



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:03 PM UTC

PDB ID : 3GR1 / pdb_00003gr1
Title : Periplasmic domain of the T3SS inner membrane protein PrgH from *S.typhimurium* (fragment 170-392)
Authors : Yip, C.K.; Vockovic, M.; Yu, A.C.; Strynadka, N.C.J.
Deposited on : 2009-03-24
Resolution : 2.80 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

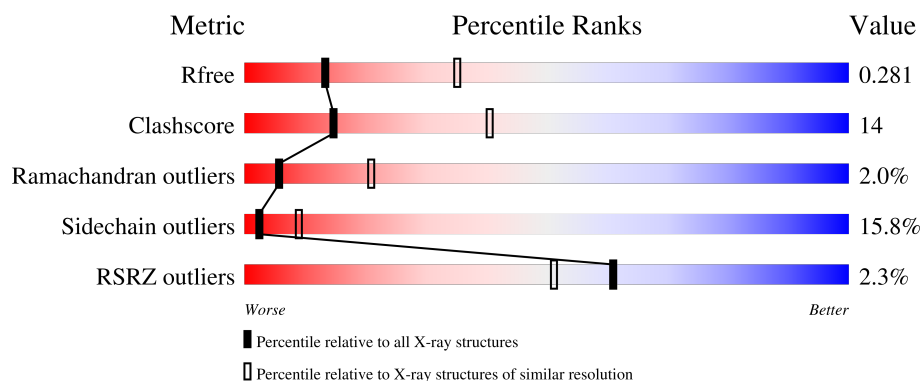
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



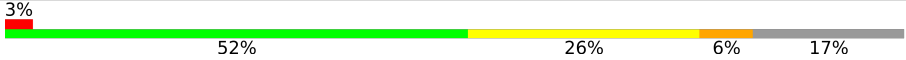
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	227	4% 60% 20% 6% 14%
1	B	227	56% 22% 6% 15%
1	C	227	56% 23% • 16%
1	D	227	53% 26% 5% 15%
1	E	227	4% 54% 24% 5% • 15%

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Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
1	H	227	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12613 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 Protein prgH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1602	1014	289	294	5			
1	B	193	Total	C	N	O	S	0	0	0
			1589	1006	287	292	4			
1	C	190	Total	C	N	O	S	0	0	0
			1570	995	284	287	4			
1	D	193	Total	C	N	O	S	0	0	0
			1589	1006	287	292	4			
1	E	192	Total	C	N	O	S	0	0	0
			1584	1003	286	291	4			
1	F	189	Total	C	N	O	S	0	0	0
			1554	986	281	283	4			
1	G	189	Total	C	N	O	S	0	0	0
			1554	986	281	283	4			
1	H	191	Total	C	N	O	S	0	0	0
			1571	996	285	285	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	-	expression tag	UNP P41783
A	167	SER	-	expression tag	UNP P41783
A	168	HIS	-	expression tag	UNP P41783
A	169	MET	-	expression tag	UNP P41783
B	166	GLY	-	expression tag	UNP P41783
B	167	SER	-	expression tag	UNP P41783
B	168	HIS	-	expression tag	UNP P41783
B	169	MET	-	expression tag	UNP P41783
C	166	GLY	-	expression tag	UNP P41783
C	167	SER	-	expression tag	UNP P41783
C	168	HIS	-	expression tag	UNP P41783
C	169	MET	-	expression tag	UNP P41783
D	166	GLY	-	expression tag	UNP P41783

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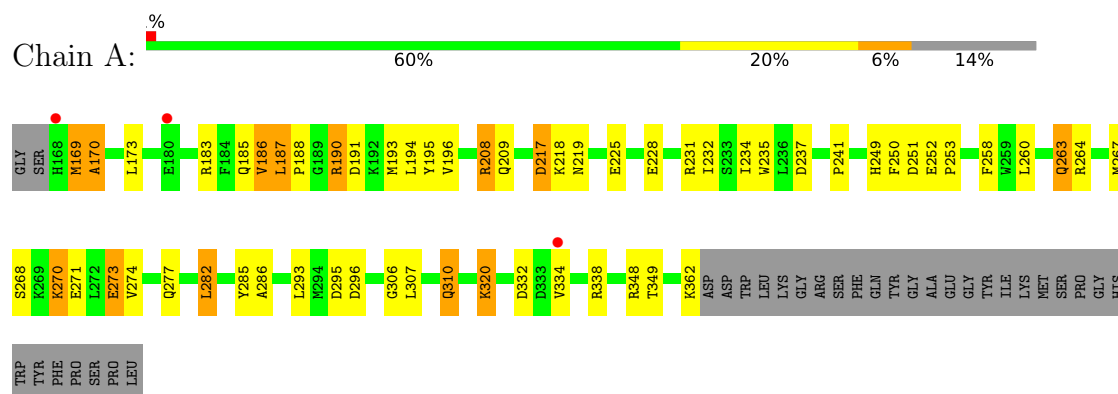
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Chain	Residue	Modelled	Actual	Comment	Reference
D	167	SER	-	expression tag	UNP P41783
D	168	HIS	-	expression tag	UNP P41783
D	169	MET	-	expression tag	UNP P41783
E	166	GLY	-	expression tag	UNP P41783
E	167	SER	-	expression tag	UNP P41783
E	168	HIS	-	expression tag	UNP P41783
E	169	MET	-	expression tag	UNP P41783
F	166	GLY	-	expression tag	UNP P41783
F	167	SER	-	expression tag	UNP P41783
F	168	HIS	-	expression tag	UNP P41783
F	169	MET	-	expression tag	UNP P41783
G	166	GLY	-	expression tag	UNP P41783
G	167	SER	-	expression tag	UNP P41783
G	168	HIS	-	expression tag	UNP P41783
G	169	MET	-	expression tag	UNP P41783
H	166	GLY	-	expression tag	UNP P41783
H	167	SER	-	expression tag	UNP P41783
H	168	HIS	-	expression tag	UNP P41783
H	169	MET	-	expression tag	UNP P41783

