Worldwide PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 12:57 AM EST

PDB ID	:	4GR4
Title	:	Crystal structure of SlgN1deltaAsub
Authors	:	Herbst, D.A.; Zocher, G.; Stehle, T.
Deposited on	:	2012-08-24
Resolution	:	2.44 Å(reported)

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

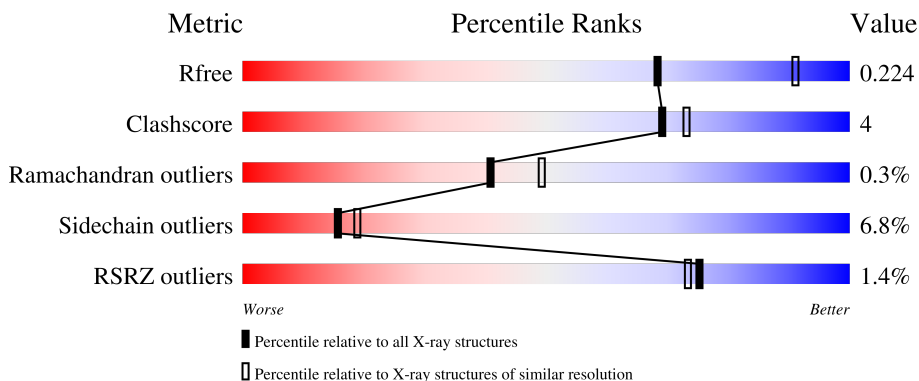|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.44 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		6.8%
RSRZ outliers		1.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	A	469	.% 84% 11% ··
1	B	469	.% 84% 10% ··
1	C	469	3% 86% 11% ··
1	D	469	.% 83% 11% · 5%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13783 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 Non-ribosomal peptide synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total 3357	C 2122	N 599	O 623	S 13	0	0	0
1	B	451	Total 3339	C 2109	N 595	O 623	S 12	0	0	0
1	C	458	Total 3353	C 2121	N 595	O 625	S 12	0	0	0
1	D	444	Total 3291	C 2080	N 585	O 614	S 12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D1GLU5
A	-1	SER	-	expression tag	UNP D1GLU5
A	0	HIS	-	expression tag	UNP D1GLU5
B	-2	GLY	-	expression tag	UNP D1GLU5
B	-1	SER	-	expression tag	UNP D1GLU5
B	0	HIS	-	expression tag	UNP D1GLU5
C	-2	GLY	-	expression tag	UNP D1GLU5
C	-1	SER	-	expression tag	UNP D1GLU5
C	0	HIS	-	expression tag	UNP D1GLU5
D	-2	GLY	-	expression tag	UNP D1GLU5
D	-1	SER	-	expression tag	UNP D1GLU5
D	0	HIS	-	expression tag	UNP D1GLU5

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total 139	O 139	0	0
3	B	108	Total 108	O 108	0	0
3	C	85	Total 85	O 85	0	0
3	D	110	Total 110	O 110	0	0

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: Non-ribosomal peptide synthetase
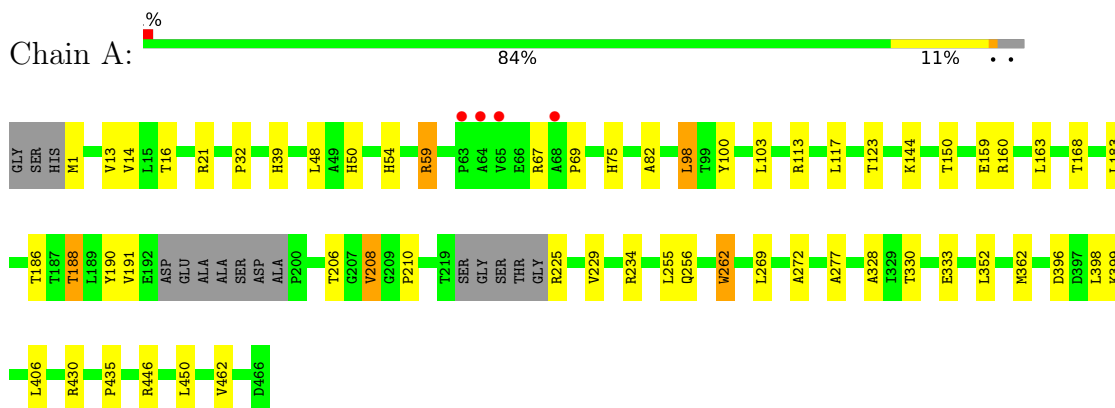
Chain A:

• Molecule 1: Non-ribosomal peptide synthetase

Chain B:

• Molecule 1: Non-ribosomal peptide synthetase

Chain C:

V432 G440 R443 R446 R454 V458 V462 A465 ASP

• Molecule 1: Non-ribosomal peptide synthetase

Chain D:

%

83%   11%   • 5%

GLY SER HIS MET S2 D9 T16 L48 R59 P60 T61 GLY PRO ALA VAL GLU ARG ALA P69 H75 Q81 A82 A83 R84 L98 T99 Y100 N104 N108 T123 E159 L163 L183 T184 L189 E192 ASP GLU ALA ALA SER ASP ALA PRO ALA

G202 N203 T206 G207 V208 E211 V216 T219 SER GLY SER THR GLY R225 V229 M230 R234 Q243 L255 Q256 W262 L269 Q282 D288 L306 S307 A308 D316 A328 I329 T330 E333 P334 A335 S336 H339 R344 L352 M362

L375 A387 R390 L398 L406 Y410 A425 R446 R452 R453 R454 V462 D466
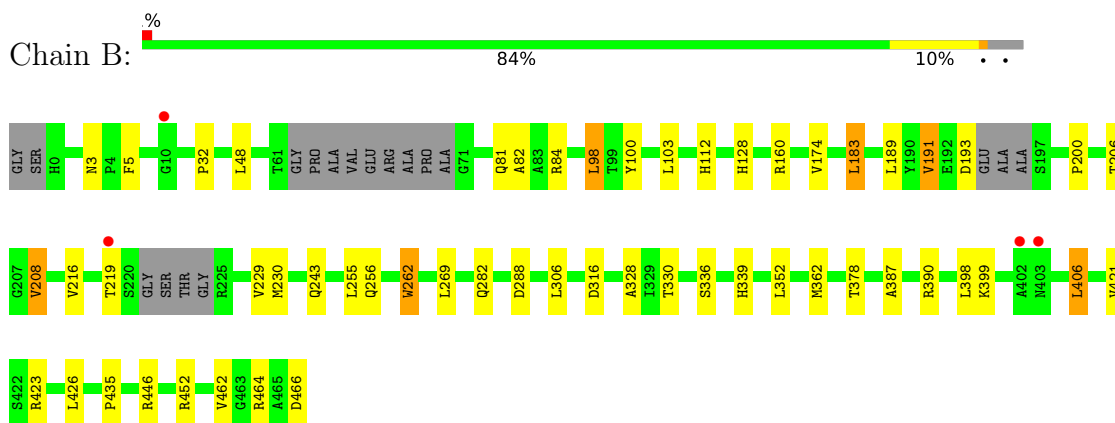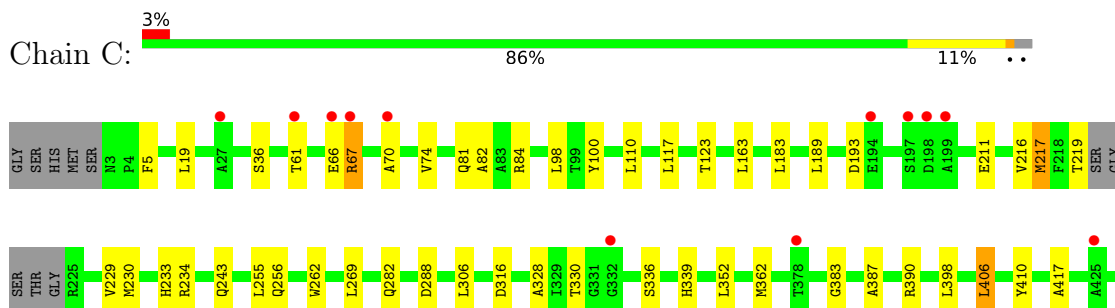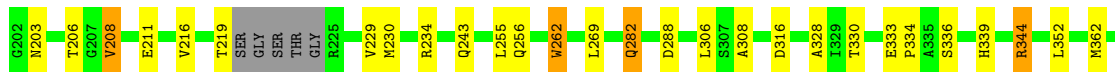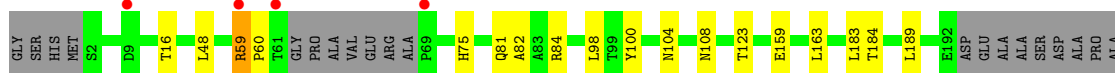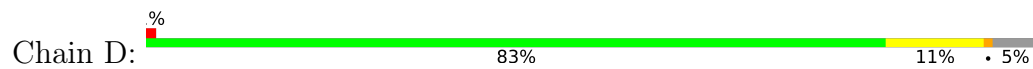
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.11Å 148.61Å 109.58Å 90.00° 113.34° 90.00°	Depositor
Resolution (Å)	35.72 – 2.44 35.63 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.72-2.44) 97.7 (35.63-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.180 , 0.213 0.192 , 0.224	Depositor DCC
R_{free} test set	4790 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 22.0	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.118 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13783	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	0.52	0/3438	0.75	0/4686
1	B	0.50	0/3419	0.72	0/4659
1	C	0.51	0/3436	0.72	1/4693 (0.0%)
1	D	0.50	0/3370	0.71	0/4591
All	All	0.51	0/13663	0.72	1/18629 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	217	MET	CB-CA-C	5.01	120.42	110.40

