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 (i)

Oct 31, 2017 – 01:03 AM EDT

|		
PDB ID	:	3RST
Title	:	Crystal structure of Bacillus subtilis signal peptide peptidase A
Authors	:	Nam, S.E.; Paetzel, M.
Deposited on	:	unknown
Resolution	:	2.37 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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.
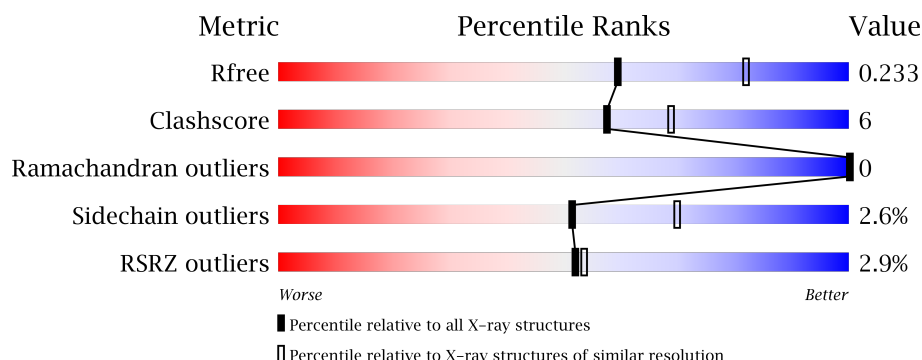
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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 <=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	240	.% / 83% 12% 5%
1	B	240	5% / 85% 8% 7%
1	C	240	2% / 81% 13% · 5%
1	D	240	3% / 83% 10% 7%
1	E	240	5% / 82% 10% · 7%

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Mol	Chain	Length	Quality of chain
1	F	240	2% / 83% / 12% / 6%
1	G	240	4% / 86% / 7% / · / 6%
1	H	240	.% / 86% / 8% / 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13957 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 Signal peptide peptidase sppA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	1	0
			1726	1084	288	345	9			
1	B	223	Total	C	N	O	S	0	0	0
			1699	1069	286	335	9			
1	C	229	Total	C	N	O	S	0	0	0
			1740	1092	291	348	9			
1	D	223	Total	C	N	O	S	0	0	0
			1687	1058	282	338	9			
1	E	223	Total	C	N	O	S	12	1	0
			1701	1068	286	338	9			
1	F	226	Total	C	N	O	S	5	1	0
			1706	1071	282	343	10			
1	G	226	Total	C	N	O	S	7	1	0
			1714	1076	289	340	9			
1	H	226	Total	C	N	O	S	0	0	0
			1727	1086	290	342	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
B	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
C	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
D	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
E	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
F	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
G	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525
H	199	ALA	LYS	ENGINEERED MUTATION	UNP O34525

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total 45	O 45	0	0
2	B	18	Total 18	O 18	0	0
2	C	33	Total 33	O 33	0	0
2	D	23	Total 23	O 23	0	0
2	E	27	Total 27	O 27	0	0
2	F	46	Total 46	O 46	0	0
2	G	35	Total 35	O 35	0	0
2	H	30	Total 30	O 30	0	0