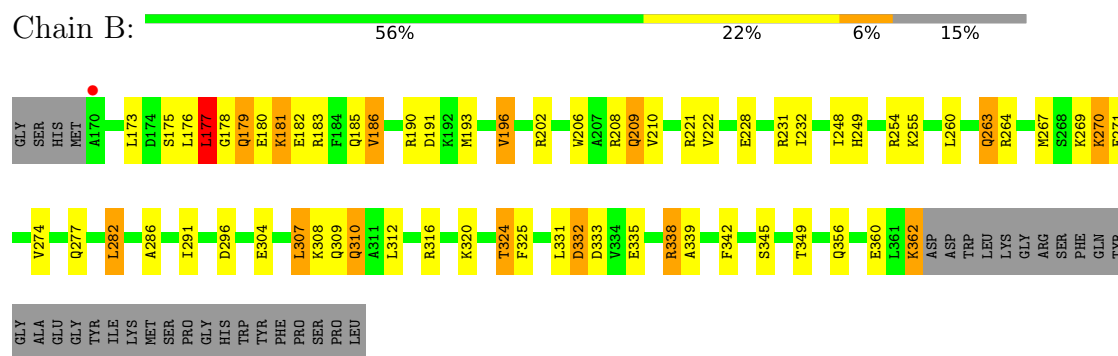
3 Residue-property plots [i](#)

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.

