



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:06 AM UTC

PDB ID : 2P5T / pdb_00002p5t
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)

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
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

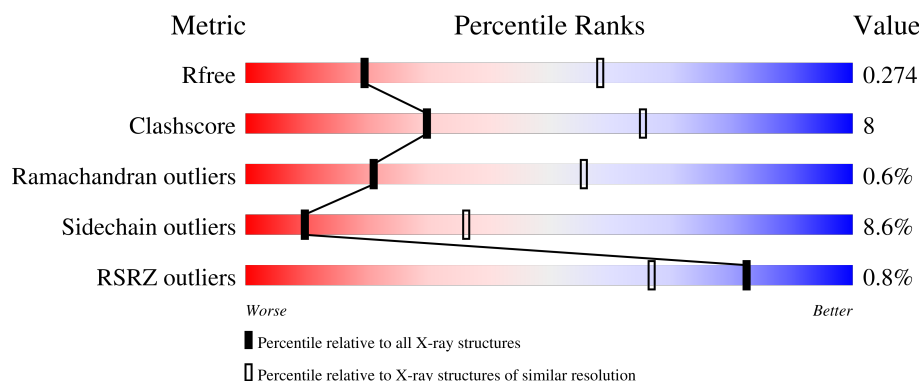
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	X	33	
2	A	158	
2	C	158	
2	E	158	
2	G	158	

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Mol	Chain	Length	Quality of chain
3	B	253	73% 20%
3	D	253	72% 22%
3	F	253	% 77% 16% 5%
3	H	253	2% 69% 24%

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	C	N	O	0	0	0
			132	66	33	33			

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

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

- Molecule 3 is a protein called PezT.

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

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

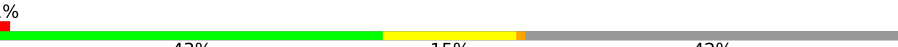
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

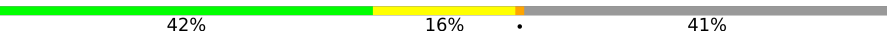
- Molecule 2: Putative transcriptional regulator PezA

Chain A:  %

MET ILE GLY GLU ASP LYS ASN ILE LYS SER LEU ARG THR HIS ASP LEU THR GLN LEU GLU PHE ALA ARG ILE ILE VAL GLY ILE SER ARG ASN SER LEU SER ARG TYR I126 GLU ASN THR SER SER VAL SER THR LEU ILE ASP I155 ILE ILE CYS GLN LYS PHE ASN VAL SER TYR VAL ASP ILE

VAL GLY GLU ASP LYS MET L67 N68 P69 L75 I79 E80 K83 S91 R95 D106 P110 L113 M114 S115 D116 L121 M125 I126 Y127 I135 S139 G140 D143 I144 I145 I151 R155 M156 V157 A158

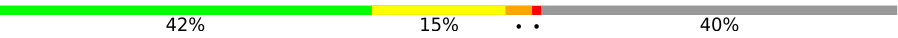
- Molecule 2: Putative transcriptional regulator PezA

Chain C:  %

MET ILE GLY GLU ASP LYS ASN ILE LYS SER LEU ARG THR HIS ASP LEU THR GLN LEU GLU PHE ALA ARG ILE ILE VAL GLY ILE SER ARG ASN SER LEU SER ARG TYR I135 GLU ASN THR SER SER VAL SER THR LEU ILE ASP I155 ILE ILE CYS GLN LYS PHE ASN VAL SER TYR VAL ASP ILE

VAL GLY GLU ASP LYS MET M66 V70 I79 E80 R92 Y96 I104 S108 N109 W111 P110 D120 L121 N125 I126 T131 F132 D133 E134 I135 E136 R137 Y138 Y141 M148 L149 E150 K154 R155 M156 V157 A158

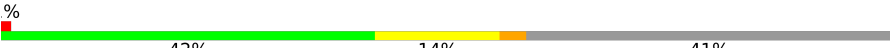
- Molecule 2: Putative transcriptional regulator PezA

Chain E:  %

MET ILE GLY GLU ASP LYS ASN ILE LYS SER LEU ARG THR HIS ASP LEU THR GLN LEU GLU PHE ALA ARG ILE ILE VAL GLY ILE SER ARG ASN SER LEU SER ARG TYR I126 GLU ASN THR SER SER VAL SER THR LEU ILE ASP I155 ILE ILE CYS GLN LYS PHE ASN VAL SER TYR VAL ASP ILE

VAL GLY GLU D84 L67 N68 E71 K78 V82 L90 Y96 Q97 D98 S99 P110 W111 I112 L113 M114 S115 L118 I121 I122 M125 I126 Y127 L128 V129 E134 I135 Y138 S139 G140 M148 L149 E150 I151 S152 M156 V157 A158

- Molecule 2: Putative transcriptional regulator PezA

Chain G:  %

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

VAL GLY GLU ASP M66 M67 M68 M69 V70 Y73 K78 I79 K83 G86 D98 I104 P110 M114 S115 D116 L121 I122 N125 I126 Y127 L128 V129 D133 E134 I135 E136 R137 Y141 I145 L149 E150 I151 R155 M156 V157 A158