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 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 contai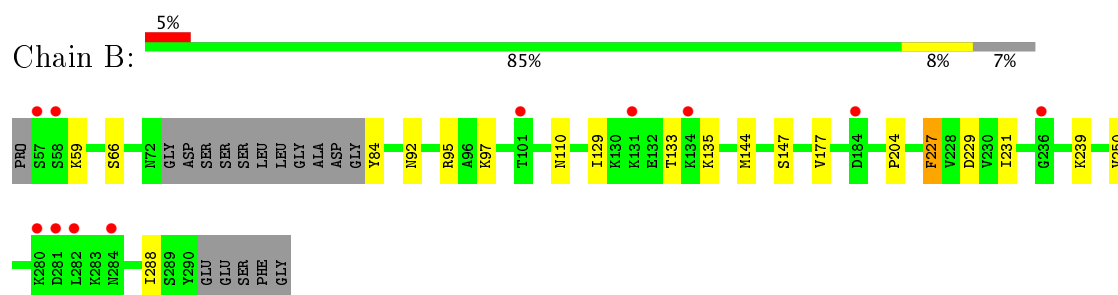n at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
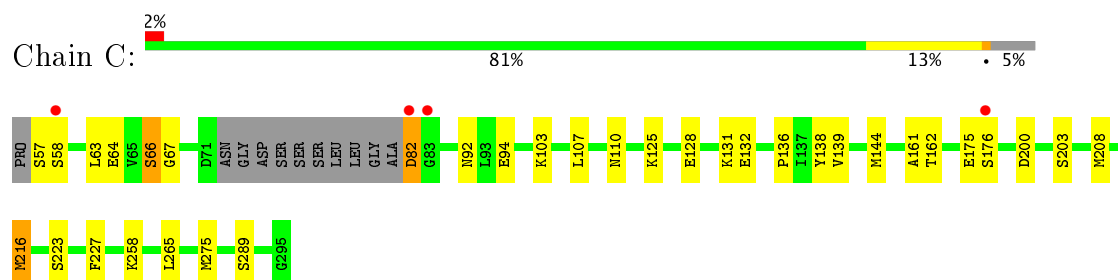
- Molecule 1: Signal peptide peptidase sppA

- Molecule 1: Signal peptide peptidase sppA

- Molecule 1: Signal peptide peptidase sppA

- Molecule 1: Signal peptide peptidase sppA

P204 M208 M216 F227 S286 V287 Y290 GLU GLU SER PHE GLY

• Molecule 1: Signal peptide peptidase sppA

Chain E:

5%

82% 10% 7%

PRO S57 S58 K59 I60 A61 D71 ASN GLY ASP SER SER SER LEU LEU GLY ALA ASP G83 L93 E94 K97 K100 T101 L107 K125 E128 I129 E132 L166 N178 Y179 S180 I201 M202 E212 M216 F227 K244 Y268 I272 T273 A274

M275 K276 K277 D278 H279 K280 D281 L282 K283 N284 Y290 GLU GLU SER PHE GLY

• Molecule 1: Signal peptide peptidase sppA

Chain F:

2%

83% 12% 6%

PRO S57 S58 K59 E64 V65 N72 GLY ASP SER SER SER LEU LEU GLY ALA D82 G83 V106 L107 P112 V139 M144 A156 A161 T162 P163 L166 S169 E175 S176 V177 S189 I201 M202 M208 K213 M216 F227 G248 G253

L265 I272 I288 E291 GLU SER PHE GLY

• Molecule 1: Signal peptide peptidase sppA

Chain G:

4%

86% 7% 6%

PRO S57 S58 N72 GLY ASP SER SER SER LEU LEU GLY ALA D82 G83 R95 D98 K103 T133 K134 K135 T162 S169 M174 E175 S176 E191 I201 M216 M219 V220 F227 G248 G253 R254 Y268 I272 L282 I288 S289 Y290

E291 GLU SER PHE GLY

• Molecule 1: Signal peptide peptidase sppA

Chain H:

.%

86% 8% 6%

P56 L63 S66 N72 GLY ASP SER SER SER LEU LEU GLY ALA ASP G83 Y84 E94 K125 T162 S169 M174 E175 S176 V177 N178 E191 R206 E207 M208 T209 K210 K213 F227 G248 Y268 I272 V287 I288 S289 Y290 E291 GLU SER PHE