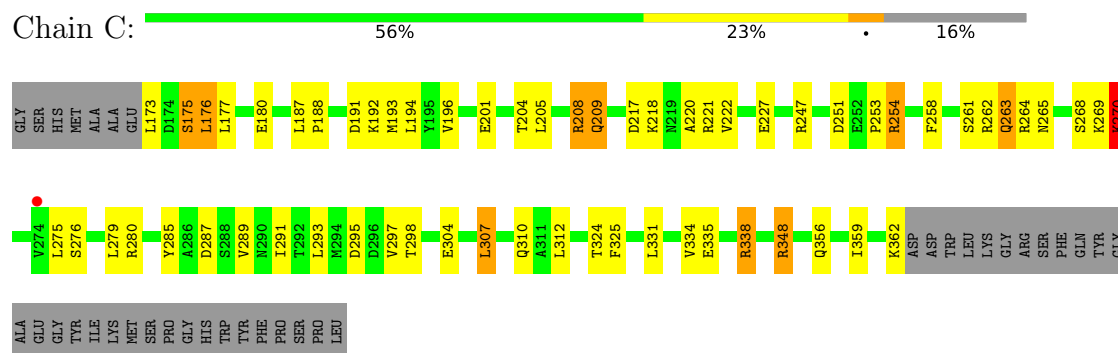
• Molecule 1: Protein prgH



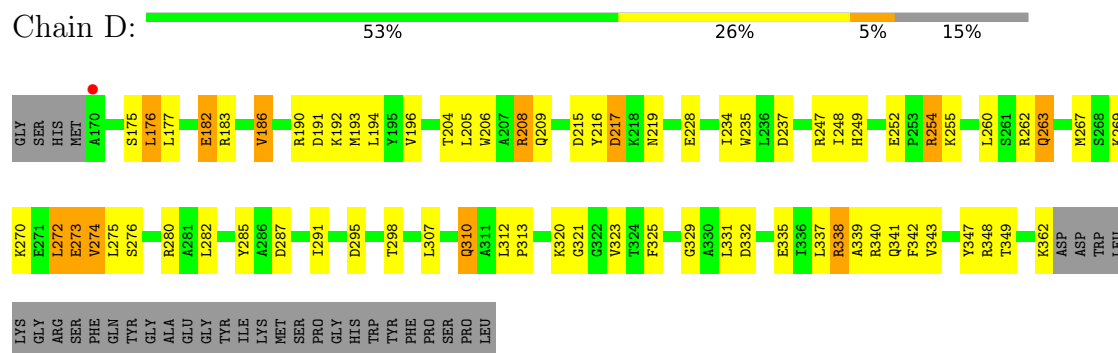
• Molecule 1: Protein prgH



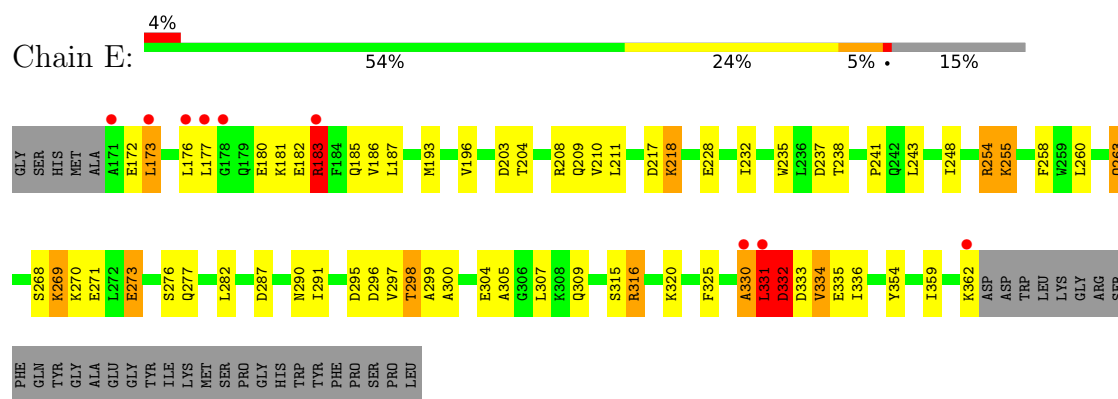
• Molecule 1: Protein prgH



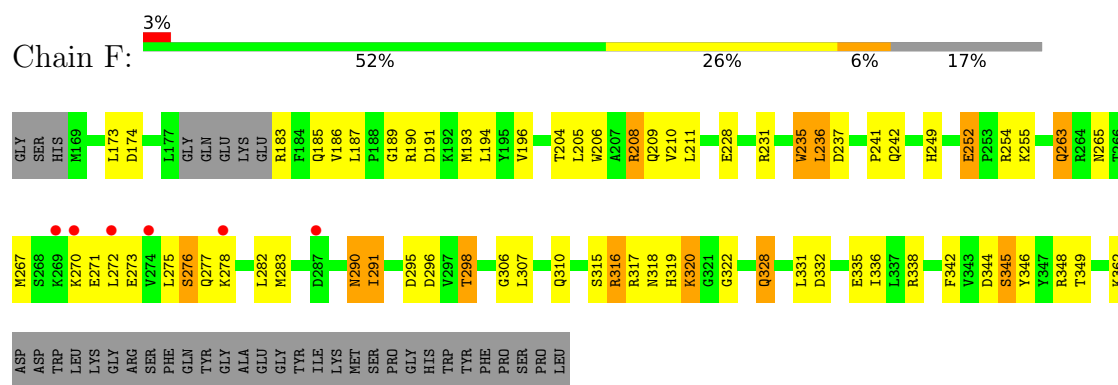
● Molecule 1: Protein prgH



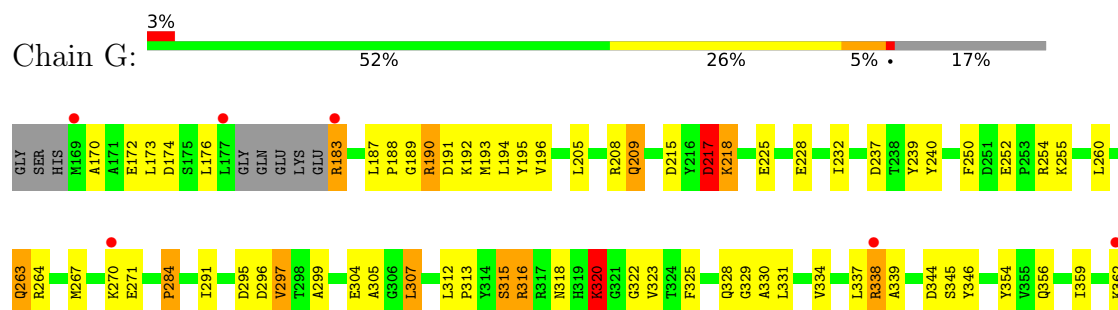
● Molecule 1: Protein prgH



● Molecule 1: Protein prgH



● Molecule 1: Protein prgH



ASP	ASP	TRP	LEU	LYS	GLY	ARG	SER	PHE	GLN	TYR	GLY	ALA	GLU	GLY	TYR	ILE	LYS	MET	SER	PRO	GLY	HIS	TRP	TYR	PHE	PRO	SER	PRO	LEU
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● Molecule 1: Protein prgH



GLY	SER	H168	M169	A170	L173	D174	S175	L176	L177	G178	GLN	GLU	LYS	GLU	R183	V186	L187	R190	D191	K192	M193	L194	Y195	V196	L205	R208	Q209	V210	G214	D215	Y216	D217	K218	V222	S233	L236	Y240	I248	H249	F250	D251	E252	P253	R254	K255	P256	L260
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S261	R262	Q263	R264	S268	K269	K270	E271	L272	E273	K278	L279	R280	A281	L282	M283	P284	Y285	A286	D287	N290	I291	T292	L293	M294	D295	D296	Y297	T298	E304	A305	G306	L307	K308	Q309	Q310	R316	R317	N318	H319	K320	G321	G322	F325	A330	L331	D332	D333	V334	R338	A339	R340
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Q341	R348	T349	Q356	K362	ASP	ASP	TRP	LEU	LYS	GLY	ARG	SER	PHE	GLN	TYR	GLY	ALA	GLU	GLY	TYR	ILE	LYS	MET	SER	PRO	GLY	HIS	TRP	TYR	PHE	PRO	SER	PRO	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.61Å 188.75Å 305.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.50 – 2.80 152.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (152.50-2.80) 96.5 (152.50-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.295 0.237 , 0.281	Depositor DCC
R_{free} test set	2812 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12613	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.51% 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