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	A	3357	0	3277	20	0
1	B	3339	0	3243	26	0
1	C	3353	0	3244	25	0
1	D	3291	0	3195	28	0
2	B	1	0	0	0	0
3	A	139	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	108	0	0	0	0
3	C	85	0	0	0	0
3	D	110	0	0	0	0
All	All	13783	0	12959	98	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 4.

All (98) 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:C:110:LEU:HD11	1:C:189:LEU:HD21	1.57	0.84
1:D:104:ASN:HD21	1:D:203:ASN:HD21	1.33	0.76
1:C:406:LEU:HD11	1:C:462:VAL:HG11	1.72	0.71
1:B:406:LEU:HD11	1:B:462:VAL:HG11	1.74	0.70
1:D:406:LEU:HD11	1:D:462:VAL:HG11	1.75	0.68
1:D:108:ASN:HD21	1:D:203:ASN:HD22	1.42	0.67
1:C:282:GLN:HE22	1:C:288:ASP:H	1.42	0.67
1:D:219:THR:HG22	1:D:262:TRP:HH2	1.58	0.66
1:C:243:GLN:HE22	1:C:387:ALA:H	1.43	0.66
1:B:282:GLN:HE22	1:B:288:ASP:H	1.44	0.66
1:C:5:PHE:CZ	1:C:432:VAL:HG11	2.32	0.65
1:D:211:GLU:OE1	1:D:234:ARG:HD3	1.97	0.64
1:D:243:GLN:HE22	1:D:387:ALA:H	1.44	0.64
1:C:211:GLU:OE1	1:C:234:ARG:HD3	1.98	0.63
1:D:282:GLN:HE22	1:D:288:ASP:H	1.46	0.62
1:B:216:VAL:HG22	1:B:230:MET:HB3	1.80	0.61
1:B:219:THR:HG22	1:B:262:TRP:HH2	1.66	0.60
1:C:216:VAL:HG22	1:C:230:MET:HB3	1.84	0.60
1:D:216:VAL:HG22	1:D:230:MET:HB3	1.84	0.59
1:B:243:GLN:HE22	1:B:387:ALA:H	1.47	0.59
1:D:108:ASN:HD21	1:D:203:ASN:ND2	2.01	0.59
1:A:186:THR:O	1:A:188:THR:HG22	2.04	0.57
1:C:410:TYR:CE2	1:C:446:ARG:HB3	2.40	0.55
1:D:219:THR:HG22	1:D:262:TRP:CH2	2.38	0.55
1:D:410:TYR:CE2	1:D:446:ARG:HB3	2.42	0.55
1:C:74:VAL:H	1:C:233:HIS:HD2	1.56	0.54
1:B:219:THR:HG22	1:B:262:TRP:CH2	2.43	0.54
1:A:272:ALA:HA	1:A:277:ALA:HB3	1.90	0.53
1:A:450:LEU:C	1:A:462:VAL:HG22	2.27	0.53