GLY

4 Data and refinement statistics (i)

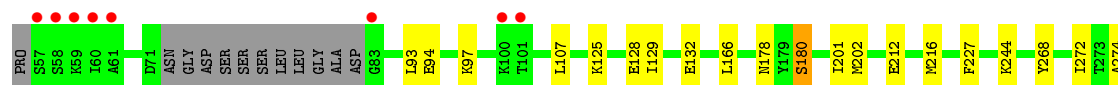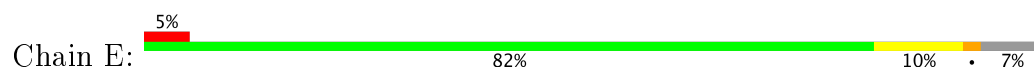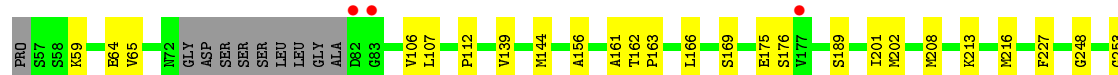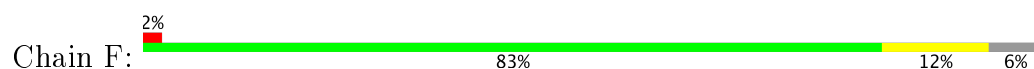| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	87.78Å 131.07Å 207.26Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	50.00 – 2.37	Depositor
	40.65 – 2.37	EDS
% Data completeness	98.2 (50.00-2.37)	Depositor
(in resolution range)	98.1 (40.65-2.37)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	8.33 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.241	Depositor
	0.200 , 0.233	DCC
R_{free} test set	4804 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.7	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13957	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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 (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	#$|Z| > 5$
1	A	0.50	0/1752	0.59	0/2350
1	B	0.43	0/1721	0.55	0/2307
1	C	0.49	0/1763	0.57	0/2364
1	D	0.49	0/1709	0.55	0/2293
1	E	0.51	0/1729	0.56	0/2317
1	F	0.53	0/1733	0.58	0/2327
1	G	0.49	0/1743	0.59	0/2337
1	H	0.51	0/1750	0.59	0/2344
All	All	0.49	0/13900	0.57	0/18639

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1726	0	1721	20	0
1	B	1699	0	1718	11	0
1	C	1740	0	1739	23	0
1	D	1687	0	1676	16	0
1	E	1701	0	1709	33	0
1	F	1706	0	1692	29	0
1	G	1714	0	1714	24	0
1	H	1727	0	1750	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	45	0	0	0	0
2	B	18	0	0	1	0
2	C	33	0	0	0	0
2	D	23	0	0	0	0
2	E	27	0	0	1	0
2	F	46	0	0	0	0
2	G	35	0	0	0	0
2	H	30	0	0	0	0
All	All	13957	0	13719	154	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 6.