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
1	A	0.90	1/1634 (0.1%)	1.07	3/2206 (0.1%)
1	B	0.91	0/1621	1.11	5/2189 (0.2%)
1	C	0.86	0/1602	1.08	1/2163 (0.0%)
1	D	0.81	0/1621	1.07	3/2189 (0.1%)
1	E	0.83	0/1616	1.06	2/2182 (0.1%)
1	F	0.83	0/1585	1.07	5/2141 (0.2%)
1	G	0.84	1/1585 (0.1%)	1.03	1/2141 (0.0%)
1	H	0.79	0/1603	1.06	4/2164 (0.2%)
All	All	0.85	2/12867 (0.0%)	1.07	24/17375 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	330	ALA	CA-CB	6.29	1.63	1.53
1	A	274	VAL	CA-CB	5.11	1.60	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	GLY	N-CA-C	-6.93	96.75	113.18
1	D	252	GLU	CA-C-N	6.88	126.48	119.19
1	D	252	GLU	C-N-CA	6.88	126.48	119.19
1	E	330	ALA	N-CA-C	-6.65	95.92	107.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	LEU	N-CA-C	6.36	120.15	107.62
1	F	331	LEU	N-CA-C	6.23	119.06	108.90
1	B	177	LEU	CA-C-N	-5.86	118.14	122.18
1	B	177	LEU	C-N-CA	-5.86	118.14	122.18
1	H	191	ASP	N-CA-C	-5.74	105.67	114.16
1	A	274	VAL	N-CA-C	-5.67	105.09	110.42
1	H	320	LYS	CA-C-N	5.49	126.19	119.99
1	H	320	LYS	C-N-CA	5.49	126.19	119.99
1	A	208	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	B	274	VAL	N-CA-C	-5.30	105.55	110.53
1	C	289	VAL	N-CA-C	5.26	114.88	106.88
1	F	283	MET	CA-C-N	5.25	126.40	119.84
1	F	283	MET	C-N-CA	5.25	126.40	119.84
1	G	313	PRO	N-CA-C	-5.23	103.56	111.41
1	E	354	TYR	N-CA-C	-5.14	105.24	112.12
1	F	252	GLU	CA-C-N	5.12	124.92	119.28
1	F	252	GLU	C-N-CA	5.12	124.92	119.28
1	A	234	ILE	N-CA-C	-5.10	105.53	110.42
1	B	186	VAL	N-CA-C	5.09	114.90	107.37
1	H	262	ARG	N-CA-C	-5.07	105.45	110.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	320	LYS	Peptide
1	E	331	LEU	Peptide

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	1602	0	1588	38	0
1	B	1589	0	1577	48	0
1	C	1570	0	1561	39	0
1	D	1589	0	1577	51	0
1	E	1584	0	1572	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1554	0	1542	46	0
1	G	1554	0	1542	42	0
1	H	1571	0	1559	55	0
All	All	12613	0	12518	349	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 14.

