2	3:D:60:ILE:HG22	2.35	0.42
3:H:51:ILE:HG13	3:H:207:ARG:HD2	2.02	0.42
3:H:221:ALA:HA	3:H:224:LEU:HD12	2.02	0.41
3:H:106:SER:HA	3:H:136:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:78:LYS:HB3	2:G:135:ILE:HG21	2.02	0.41
3:H:84:LYS:H	3:H:84:LYS:HE2	1.85	0.41
3:F:46:THR:HA	3:F:49:HIS:CD2	2.56	0.41
3:F:46:THR:HA	3:F:49:HIS:HD2	1.85	0.41
3:H:94:ALA:O	3:H:98:VAL:HG23	2.20	0.41
2:E:110:PRO:HB2	2:G:110:PRO:HG2	2.01	0.41
3:H:37:LEU:HD21	3:H:113:LEU:HD11	2.02	0.41
3:F:118:LEU:HD22	3:F:124:PRO:HG3	2.03	0.41
3:B:198:GLU:H	3:B:198:GLU:HG2	1.67	0.41
2:C:96:TYR:OH	2:C:155:ARG:NH2	2.38	0.41
3:D:140:LEU:HB3	3:D:200:ILE:HG23	2.02	0.41
3:D:165:ASN:HB3	3:D:168:GLN:HB2	2.02	0.41
3:D:210:VAL:O	3:D:210:VAL:HG12	2.21	0.41
2:G:86:GLY:HA3	2:G:122:ILE:HD13	2.03	0.41
3:H:182:ASN:OD1	3:H:182:ASN:N	2.54	0.41
2:E:90:LEU:HD13	2:E:118:LEU:HG	2.03	0.41
3:B:248:ASN:O	3:B:251:LEU:HB3	2.21	0.40
3:B:79:GLN:C	3:B:81:GLU:H	2.24	0.40
3:F:245:LYS:O	3:F:249:GLU:HB2	2.22	0.40
2:G:127:TYR:CE2	3:H:62:ILE:HD13	2.56	0.40
2:A:143:ASP:HB3	2:C:137:ARG:HH12	1.83	0.40
3:B:20:ARG:O	3:B:24:ARG:HG2	2.21	0.40
2:C:136:GLU:O	2:C:137:ARG:C	2.60	0.40
2:E:129:VAL:HG22	2:E:134:GLU:HB3	2.04	0.40
3:F:19:LEU:O	3:F:23:THR:HB	2.20	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	
2	A	90/158 (57%)	84 (93%)	5 (6%)	1 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	91/158 (58%)	87 (96%)	3 (3%)	1 (1%)	14	51
2	E	93/158 (59%)	88 (95%)	5 (5%)	0	100	100
2	G	91/158 (58%)	87 (96%)	4 (4%)	0	100	100
3	B	240/253 (95%)	218 (91%)	21 (9%)	1 (0%)	34	69
3	D	243/253 (96%)	226 (93%)	15 (6%)	2 (1%)	19	58
3	F	236/253 (93%)	221 (94%)	13 (6%)	2 (1%)	19	58
3	H	238/253 (94%)	224 (94%)	13 (6%)	1 (0%)	34	69
All	All	1322/1644 (80%)	1235 (93%)	79 (6%)	8 (1%)	25	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	164	ILE
3	F	24	ARG
2	A	106	ASP
2	C	104	ILE
3	D	177	HIS
3	F	83	GLY
3	D	166	PRO
3	H	83	GLY

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	
2	A	86/147 (58%)	83 (96%)	3 (4%)	36	69
2	C	87/147 (59%)	85 (98%)	2 (2%)	50	78
2	E	89/147 (60%)	83 (93%)	6 (7%)	16	50
2	G	87/147 (59%)	81 (93%)	6 (7%)	15	49
3	B	219/226 (97%)	203 (93%)	16 (7%)	14	46
3	D	222/226 (98%)	204 (92%)	18 (8%)	11	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	215/226 (95%)	198 (92%)	17 (8%)	12	43
3	H	217/226 (96%)	194 (89%)	23 (11%)	6	27
All	All	1222/1492 (82%)	1131 (93%)	91 (7%)	13	46