All (154) 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:281:ASP:C	1:E:282:LEU:HD22	1.53	1.27
1:E:281:ASP:O	1:E:282:LEU:HD22	1.38	1.19
1:E:281:ASP:C	1:E:282:LEU:CD2	2.14	1.15
1:G:201:ILE:CD1	1:G:216:MET:HE1	1.87	1.03
1:G:201:ILE:HD13	1:G:216:MET:HE1	1.38	1.00
1:G:268:TYR:CZ	1:G:272:ILE:HD11	2.01	0.94
1:G:201:ILE:CD1	1:G:216:MET:CE	2.46	0.93
1:G:201:ILE:HD11	1:G:216:MET:CE	2.00	0.91
1:E:277:LYS:HD2	1:E:277:LYS:O	1.75	0.87
1:E:282:LEU:CD2	1:E:282:LEU:N	2.34	0.87
1:F:166:LEU:HD11	1:G:219:MET:HE1	1.59	0.85
1:E:279:HIS:HB2	1:E:282:LEU:HG	1.61	0.81
1:E:281:ASP:C	1:E:282:LEU:HD23	2.01	0.78
1:E:282:LEU:HD23	1:E:282:LEU:N	1.99	0.77
1:C:67:GLY:HA3	1:C:82:ASP:HB3	1.67	0.76
1:H:208:MET:HE2	1:H:213:LYS:HA	1.67	0.76
1:F:201:ILE:HD13	1:F:216:MET:CE	2.15	0.75
1:D:201:ILE:CD1	1:D:216:MET:HE2	2.21	0.71
1:D:65:VAL:HG23	1:D:107:LEU:HD11	1.71	0.71
1:F:166:LEU:CD1	1:G:219:MET:HE1	2.22	0.70
1:E:279:HIS:CB	1:E:282:LEU:HG	2.21	0.69
1:H:268:TYR:CZ	1:H:272:ILE:HD11	2.27	0.69
1:C:67:GLY:HA3	1:C:82:ASP:CB	2.23	0.68
1:D:201:ILE:HD13	1:D:216:MET:HE2	1.76	0.68
1:F:202[B]:MET:HE1	1:F:208:MET:SD	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:MET:CE	1:C:216:MET:HA	2.23	0.67
1:E:268:TYR:CZ	1:E:272:ILE:HD11	2.30	0.67
1:C:216:MET:HA	1:C:216:MET:HE3	1.77	0.67
1:G:174:MET:CE	1:G:220:VAL:HG23	2.26	0.66
1:C:63:LEU:HD21	1:C:92:ASN:HB3	1.78	0.64
1:H:63:LEU:HD21	1:H:290:TYR:HD2	1.63	0.64
1:E:93:LEU:HD23	1:E:125:LYS:HG2	1.80	0.63
1:D:201:ILE:HD13	1:D:216:MET:CE	2.28	0.63
1:F:208:MET:HE2	1:F:213:LYS:HA	1.82	0.61
1:F:208:MET:HE1	1:F:216:MET:HG3	1.81	0.61
1:E:201:ILE:CD1	1:E:216:MET:HE3	2.31	0.61
1:E:97:LYS:HG3	1:E:129:ILE:HG12	1.81	0.61
1:E:274:ALA:O	1:E:278:ASP:HB2	2.00	0.60
1:F:112:PRO:HA	1:F:144:MET:HE1	1.83	0.59
1:C:216:MET:CA	1:C:216:MET:HE3	2.32	0.59
1:A:191:GLU:HB3	1:H:176:SER:OG	2.03	0.59
1:E:201:ILE:HG13	1:E:212:GLU:HG2	1.84	0.58
1:F:65:VAL:HG23	1:F:107:LEU:HD11	1.86	0.58
1:A:201:ILE:HG12	1:A:216:MET:HE2	1.87	0.56
1:H:178:ASN:ND2	1:H:206:ARG:O	2.38	0.56
1:F:201:ILE:CD1	1:F:216:MET:HE2	2.36	0.56
1:E:277:LYS:CD	1:E:277:LYS:O	2.51	0.55
1:E:125:LYS:HD2	2:E:315:HOH:O	2.07	0.55
1:A:202:MET:HG2	1:A:216:MET:CE	2.36	0.55
1:F:201:ILE:CD1	1:F:216:MET:CE	2.85	0.55
1:G:201:ILE:HD11	1:G:216:MET:HE3	1.89	0.54
1:E:268:TYR:CE1	1:E:272:ILE:HD11	2.42	0.54
1:F:176:SER:OG	1:G:191:GLU:HB3	2.07	0.54
1:C:64:GLU:OE2	1:D:87:ARG:NH1	2.41	0.53
1:E:201:ILE:HG12	1:E:216:MET:HE3	1.90	0.53