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLN:HG2	1:B:191:ASP:HA	1.36	1.07
1:G:316:ARG:HD3	1:G:318:ASN:HD21	1.21	1.05
1:E:330:ALA:CA	1:E:331:LEU:HB2	1.89	1.02
1:E:330:ALA:HA	1:E:331:LEU:HB2	1.02	1.02
1:E:330:ALA:HA	1:E:331:LEU:CB	1.90	1.01
1:A:191:ASP:HA	1:B:277:GLN:HG2	1.38	1.01
1:H:332:ASP:OD2	1:H:334:VAL:HG12	1.60	1.01
1:B:263:GLN:H	1:B:263:GLN:HE21	1.00	0.99
1:H:263:GLN:H	1:H:263:GLN:HE21	1.02	0.99
1:H:253:PRO:O	1:H:256:PRO:HD3	1.64	0.97
1:C:263:GLN:H	1:C:263:GLN:HE21	1.04	0.95
1:G:263:GLN:H	1:G:263:GLN:HE21	0.97	0.95
1:B:267:MET:HE2	1:B:271:GLU:HB3	1.51	0.91
1:C:263:GLN:HE21	1:C:263:GLN:N	1.71	0.88
1:G:316:ARG:HD3	1:G:318:ASN:ND2	1.87	0.88
1:H:254:ARG:HG2	1:H:254:ARG:HH21	1.38	0.85
1:C:254:ARG:HH21	1:C:254:ARG:HG3	1.40	0.84
1:B:349:THR:OG1	1:D:209:GLN:NE2	2.11	0.84
1:E:173:LEU:H	1:E:173:LEU:HD12	1.43	0.84
1:E:263:GLN:H	1:E:263:GLN:HE21	1.25	0.83
1:E:263:GLN:H	1:E:263:GLN:NE2	1.74	0.83
1:F:263:GLN:H	1:F:263:GLN:HE21	1.23	0.83
1:D:254:ARG:HH21	1:D:254:ARG:HG3	1.45	0.82
1:H:263:GLN:HE21	1:H:263:GLN:N	1.78	0.82
1:G:263:GLN:HE21	1:G:263:GLN:N	1.75	0.81
1:H:254:ARG:HH21	1:H:254:ARG:CG	1.93	0.80
1:E:182:GLU:O	1:E:183:ARG:HB2	1.81	0.78
1:B:264:ARG:HD3	1:B:296:ASP:OD2	1.84	0.78
1:F:315:SER:OG	1:F:317:ARG:NH1	2.16	0.78
1:E:273:GLU:HA	1:E:276:SER:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:ASP:HB3	1:E:335:GLU:H	1.50	0.76
1:A:185:GLN:HG2	1:A:187:LEU:HD21	1.68	0.76
1:D:254:ARG:CD	1:H:287:ASP:OD2	2.33	0.76
1:B:263:GLN:HE21	1:B:263:GLN:N	1.81	0.75
1:C:295:ASP:HB3	1:C:298:THR:OG1	1.87	0.74
1:D:206:TRP:O	1:D:209:GLN:HB3	1.87	0.74
1:B:190:ARG:NH2	1:B:286:ALA:O	2.21	0.74
1:H:317:ARG:HG2	1:H:317:ARG:HH11	1.53	0.74
1:D:254:ARG:HD3	1:H:287:ASP:OD2	1.89	0.72
1:A:320:LYS:HE2	1:A:320:LYS:HA	1.70	0.72
1:D:254:ARG:HH21	1:D:254:ARG:CG	2.03	0.72
1:C:263:GLN:H	1:C:263:GLN:NE2	1.84	0.72
1:H:193:MET:HE1	1:H:218:LYS:O	1.89	0.72
1:E:254:ARG:CG	1:E:254:ARG:HH21	2.02	0.72
1:F:206:TRP:O	1:F:209:GLN:HB3	1.90	0.72
1:E:254:ARG:HH21	1:E:254:ARG:HG3	1.53	0.71
1:F:320:LYS:NZ	1:F:320:LYS:HA	2.05	0.71
1:G:183:ARG:C	1:G:183:ARG:HD3	2.16	0.71
1:B:185:GLN:HE21	1:B:254:ARG:HH11	1.39	0.70
1:D:182:GLU:OE2	1:D:182:GLU:HA	1.90	0.70
1:D:339:ALA:O	1:D:343:VAL:HG23	1.93	0.69
1:C:254:ARG:HH21	1:C:254:ARG:CG	2.05	0.69
1:A:267:MET:HE2	1:A:271:GLU:HB3	1.75	0.68
1:G:307:LEU:HD12	1:G:312:LEU:HD12	1.76	0.68
1:H:264:ARG:HD3	1:H:296:ASP:OD2	1.93	0.68
1:C:191:ASP:O	1:C:192:LYS:HB2	1.93	0.67
1:C:193:MET:HE1	1:C:218:LYS:O	1.94	0.67
1:B:181:LYS:HE3	1:B:182:GLU:H	1.59	0.66
1:E:332:ASP:HB3	1:E:334:VAL:H	1.59	0.66
1:B:231:ARG:HH22	1:B:282:LEU:HD22	1.61	0.65
1:D:263:GLN:H	1:D:263:GLN:HE21	1.44	0.65
1:A:263:GLN:H	1:A:263:GLN:HE21	1.42	0.65
1:C:254:ARG:CD	1:E:287:ASP:OD2	2.45	0.64
1:A:277:GLN:CG	1:B:191:ASP:HA	2.22	0.64