1:A:14:VAL:HB	1:A:39:HIS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HA	1:C:61:THR:HG22	1.90	0.53
1:B:336:SER:OG	1:B:339:HIS:HD2	1.92	0.52
1:C:336:SER:OG	1:C:339:HIS:HD2	1.93	0.52
1:B:306:LEU:O	1:B:330:THR:HA	2.10	0.52
1:D:308:ALA:HB3	1:D:333:GLU:HG2	1.93	0.51
1:D:336:SER:OG	1:D:339:HIS:HD2	1.94	0.51
1:A:450:LEU:HB2	1:A:462:VAL:CG2	2.41	0.51
1:B:328:ALA:HB3	1:B:352:LEU:HD23	1.93	0.51
1:D:59:ARG:HD2	1:D:60:PRO:HD2	1.93	0.51
1:B:3:ASN:ND2	1:B:446:ARG:HD3	2.26	0.51
1:C:74:VAL:H	1:C:233:HIS:CD2	2.29	0.51
1:D:328:ALA:HB3	1:D:352:LEU:HD23	1.93	0.50
1:A:328:ALA:HB3	1:A:352:LEU:HD23	1.93	0.50
1:A:82:ALA:HA	1:A:100:TYR:HB3	1.93	0.50
1:A:117:LEU:HD22	1:C:117:LEU:HD22	1.93	0.50
1:B:316:ASP:OD2	1:B:339:HIS:HE1	1.95	0.50
1:A:21:ARG:NE	3:A:630:HOH:O	2.44	0.50
1:B:174:VAL:CG1	1:B:191:VAL:HG13	2.42	0.49
1:A:113:ARG:NH1	1:A:190:TYR:O	2.46	0.49
1:A:150:THR:HG21	1:A:168:THR:HG21	1.95	0.49
1:C:328:ALA:HB3	1:C:352:LEU:HD23	1.93	0.49
1:C:316:ASP:OD2	1:C:339:HIS:HE1	1.96	0.48
1:B:406:LEU:HD12	1:B:452:ARG:CZ	2.44	0.48
1:D:81:GLN:NE2	1:D:84:ARG:HH21	2.12	0.48
1:C:67:ARG:HH12	1:C:440:GLY:HA3	1.78	0.48
1:D:406:LEU:HB2	1:D:452:ARG:HH21	1.79	0.48
1:C:383:GLY:HA2	1:C:458:VAL:HG13	1.96	0.47
1:C:81:GLN:HE22	1:C:84:ARG:HH21	1.61	0.47
1:D:82:ALA:HA	1:D:100:TYR:HB3	1.97	0.47
1:B:206:THR:OG1	1:B:208:VAL:HG22	2.15	0.47
1:C:81:GLN:NE2	1:C:84:ARG:HH21	2.12	0.47
1:A:98:LEU:HD13	1:A:103:LEU:HB2	1.95	0.47
1:D:333:GLU:HB2	1:D:334:PRO:HD2	1.97	0.47
1:C:5:PHE:CZ	1:C:398:LEU:HD11	2.50	0.47
1:B:81:GLN:NE2	1:B:84:ARG:HH21	2.13	0.46
1:B:32:PRO:HB3	1:B:435:PRO:HA	1.97	0.46
1:D:316:ASP:OD2	1:D:339:HIS:HE1	1.99	0.46
1:D:406:LEU:HD12	1:D:452:ARG:NH2	2.31	0.46