1:F:201:ILE:HD13	1:F:216:MET:HE2	1.89	0.53
1:F:201:ILE:O	1:F:202[A]:MET:HB2	2.09	0.53
1:E:274:ALA:O	1:E:278:ASP:N	2.42	0.53
1:E:128:GLU:O	1:E:132:GLU:HG2	2.08	0.53
1:E:178:ASN:OD1	1:E:180:SER:HB3	2.09	0.52
1:C:94:GLU:OE1	1:C:125:LYS:HE2	2.10	0.52
1:G:176:SER:OG	1:H:191:GLU:HB3	2.10	0.51
1:F:201:ILE:O	1:F:202[B]:MET:HB2	2.10	0.51
1:F:201:ILE:HD13	1:F:216:MET:HE3	1.90	0.51
1:G:174:MET:HE3	1:G:220:VAL:HG23	1.91	0.51
1:E:201:ILE:O	1:E:202:MET:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:TYR:CE2	1:G:272:ILE:HD11	2.44	0.51
1:G:174:MET:CE	1:G:220:VAL:CG2	2.90	0.50
1:D:128:GLU:O	1:D:132:GLU:HG2	2.11	0.50
1:B:92:ASN:HA	1:B:95:ARG:HD3	1.92	0.50
1:A:177:VAL:O	1:A:204:PRO:HA	2.11	0.50
1:D:179:TYR:CE2	1:D:204:PRO:HB2	2.47	0.50
1:E:201:ILE:HD11	1:E:216:MET:CE	2.42	0.50
1:C:107:LEU:HB2	1:C:139:VAL:HG22	1.94	0.49
1:A:225:GLU:OE2	1:A:243:LYS:NZ	2.36	0.49
1:A:191:GLU:HB3	1:H:176:SER:HG	1.78	0.49
1:A:208:MET:HE1	1:A:216:MET:HG3	1.94	0.48
1:G:201:ILE:CD1	1:G:216:MET:HE3	2.38	0.48
1:C:176:SER:OG	1:D:191:GLU:HB3	2.12	0.48
1:F:166:LEU:CD1	1:G:219:MET:CE	2.91	0.48
1:F:161:ALA:O	1:F:265:LEU:HA	2.14	0.48
1:D:208:MET:HE1	1:D:216:MET:HG3	1.96	0.48
1:A:201:ILE:O	1:A:202:MET:HB2	2.14	0.47
1:E:201:ILE:CD1	1:E:216:MET:CE	2.92	0.47
1:A:202:MET:HG2	1:A:216:MET:HE3	1.95	0.47
1:B:110:ASN:HA	1:B:144:MET:O	2.15	0.47
1:E:201:ILE:CD1	1:E:212:GLU:HG2	2.44	0.47
1:D:105:ILE:HB	1:D:137:ILE:HG12	1.97	0.46
1:A:161:ALA:O	1:A:265:LEU:HA	2.15	0.46
1:G:268:TYR:CE1	1:G:272:ILE:HD11	2.46	0.46
1:B:97:LYS:HG3	1:B:129:ILE:HG12	1.98	0.46
1:G:162:THR:O	1:G:253:GLY:HA3	2.16	0.46
1:A:162:THR:O	1:A:253:GLY:HA3	2.16	0.46
1:F:162:THR:HB	1:F:163:PRO:HD2	1.98	0.46
1:F:169:SER:HA	1:F:248:GLY:O	2.16	0.46
1:F:162:THR:O	1:F:253:GLY:HA3	2.15	0.46
1:F:59:LYS:HD3	1:F:288:ILE:HG12	1.98	0.46
1:C:110:ASN:HA	1:C:144:MET:O	2.16	0.45
1:E:276:LYS:HG2	1:E:282:LEU:O	2.16	0.45
1:D:167:THR:HG23	1:D:168:GLY:N	2.30	0.45
1:A:65:VAL:HG23	1:A:107:LEU:HD11	1.97	0.45
1:G:174:MET:HE2	1:G:220:VAL:CG2	2.48	0.44
1:C:128:GLU:O	1:C:132:GLU:HG2	2.17	0.44
1:E:94:GLU:OE1	1:E:125:LYS:HE3	2.17	0.44
1:C:162:THR:HG21	1:D:117:TYR:HE1	1.81	0.44
1:E:201:ILE:CG1	1:E:216:MET:HE3	2.47	0.44
1:G:133:THR:HB	1:G:135:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:268:TYR:OH	1:H:272:ILE:HD11	2.18	0.44
1:C:162:THR:HG21	1:D:117:TYR:CE1	2.52	0.44
1:E:281:ASP:N	1:E:282:LEU:HD23	2.32	0.44
1:G:95:ARG:HG2	1:G:290:TYR:CE1	2.53	0.43
1:A:139:VAL:HG23	1:A:156:ALA:HB2	1.98	0.43