1:A:332:ASP:OD2	1:A:334:VAL:HG12	1.97	0.64
1:A:190:ARG:NH2	1:A:286:ALA:O	2.31	0.64
1:F:263:GLN:H	1:F:263:GLN:NE2	1.94	0.63
1:G:189:GLY:C	1:G:191:ASP:H	2.06	0.63
1:D:341:GLN:O	1:D:342:PHE:C	2.41	0.63
1:A:270:LYS:HA	1:A:273:GLU:HG3	1.81	0.62
1:H:170:ALA:O	1:H:174:ASP:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:306:GLY:HA2	1:H:309:GLN:OE1	2.00	0.62
1:A:320:LYS:HA	1:A:320:LYS:CE	2.27	0.62
1:G:228:GLU:O	1:G:232:ILE:HG12	2.00	0.62
1:E:268:SER:HB2	1:H:270:LYS:HG2	1.80	0.62
1:C:254:ARG:HD3	1:E:287:ASP:OD2	1.99	0.62
1:B:181:LYS:HE3	1:B:182:GLU:N	2.15	0.62
1:H:290:ASN:C	1:H:291:ILE:HD12	2.26	0.61
1:H:317:ARG:HG2	1:H:317:ARG:NH1	2.15	0.61
1:F:235:TRP:CD2	1:F:282:LEU:HD11	2.35	0.61
1:G:267:MET:HB3	1:G:271:GLU:HB2	1.83	0.61
1:F:273:GLU:O	1:F:277:GLN:HB2	2.01	0.60
1:B:249:HIS:HE1	1:B:349:THR:O	1.83	0.60
1:H:195:TYR:OH	1:H:284:PRO:HG2	2.00	0.60
1:A:187:LEU:HD11	1:A:253:PRO:HB2	1.82	0.60
1:F:295:ASP:HB3	1:F:298:THR:OG1	2.02	0.59
1:G:217:ASP:OD2	1:G:217:ASP:N	2.34	0.59
1:E:263:GLN:NE2	1:E:263:GLN:N	2.49	0.59
1:B:173:LEU:HD12	1:D:194:LEU:HD13	1.83	0.59
1:B:209:GLN:HE21	1:C:348:ARG:HH21	1.50	0.59
1:E:248:ILE:HG12	1:E:258:PHE:CD1	2.36	0.59
1:D:280:ARG:NE	1:D:287:ASP:O	2.30	0.59
1:B:263:GLN:H	1:B:263:GLN:NE2	1.85	0.59
1:C:287:ASP:OD2	1:E:254:ARG:CD	2.51	0.59
1:F:290:ASN:OD1	1:F:290:ASN:C	2.46	0.59
1:A:277:GLN:HG2	1:B:191:ASP:CA	2.24	0.59
1:B:232:ILE:HG21	1:B:248:ILE:HD11	1.84	0.58
1:E:332:ASP:CB	1:E:335:GLU:H	2.16	0.58
1:E:304:GLU:HG2	1:E:325:PHE:CE2	2.38	0.58
1:D:263:GLN:HE21	1:D:263:GLN:N	2.01	0.58
1:H:295:ASP:HB3	1:H:298:THR:OG1	2.04	0.58
1:A:263:GLN:HE22	1:A:295:ASP:HA	1.67	0.58
1:A:169:MET:O	1:A:170:ALA:CB	2.52	0.58
1:H:264:ARG:CD	1:H:296:ASP:OD2	2.52	0.58
1:E:305:ALA:O	1:E:309:GLN:HG3	2.04	0.57
1:G:252:GLU:OE2	1:G:255:LYS:HE2	2.05	0.57
1:H:264:ARG:HH21	1:H:296:ASP:CG	2.11	0.57
1:E:243:LEU:HD11	1:E:260:LEU:HD21	1.86	0.57
1:F:189:GLY:C	1:F:191:ASP:H	2.12	0.57
1:E:331:LEU:HD13	1:E:336:ILE:HG12	1.87	0.56
1:A:264:ARG:HD3	1:A:296:ASP:OD2	2.06	0.56
1:H:216:TYR:C	1:H:218:LYS:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLN:H	1:D:263:GLN:NE2	2.04	0.55
1:D:193:MET:SD	1:D:219:ASN:O	2.63	0.55
1:G:296:ASP:O	1:G:299:ALA:N	2.39	0.55
1:B:173:LEU:O	1:B:177:LEU:HB2	2.06	0.55
1:G:320:LYS:HD3	1:G:320:LYS:N	2.21	0.55
1:E:332:ASP:C	1:E:334:VAL:H	2.13	0.55
1:H:278:LYS:O	1:H:281:ALA:HB3	2.07	0.55
1:H:208:ARG:HD2	1:H:222:VAL:HB	1.88	0.55
1:B:206:TRP:O	1:B:209:GLN:HB3	2.06	0.55
1:A:263:GLN:H	1:A:263:GLN:NE2	2.04	0.54
1:E:332:ASP:HB2	1:E:335:GLU:HB2	1.88	0.54
1:H:251:ASP:O	1:H:253:PRO:HD3	2.07	0.54
1:B:180:GLU:HG2	1:B:181:LYS:N	2.22	0.54
1:F:276:SER:HB2	1:F:291:ILE:HD13	1.90	0.54
1:B:196:VAL:HG22	1:B:222:VAL:HG13	1.89	0.54
1:G:320:LYS:O	1:G:320:LYS:HG2	2.08	0.54
1:D:216:TYR:O	1:D:219:ASN:N	2.33	0.54
1:H:190:ARG:HD3	1:H:280:ARG:HH22	1.73	0.53