• Molecule 3: PezT

Chain B: 73% 20%

MET GLU I3 Q4 R20 S21 L22 L23 R24 P32 I33 Q40 K45 T46 Q53 Q58 I62 R69 S70 Q79 Q80 E81 Y82 G83 K84 V87 E88 Y89 M111 L112 L113 T117 L118 R119 T120 V121 D122 V123 L131 Y136 E137 V138 T143 A144 T145

S153 R157 E160 L161 T164 N165 Q168 A168 ARG A168 THR PRO LYS H176 H177 D178 F179 I180 E198 R199 Q204 Q205 D206 Y207 S208 Y211 D212 S213 S214 K214 E215 N216 V223 L227 E238 N248 E249 L250 L251 E252 K253

• Molecule 3: PezT

Chain D: 72% 22%

M1 E2 I3 T7 R17 R24 Q25 A141 K26 T35 L36 L37 T46 T51 K52 Q53 Q58 N59 I60 V61 I62 I63 D64 G65 D66 R69 S70 Q71 H72 H73 H74 H75 Q79 Q87 E88 T89 K91 G95 E99 S100 L108 L113 T114 E115 L118

R119 T120 V121 L131 Y136 L140 A141 L142 T145 K146 P147 Y151 R157 N165 P166 Q168 A168 ARG THR A168 K174 E175 H176 H177 L200 Q201 L202 Y203 Q204 V210 V211 T218 S219 D222 V223 F229 V235 E236 K237 E244 L251 LYS

• Molecule 3: PezT

Chain F: 77% 16% 5%

MET E2 I3 T7 D8 K12 L19 L23 R24 T23 K27 S28 S41 T46 H49 N59 I60 S70 Q79 Y82 G83 M111 L112 L113 T117 L118 R119 T120 V121 D122 V123 P124 A144 T145 K146 S150 E160 I163 I164 H165 PRO ASN GLN

ALA ARG THR PRO LYS HIS D178 F179 I180 V185 E198 D212 E215 Q225 F228 W232 S233 E236 K245 E249 K253

• Molecule 3: PezT

Chain H: 2% 69% 24%

M1 T7 D8 S9 H13 A14 R17 R18 S21 R24 G25 K26 P32 I35 L36 L37 Q40 S41 G42 A43 R50 I51 K54 G58 I62 S70 H74 Q79 G83 R84 E88 A94 V98 S106 L113 L118 R119 T120

V121 D122 P124 K125 Q129 Y136 Q139 T145 E148 L152 G153 T154 L155 E159 I163 T164 N165 P166 ASN GLN ALA ALA THR PRO LYS GLU HIS D178 F179 M182 H183 I196 R199 Q204 R205 D206 R207 V210 T217 A221

L224 W232 L240 Q241 E244 K245 R246 L250 L251 E252 K253

4 Data and refinement statistics

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 47.67 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-3.20) 98.4 (47.67-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/770	0.91	0/1039
2	C	0.48	0/778	0.86	0/1049
2	E	0.52	0/795	0.93	2/1071 (0.2%)
2	G	0.53	0/778	0.92	1/1049 (0.1%)
3	B	0.49	0/2010	0.85	0/2703
3	D	0.49	0/2034	0.84	0/2736
3	F	0.49	0/1972	0.86	0/2650
3	H	0.54	0/1988	0.89	0/2672
All	All	0.50	0/11125	0.87	3/14969 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	125	ASN	N-CA-C	6.54	119.40	111.82
2	E	125	ASN	N-CA-C	6.23	118.07	111.28
2	E	126	ILE	CB-CA-C	-5.61	104.70	112.04

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	X	132	0	2	0	0
2	A	759	0	740	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	767	0	749	22	0
2	E	784	0	766	19	0
2	G	767	0	749	23	0
3	B	1979	0	1997	33	0
3	D	2002	0	2023	38	0
3	F	1944	0	1968	20	0
3	H	1959	0	1987	43	0
All	All	11093	0	10981	187	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 (187) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:146:LYS:HZ1	3:F:232:TRP:CD1	2.23	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
3:F:59:ASN:CG	3:F:59:ASN:O	2.49	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
2:E:99:SER:HB3	2:E:156:MET:HE3	1.89	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
3:D:204:GLN:CD	3:D:210:VAL:HG21	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:OD1	3:F:122:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:1:MET:HE1	3:H:74:HIS:CE1	2.50	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
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:A:83:LYS:HZ3	3:B:46:THR:HG22	1.82	0.45
3:B:79:GLN:C	3:B:81:GLU:H	2.24	0.45
2:C:136:GLU:O	2:C:137:ARG:C	2.60	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:D:165:ASN:C	3:D:167:ASN:H	2.24	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:F:82:TYR:O	3:F:83:GLY:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:148:MET:HE2	2:G:114:MET:HA	2.01	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
2:A:114:MET:HE3	2:A:145:ILE:HG12	2.01	0.41
3:H:106:SER:HA	3:H:136:TYR:OH	2.20	0.41
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:122:ASP:O	3:B:123:VAL:C	2.64	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: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: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%)	11	43
2	C	91/158 (58%)	87 (96%)	3 (3%)	1 (1%)	11	43
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%)	30	62
3	D	243/253 (96%)	226 (93%)	15 (6%)	2 (1%)	16	50
3	F	236/253 (93%)	221 (94%)	13 (6%)	2 (1%)	16	50
3	H	238/253 (94%)	224 (94%)	13 (6%)	1 (0%)	30	62
All	All	1322/1644 (80%)	1235 (93%)	79 (6%)	8 (1%)	21	56