1:A:32:PRO:HB3	1:A:435:PRO:HA	1.98	0.46
1:A:69:PRO:HB2	1:A:210:PRO:HG2	1.98	0.45
1:A:262:TRP:HA	1:A:262:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ALA:HA	1:C:100:TYR:HB3	1.97	0.45
1:B:128:HIS:CD2	1:B:183:LEU:HD22	2.52	0.45
1:D:406:LEU:HD12	1:D:452:ARG:HH21	1.82	0.44
1:D:81:GLN:HE22	1:D:84:ARG:HH21	1.64	0.44
1:D:206:THR:OG1	1:D:208:VAL:HG22	2.18	0.44
1:C:306:LEU:O	1:C:330:THR:HA	2.18	0.44
1:B:82:ALA:HA	1:B:100:TYR:HB3	1.99	0.44
1:A:75:HIS:CD2	1:A:144:LYS:HA	2.53	0.44
1:B:5:PHE:HE2	1:B:398:LEU:HD21	1.83	0.44
1:D:344:ARG:HD3	1:D:375:LEU:HD11	1.98	0.44
1:B:262:TRP:HA	1:B:262:TRP:CE3	2.53	0.43
1:A:59:ARG:H	1:A:59:ARG:HG2	1.66	0.43
1:A:1:MET:HG2	1:A:396:ASP:OD1	2.18	0.43
1:A:206:THR:OG1	1:A:208:VAL:HG22	2.18	0.43
1:B:423:ARG:HH21	1:B:426:LEU:HD22	1.82	0.43
1:D:75:HIS:H	1:D:75:HIS:CD2	2.37	0.43
1:B:81:GLN:HE22	1:B:84:ARG:HH21	1.68	0.42
1:C:110:LEU:CD1	1:C:189:LEU:HD21	2.40	0.42
1:D:262:TRP:HA	1:D:262:TRP:CE3	2.55	0.42
1:A:50:HIS:CE1	1:A:54:HIS:CD2	3.08	0.42
1:D:48:LEU:HD22	1:D:425:ALA:HB1	2.01	0.41
1:C:417:ALA:O	1:C:443:ARG:NH2	2.53	0.41
1:B:3:ASN:HD21	1:B:446:ARG:HD3	1.85	0.41
1:B:98:LEU:HD13	1:B:103:LEU:HB2	2.03	0.41
1:C:219:THR:HA	1:C:262:TRP:CZ3	2.56	0.40
1:B:112:HIS:CE1	1:B:200:PRO:HG2	2.56	0.40
1:B:174:VAL:HG12	1:B:191:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/469 (96%)	439 (98%)	8 (2%)	1 (0%)	47	57
1	B	443/469 (94%)	434 (98%)	8 (2%)	1 (0%)	47	57
1	C	454/469 (97%)	441 (97%)	11 (2%)	2 (0%)	34	41
1	D	436/469 (93%)	430 (99%)	5 (1%)	1 (0%)	47	57
All	All	1781/1876 (95%)	1744 (98%)	32 (2%)	5 (0%)	41	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	MET
1	B	362	MET
1	C	362	MET
1	D	362	MET
1	C	70	ALA