1:A:263:GLN:HE21	1:A:263:GLN:N	2.05	0.53
1:H:338:ARG:HG2	1:H:339:ALA:N	2.23	0.53
1:D:262:ARG:HB3	1:D:263:GLN:HE21	1.74	0.53
1:G:320:LYS:HD3	1:G:320:LYS:H	1.74	0.53
1:C:254:ARG:NE	1:E:287:ASP:OD2	2.41	0.53
1:G:189:GLY:O	1:G:191:ASP:N	2.41	0.53
1:B:202:ARG:HB3	1:B:202:ARG:CZ	2.38	0.53
1:F:237:ASP:O	1:F:241:PRO:HB3	2.09	0.53
1:F:306:GLY:HA3	1:F:342:PHE:CZ	2.43	0.52
1:F:320:LYS:HA	1:F:320:LYS:HZ2	1.73	0.52
1:H:304:GLU:HG2	1:H:325:PHE:CE2	2.44	0.52
1:D:295:ASP:HB3	1:D:298:THR:OG1	2.09	0.52
1:E:228:GLU:O	1:E:232:ILE:HG12	2.10	0.52
1:A:188:PRO:HA	1:A:194:LEU:HD23	1.92	0.52
1:B:324:THR:HG23	1:B:356:GLN:HB2	1.91	0.52
1:C:307:LEU:HD12	1:C:312:LEU:HD12	1.92	0.52
1:D:254:ARG:NH2	1:D:285:TYR:O	2.43	0.52
1:D:287:ASP:OD2	1:H:254:ARG:NE	2.43	0.51
1:E:298:THR:O	1:E:299:ALA:C	2.53	0.51
1:F:191:ASP:C	1:F:193:MET:H	2.17	0.51
1:H:262:ARG:HB3	1:H:263:GLN:NE2	2.26	0.51
1:C:304:GLU:HG2	1:C:325:PHE:CE2	2.45	0.51
1:E:238:THR:O	1:E:241:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:MET:HE1	1:G:218:LYS:O	2.10	0.51
1:A:191:ASP:OD1	1:A:195:TYR:OH	2.25	0.51
1:C:247:ARG:HG3	1:C:247:ARG:HH11	1.76	0.51
1:C:335:GLU:HA	1:C:338:ARG:HD3	1.93	0.51
1:A:258:PHE:CE2	1:A:260:LEU:HD11	2.45	0.51
1:F:267:MET:HE2	1:F:271:GLU:HB3	1.92	0.51
1:E:304:GLU:HG2	1:E:325:PHE:HE2	1.76	0.51
1:E:185:GLN:HE21	1:E:187:LEU:HD21	1.75	0.50
1:F:235:TRP:CG	1:F:282:LEU:HD11	2.46	0.50
1:F:315:SER:HG	1:F:317:ARG:HH12	1.55	0.50
1:H:254:ARG:HG2	1:H:254:ARG:NH2	2.15	0.50
1:A:185:GLN:HG2	1:A:187:LEU:CD2	2.39	0.50
1:F:275:LEU:C	1:F:277:GLN:H	2.20	0.50
1:G:225:GLU:HG3	1:G:250:PHE:HD1	1.76	0.50
1:D:331:LEU:HD23	1:D:335:GLU:HB3	1.93	0.50
1:A:169:MET:O	1:A:170:ALA:HB2	2.12	0.50
1:D:337:LEU:O	1:D:340:ARG:N	2.45	0.50
1:H:191:ASP:OD2	1:H:193:MET:HB2	2.12	0.50
1:D:254:ARG:CG	1:D:254:ARG:NH2	2.70	0.50
1:E:273:GLU:O	1:E:277:GLN:HB2	2.11	0.50
1:E:295:ASP:HB3	1:E:298:THR:OG1	2.11	0.50
1:G:322:GLY:HA2	1:G:354:TYR:CE1	2.47	0.50
1:H:233:SER:HA	1:H:236:LEU:HD12	1.93	0.50
1:C:262:ARG:HA	1:C:293:LEU:HD22	1.93	0.50
1:D:287:ASP:OD2	1:H:254:ARG:CD	2.59	0.50
1:D:332:ASP:HB3	1:D:335:GLU:H	1.77	0.50
1:C:175:SER:O	1:C:177:LEU:N	2.45	0.49
1:E:276:SER:HB2	1:E:291:ILE:HD13	1.94	0.49
1:G:296:ASP:O	1:G:297:VAL:C	2.54	0.49
1:G:239:TYR:O	1:G:240:TYR:CD2	2.66	0.49
1:E:193:MET:HE1	1:E:218:LYS:O	2.11	0.49
1:F:228:GLU:OE2	1:F:231:ARG:NH1	2.37	0.49
1:A:225:GLU:HG3	1:A:250:PHE:HD1	1.78	0.48
1:H:283:MET:O	1:H:284:PRO:C	2.55	0.48
1:A:228:GLU:O	1:A:232:ILE:HG12	2.13	0.48
1:B:264:ARG:CD	1:B:296:ASP:OD2	2.60	0.48
1:F:265:ASN:HD21	1:F:267:MET:HB2	1.77	0.48
1:A:186:VAL:C	1:A:187:LEU:HD23	2.38	0.48
1:G:295:ASP:O	1:G:296:ASP:C	2.56	0.48
1:D:254:ARG:NE	1:H:287:ASP:OD2	2.46	0.48
1:C:258:PHE:CD2	1:C:279:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:GLN:HE22	1:F:295:ASP:HA	1.79	0.48