1:A:64:GLU:HG2	1:A:108:LYS:HB2	2.01	0.43
1:A:202:MET:HG2	1:A:216:MET:HE2	2.00	0.43
1:B:59:LYS:HD3	1:B:288:ILE:HD12	1.99	0.43
1:B:250:VAL:HG23	1:C:216:MET:HE1	2.00	0.43
1:C:216:MET:N	1:C:216:MET:HE3	2.33	0.43
1:F:202[B]:MET:HE1	1:F:208:MET:CE	2.48	0.43
1:C:138:TYR:CD1	1:C:275:MET:HE2	2.54	0.43
1:C:216:MET:CE	1:C:216:MET:CA	2.92	0.43
1:C:66:SER:HA	1:C:110:ASN:O	2.19	0.42
1:A:213:LYS:HB2	1:A:213:LYS:HE3	1.85	0.42
1:E:201:ILE:CG1	1:E:212:GLU:HG2	2.49	0.42
1:G:169:SER:HA	1:G:248:GLY:O	2.19	0.42
1:D:95:ARG:O	1:D:99:ASP:HB2	2.19	0.42
1:H:94:GLU:OE1	1:H:125:LYS:HE2	2.20	0.42
1:A:110:ASN:HA	1:A:144:MET:O	2.20	0.42
1:B:229:ASP:OD1	1:B:239:LYS:NZ	2.52	0.42
1:A:276:LYS:O	1:A:283:LYS:HE2	2.20	0.42
1:B:147:SER:OG	2:B:307:HOH:O	2.20	0.42
1:F:139:VAL:HG23	1:F:156:ALA:HB2	2.00	0.42
1:F:176:SER:HG	1:G:191:GLU:HB3	1.85	0.42
1:A:201:ILE:HD13	1:A:216:MET:HE1	2.00	0.42
1:H:169:SER:HA	1:H:248:GLY:O	2.19	0.42
1:B:177:VAL:O	1:B:204:PRO:HA	2.19	0.42
1:B:66:SER:O	1:B:84:TYR:HB2	2.20	0.41
1:C:200:ASP:O	1:C:203:SER:HB2	2.20	0.41
1:F:106:VAL:HG21	1:F:272:ILE:HD13	2.02	0.41
1:A:128:GLU:O	1:A:132:GLU:HB2	2.21	0.41
1:C:208:MET:HE3	1:C:216:MET:HG3	2.02	0.41
1:H:66:SER:O	1:H:84:TYR:HB2	2.19	0.41
1:B:133:THR:HB	1:B:135:LYS:HE3	2.02	0.41
1:C:161:ALA:O	1:C:265:LEU:HA	2.21	0.41
1:D:201:ILE:O	1:D:202:MET:HB2	2.21	0.41
1:E:97:LYS:CG	1:E:129:ILE:HG12	2.49	0.41
1:C:103:LYS:O	1:C:136:PRO:HD2	2.20	0.41
1:D:85:ASN:HB3	1:D:88:THR:HB	2.03	0.41
1:B:227:PHE:O	1:B:231:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:MET:HB2	1:E:216:MET:HE2	1.89	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	224/240 (93%)	219 (98%)	5 (2%)	0	100	100
1	B	219/240 (91%)	212 (97%)	7 (3%)	0	100	100
1	C	225/240 (94%)	219 (97%)	6 (3%)	0	100	100
1	D	219/240 (91%)	213 (97%)	6 (3%)	0	100	100
1	E	220/240 (92%)	213 (97%)	7 (3%)	0	100	100
1	F	223/240 (93%)	218 (98%)	5 (2%)	0	100	100
1	G	223/240 (93%)	218 (98%)	5 (2%)	0	100	100
1	H	222/240 (92%)	215 (97%)	7 (3%)	0	100	100
All	All	1775/1920 (92%)	1727 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/201 (92%)	183 (99%)	2 (1%)	78	89
1	B	184/201 (92%)	183 (100%)	1 (0%)	91	96
1	C	188/201 (94%)	177 (94%)	11 (6%)	23	34
1	D	180/201 (90%)	176 (98%)	4 (2%)	57	75
1	E	184/201 (92%)	175 (95%)	9 (5%)	29	43
1	F	183/201 (91%)	179 (98%)	4 (2%)	57	75
1	G	184/201 (92%)	179 (97%)	5 (3%)	50	68
1	H	188/201 (94%)	184 (98%)	4 (2%)	59	76
All	All	1476/1608 (92%)	1436 (97%)	40 (3%)	51	68