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%)	32	64
2	C	87/147 (59%)	84 (97%)	3 (3%)	32	64
2	E	89/147 (60%)	81 (91%)	8 (9%)	9	34
2	G	87/147 (59%)	78 (90%)	9 (10%)	7	28
3	B	219/226 (97%)	198 (90%)	21 (10%)	8	32
3	D	222/226 (98%)	200 (90%)	22 (10%)	7	31
3	F	215/226 (95%)	199 (93%)	16 (7%)	13	43
3	H	217/226 (96%)	194 (89%)	23 (11%)	6	27
All	All	1222/1492 (82%)	1117 (91%)	105 (9%)	10	36

All (105) 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	46	THR
3	B	70	SER
3	B	84	LYS
3	B	87	VAL
3	B	117	THR
3	B	118	LEU
3	B	120	THR
3	B	121	VAL
3	B	123	VAL
3	B	138	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	70	VAL
2	C	108	SER
2	C	157	VAL

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Mol	Chain	Res	Type
3	D	7	THR
3	D	26	LYS
3	D	46	THR
3	D	64	ASP
3	D	70	SER
3	D	79	GLN
3	D	88	GLU
3	D	90	THR
3	D	99	GLU
3	D	100	SER
3	D	108	LEU
3	D	118	LEU
3	D	119	ARG
3	D	121	VAL
3	D	145	THR
3	D	157	ARG
3	D	175	GLU
3	D	218	THR
3	D	219	SER
3	D	235	VAL
3	D	237	LYS
3	D	244	GLU
2	E	113	LEU
2	E	115	SER
2	E	121	LEU
2	E	126	ILE
2	E	134	GLU
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	118	LEU
3	F	120	THR
3	F	121	VAL
3	F	122	ASP

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Mol	Chain	Res	Type
3	F	150	SER
3	F	163	ILE
3	F	198	GLU
3	F	253	LYS
2	G	68	ASN
2	G	70	VAL
2	G	83	LYS
2	G	104	ILE
2	G	122	ILE
2	G	126	ILE
2	G	129	VAL
2	G	133	ASP
2	G	149	LEU
3	H	1	MET
3	H	21	SER
3	H	41	SER
3	H	70	SER
3	H	79	GLN
3	H	84	LYS
3	H	88	GLU
3	H	118	LEU
3	H	120	THR
3	H	122	ASP
3	H	123	VAL
3	H	129	GLN
3	H	145	THR
3	H	154	THR
3	H	159	GLU
3	H	178	ASP
3	H	182	ASN
3	H	196	ILE
3	H	204	GLN
3	H	210	VAL
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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	125	ASN
3	B	53	GLN

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Mol	Chain	Res	Type
3	B	111	ASN
3	B	204	GLN
3	B	216	ASN
3	D	53	GLN
3	D	72	HIS
3	D	129	GLN
3	D	176	HIS
3	D	182	ASN
2	E	125	ASN
3	F	31	GLN
3	F	59	ASN
3	F	204	GLN
2	G	100	GLN
2	G	123	HIS
3	H	49	HIS
3	H	129	GLN
3	H	133	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	0/33	-	-	-	-
2	A	92/158 (58%)	-0.14	2 (2%) 62 42	78, 88, 97, 104	0
2	C	93/158 (58%)	-0.18	0 100 100	79, 90, 105, 112	0
2	E	95/158 (60%)	-0.24	0 100 100	79, 89, 107, 114	0
2	G	93/158 (58%)	-0.17	1 (1%) 78 61	79, 89, 108, 111	0
3	B	244/253 (96%)	-0.03	1 (0%) 88 79	78, 91, 106, 115	0
3	D	247/253 (97%)	-0.24	1 (0%) 88 79	79, 89, 105, 114	0
3	F	240/253 (94%)	-0.23	2 (0%) 82 67	74, 89, 114, 123	0
3	H	242/253 (95%)	-0.19	4 (1%) 69 49	75, 90, 112, 130	0
All	All	1346/1677 (80%)	-0.17	11 (0%) 82 67	74, 90, 107, 130	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	178	ASP	6.6
3	F	178	ASP	4.0
3	B	3	ILE	3.6
3	H	179	PHE	3.5
3	H	164	ILE	2.8
3	F	179	PHE	2.7
2	A	127	TYR	2.6
3	H	163	ILE	2.5
3	D	3	ILE	2.4
2	G	157	VAL	2.2
2	A	67	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.