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	333/346 (96%)	305 (92%)	28 (8%)	11	12
1	B	332/346 (96%)	312 (94%)	20 (6%)	19	25
1	C	328/346 (95%)	310 (94%)	18 (6%)	21	28
1	D	327/346 (94%)	303 (93%)	24 (7%)	14	17
All	All	1320/1384 (95%)	1230 (93%)	90 (7%)	16	19

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	16	THR
1	A	48	LEU
1	A	59	ARG
1	A	67	ARG
1	A	98	LEU

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Mol	Chain	Res	Type
1	A	123	THR
1	A	159	GLU
1	A	160	ARG
1	A	163	LEU
1	A	183	LEU
1	A	188	THR
1	A	191	VAL
1	A	208	VAL
1	A	225	ARG
1	A	229	VAL
1	A	234	ARG
1	A	255	LEU
1	A	256	GLN
1	A	262	TRP
1	A	269	LEU
1	A	330	THR
1	A	333	GLU
1	A	398	LEU
1	A	399	LYS
1	A	406	LEU
1	A	430	ARG
1	A	446	ARG
1	B	48	LEU
1	B	98	LEU
1	B	160	ARG
1	B	183	LEU
1	B	189	LEU
1	B	191	VAL
1	B	193	ASP
1	B	208	VAL
1	B	229	VAL
1	B	255	LEU
1	B	256	GLN
1	B	262	TRP
1	B	269	LEU
1	B	378	THR
1	B	390	ARG
1	B	399	LYS
1	B	406	LEU
1	B	421	VAL
1	B	464	ARG
1	B	466	ASP

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Mol	Chain	Res	Type
1	C	36	SER
1	C	66	GLU
1	C	67	ARG
1	C	98	LEU
1	C	123	THR
1	C	163	LEU
1	C	183	LEU
1	C	193	ASP
1	C	217	MET
1	C	229	VAL
1	C	255	LEU
1	C	256	GLN
1	C	269	LEU
1	C	390	ARG
1	C	406	LEU
1	C	432	VAL
1	C	446	ARG
1	C	454	ARG
1	D	16	THR
1	D	59	ARG
1	D	98	LEU
1	D	123	THR
1	D	159	GLU
1	D	163	LEU
1	D	183	LEU
1	D	184	THR
1	D	189	LEU
1	D	208	VAL
1	D	229	VAL
1	D	255	LEU
1	D	256	GLN
1	D	262	TRP
1	D	269	LEU
1	D	282	GLN
1	D	306	LEU
1	D	330	THR
1	D	344	ARG
1	D	390	ARG
1	D	398	LEU
1	D	406	LEU
1	D	446	ARG
1	D	454	ARG

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

Mol	Chain	Res	Type
1	A	50	HIS
1	A	54	HIS
1	B	22	HIS
1	B	75	HIS
1	B	81	GLN
1	B	128	HIS
1	B	243	GLN
1	B	282	GLN
1	B	339	HIS
1	C	75	HIS
1	C	81	GLN
1	C	233	HIS
1	C	243	GLN
1	C	282	GLN
1	C	339	HIS
1	D	75	HIS
1	D	81	GLN
1	D	203	ASN
1	D	243	GLN
1	D	282	GLN
1	D	339	HIS

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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	454/469 (96%)	-0.20	4 (0%)	84 83	22, 36, 66, 98	0
1	B	451/469 (96%)	-0.22	4 (0%)	84 83	23, 38, 68, 96	0
1	C	458/469 (97%)	-0.07	12 (2%)	56 52	22, 41, 85, 106	0
1	D	444/469 (94%)	-0.16	5 (1%)	80 79	24, 38, 79, 109	0
All	All	1807/1876 (96%)	-0.16	25 (1%)	75 73	22, 38, 79, 109	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	ALA	6.6
1	B	402	ALA	5.6
1	A	65	VAL	5.1
1	C	198	ASP	3.7
1	A	63	PRO	3.5
1	C	199	ALA	3.3
1	D	69	PRO	3.2
1	B	403	ASN	3.1
1	C	66	GLU	2.7
1	C	194	GLU	2.7
1	B	10	GLY	2.4
1	A	68	ALA	2.4
1	B	219	THR	2.4
1	C	70	ALA	2.4
1	D	9	ASP	2.4
1	D	61	THR	2.4
1	D	59	ARG	2.2
1	C	378	THR	2.2
1	C	425	ALA	2.1
1	C	61	THR	2.1
1	C	67	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	197	SER	2.1
1	D	375	LEU	2.1
1	C	27	ALA	2.0
1	C	332	GLY	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	B	501	1/1	0.98	0.11	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.