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	PHE
1	A	289	SER
1	B	227	PHE
1	C	57	SER
1	C	58	SER
1	C	66	SER
1	C	82	ASP
1	C	131	LYS
1	C	175	GLU
1	C	216	MET
1	C	223	SER
1	C	227	PHE
1	C	258	LYS
1	C	289	SER
1	D	143	SER
1	D	169	SER
1	D	184	ASP
1	D	227	PHE
1	E	107	LEU
1	E	166	LEU
1	E	180	SER
1	E	227	PHE
1	E	244	LYS
1	E	277	LYS
1	E	278	ASP
1	E	280	LYS
1	E	282	LEU

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Mol	Chain	Res	Type
1	F	64	GLU
1	F	175	GLU
1	F	189	SER
1	F	227	PHE
1	G	174	MET
1	G	216	MET
1	G	227	PHE
1	G	254[A]	ARG
1	G	254[B]	ARG
1	H	162	THR
1	H	210	LYS
1	H	227	PHE
1	H	287	VAL

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

Mol	Chain	Res	Type
1	A	70	GLN
1	A	217	GLN
1	B	198	HIS
1	B	214	ASN
1	C	110	ASN
1	C	198	HIS
1	D	70	GLN
1	D	198	HIS
1	D	217	GLN
1	E	217	GLN
1	E	222	ASN
1	E	279	HIS
1	F	198	HIS
1	F	217	GLN
1	G	70	GLN
1	G	222	ASN
1	H	70	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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(Å²)	Q<0.9
1	A	227/240 (94%)	-0.05	2 (0%)	84	85	26, 38, 60, 77	0
1	B	223/240 (92%)	0.13	11 (4%)	30	33	32, 50, 89, 105	0
1	C	229/240 (95%)	-0.01	4 (1%)	70	71	29, 43, 63, 74	0
1	D	223/240 (92%)	0.24	8 (3%)	43	46	34, 55, 102, 112	0
1	E	223/240 (92%)	0.16	12 (5%)	26	28	27, 50, 111, 169	2 (0%)
1	F	226/240 (94%)	-0.16	4 (1%)	69	70	27, 40, 64, 81	1 (0%)
1	G	226/240 (94%)	-0.05	9 (3%)	39	42	27, 45, 81, 101	1 (0%)
1	H	226/240 (94%)	-0.11	3 (1%)	77	78	27, 43, 72, 84	0
All	All	1803/1920 (93%)	0.02	53 (2%)	52	53	26, 45, 82, 169	4 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	82	ASP	5.2
1	D	83	GLY	4.8
1	E	282	LEU	4.2
1	G	58	SER	4.2
1	E	57	SER	4.2
1	B	280	LYS	4.1
1	D	58	SER	3.5
1	F	83	GLY	3.5
1	F	82	ASP	3.4
1	B	57	SER	3.3
1	D	290	TYR	3.3
1	D	287	VAL	3.3
1	D	101	THR	3.3
1	B	58	SER	3.3
1	E	58	SER	3.2
1	E	290	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	57	SER	3.1
1	C	83	GLY	3.1
1	G	288	ILE	3.0
1	E	100	LYS	2.9
1	G	134	LYS	2.9
1	B	284	ASN	2.8
1	B	134	LYS	2.8
1	D	102	VAL	2.8
1	B	101	THR	2.8
1	B	282	LEU	2.7
1	E	101	THR	2.7
1	G	83	GLY	2.7
1	C	82	ASP	2.6
1	D	286	SER	2.6
1	B	281	ASP	2.5
1	A	56	PRO	2.5
1	B	131	LYS	2.5
1	D	59	LYS	2.5
1	E	83	GLY	2.5
1	C	58	SER	2.4
1	H	174	MET	2.3
1	A	82	ASP	2.3
1	G	282	LEU	2.3
1	B	184	ASP	2.2
1	H	83	GLY	2.2
1	E	284	ASN	2.2
1	G	98	ASP	2.2
1	F	177	VAL	2.1
1	E	61	ALA	2.1
1	C	176	SER	2.1
1	E	277	LYS	2.0
1	G	103	LYS	2.0
1	E	60	ILE	2.0
1	H	288	ILE	2.0
1	F	291	GLU	2.0
1	B	236	GLY	2.0
1	E	59	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.