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	126	ILE
2	A	139	SER
2	A	156	MET
3	B	3	ILE
3	B	21	SER
3	B	23	THR
3	B	45	LYS
3	B	70	SER
3	B	84	LYS
3	B	118	LEU
3	B	120	THR
3	B	121	VAL
3	B	145	THR
3	B	153	SER
3	B	161	LEU
3	B	180	ILE
3	B	227	LEU
3	B	238	GLU
3	B	250	LEU
2	C	67	LEU
2	C	108	SER
3	D	7	THR
3	D	26	LYS
3	D	46	THR
3	D	64	ASP
3	D	79	GLN
3	D	88	GLU
3	D	90	THR
3	D	91	LYS
3	D	99	GLU
3	D	100	SER
3	D	108	LEU
3	D	118	LEU
3	D	119	ARG

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Mol	Chain	Res	Type
3	D	121	VAL
3	D	157	ARG
3	D	175	GLU
3	D	218	THR
3	D	219	SER
2	E	115	SER
2	E	126	ILE
2	E	133	ASP
2	E	135	ILE
2	E	139	SER
2	E	150	GLU
3	F	3	ILE
3	F	7	THR
3	F	23	THR
3	F	28	SER
3	F	41	SER
3	F	70	SER
3	F	79	GLN
3	F	113	LEU
3	F	120	THR
3	F	121	VAL
3	F	122	ASP
3	F	150	SER
3	F	162	TYR
3	F	163	ILE
3	F	179	PHE
3	F	222	ASP
3	F	253	LYS
2	G	68	ASN
2	G	83	LYS
2	G	103	SER
2	G	104	ILE
2	G	126	ILE
2	G	133	ASP
3	H	21	SER
3	H	41	SER
3	H	50	ARG
3	H	70	SER
3	H	79	GLN
3	H	84	LYS
3	H	118	LEU
3	H	120	THR

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Mol	Chain	Res	Type
3	H	122	ASP
3	H	129	GLN
3	H	145	THR
3	H	154	THR
3	H	158	TYR
3	H	159	GLU
3	H	178	ASP
3	H	182	ASN
3	H	196	ILE
3	H	204	GLN
3	H	205	ARG
3	H	216	ASN
3	H	217	THR
3	H	241	GLN
3	H	251	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	125	ASN
3	B	53	GLN
3	B	111	ASN
3	B	204	GLN
3	B	216	ASN
3	D	18	ASN
3	D	53	GLN
3	D	71	GLN
3	D	72	HIS
3	D	129	GLN
3	D	176	HIS
3	D	182	ASN
2	E	125	ASN
3	F	59	ASN
3	F	204	GLN
2	G	123	HIS
3	H	49	HIS
3	H	129	GLN
3	H	183	HIS
3	H	204	GLN
3	H	241	GLN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	X	0/33	-		-		-	-
2	A	92/158 (58%)	-0.07	0	100	100	78, 88, 97, 104	0
2	C	93/158 (58%)	-0.13	0	100	100	79, 90, 105, 112	0
2	E	95/158 (60%)	-0.15	1 (1%)	80	69	79, 89, 107, 114	0
2	G	93/158 (58%)	-0.10	2 (2%)	62	48	79, 89, 108, 111	0
3	B	244/253 (96%)	0.05	9 (3%)	41	26	78, 91, 106, 115	0
3	D	247/253 (97%)	-0.15	3 (1%)	79	67	79, 89, 105, 114	0
3	F	240/253 (94%)	-0.09	4 (1%)	70	57	74, 89, 114, 123	0
3	H	242/253 (95%)	-0.06	3 (1%)	79	67	75, 90, 112, 130	0
All	All	1346/1677 (80%)	-0.08	22 (1%)	72	59	74, 90, 107, 130	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	157	VAL	5.7
2	E	64	ASP	5.1
3	H	164	ILE	4.1
3	B	253	LYS	4.0
2	G	158	ALA	4.0
3	H	178	ASP	3.9
3	F	178	ASP	3.7
3	F	253	LYS	3.4
3	B	85	ASP	2.9
3	F	162	TYR	2.9
3	B	191	LEU	2.8
3	B	196	ILE	2.7
3	H	253	LYS	2.6
3	B	167	ASN	2.5
3	D	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	72	HIS	2.3
3	B	69	ARG	2.3
3	D	117	THR	2.3
3	D	167	ASN	2.2
3	F	85	ASP	2.2
3	B	252	GLU	2.0
3	B	93	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.