1:B:231:ARG:NH2	1:B:282:LEU:HD22	2.26	0.48
1:G:345:SER:O	1:G:346:TYR:C	2.54	0.48
1:B:308:LYS:C	1:B:310:GLN:H	2.22	0.47
1:G:264:ARG:HD3	1:G:296:ASP:OD2	2.13	0.47
1:A:231:ARG:HH22	1:A:282:LEU:HD22	1.79	0.47
1:E:290:ASN:OD1	1:E:290:ASN:C	2.57	0.47
1:H:306:GLY:O	1:H:310:GLN:HB2	2.13	0.47
1:E:332:ASP:C	1:E:334:VAL:N	2.70	0.47
1:F:290:ASN:OD1	1:F:291:ILE:N	2.48	0.47
1:F:316:ARG:HD3	1:F:318:ASN:OD1	2.13	0.47
1:D:235:TRP:CD2	1:D:282:LEU:HD11	2.49	0.47
1:A:249:HIS:HE1	1:A:349:THR:O	1.96	0.47
1:D:190:ARG:NH2	1:D:280:ARG:O	2.46	0.47
1:D:287:ASP:CG	1:H:254:ARG:HE	2.23	0.47
1:E:235:TRP:CD2	1:E:282:LEU:HD11	2.50	0.47
1:F:235:TRP:O	1:F:237:ASP:N	2.48	0.47
1:G:195:TYR:CE2	1:G:284:PRO:HB2	2.50	0.47
1:E:210:VAL:O	1:E:211:LEU:C	2.58	0.47
1:E:243:LEU:HD11	1:E:260:LEU:CD2	2.44	0.47
1:G:191:ASP:OD2	1:G:193:MET:HB2	2.15	0.47
1:C:204:THR:O	1:C:208:ARG:HB2	2.14	0.46
1:F:275:LEU:C	1:F:277:GLN:N	2.73	0.46
1:H:186:VAL:O	1:H:186:VAL:HG22	2.15	0.46
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.81	0.46
1:H:254:ARG:CG	1:H:254:ARG:NH2	2.63	0.46
1:B:264:ARG:HH21	1:B:296:ASP:CG	2.23	0.46
1:F:319:HIS:CD2	1:F:322:GLY:O	2.68	0.46
1:D:267:MET:HE2	1:D:272:LEU:HD23	1.97	0.46
1:F:185:GLN:HE21	1:F:187:LEU:HD21	1.80	0.46
1:A:193:MET:HE3	1:B:270:LYS:NZ	2.31	0.46
1:E:331:LEU:HA	1:E:331:LEU:HD22	1.53	0.46
1:F:242:GLN:OE1	1:F:242:GLN:HA	2.15	0.46
1:D:247:ARG:HG2	1:D:248:ILE:N	2.30	0.46
1:E:203:ASP:O	1:E:204:THR:C	2.58	0.46
1:D:204:THR:O	1:D:208:ARG:HB2	2.16	0.46
1:D:272:LEU:O	1:D:275:LEU:N	2.49	0.46
1:A:268:SER:H	1:A:271:GLU:HB2	1.80	0.45
1:D:262:ARG:HB3	1:D:263:GLN:NE2	2.31	0.45
1:D:343:VAL:HG12	1:D:347:TYR:CE1	2.51	0.45
1:G:338:ARG:HG2	1:G:339:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:319:HIS:CE1	1:H:322:GLY:H	2.34	0.45
1:B:308:LYS:C	1:B:310:GLN:N	2.74	0.45
1:F:332:ASP:O	1:F:336:ILE:HG12	2.15	0.45
1:B:312:LEU:HD21	1:B:338:ARG:HD3	1.97	0.45
1:B:332:ASP:HB3	1:B:335:GLU:HB2	1.98	0.45
1:H:318:ASN:ND2	1:H:318:ASN:H	2.13	0.45
1:D:216:TYR:O	1:D:217:ASP:C	2.60	0.45
1:H:362:LYS:HD2	1:H:362:LYS:HA	1.81	0.45
1:C:208:ARG:HD3	1:C:222:VAL:HB	1.98	0.45
1:C:194:LEU:O	1:C:220:ALA:HA	2.17	0.45
1:C:261:SER:OG	1:C:264:ARG:HD3	2.17	0.45
1:D:323:VAL:HG11	1:D:325:PHE:CE1	2.51	0.45
1:F:235:TRP:HB3	1:F:236:LEU:H	1.64	0.45
1:F:332:ASP:HB3	1:F:335:GLU:HG3	1.98	0.45
1:C:287:ASP:OD2	1:E:254:ARG:NE	2.50	0.45
1:G:173:LEU:O	1:G:174:ASP:C	2.59	0.45
1:G:240:TYR:HE1	1:G:267:MET:HE1	1.82	0.45
1:B:228:GLU:O	1:B:232:ILE:HG12	2.17	0.45
1:H:216:TYR:O	1:H:218:LYS:N	2.50	0.45
1:C:254:ARG:NH2	1:C:285:TYR:O	2.50	0.44
1:E:263:GLN:NE2	1:E:296:ASP:OD1	2.50	0.44
1:E:330:ALA:CA	1:E:331:LEU:CB	2.66	0.44
1:D:337:LEU:O	1:D:338:ARG:C	2.59	0.44
1:B:362:LYS:HA	1:B:362:LYS:NZ	2.33	0.44
1:E:254:ARG:CG	1:E:254:ARG:NH2	2.71	0.44
1:H:291:ILE:HD12	1:H:291:ILE:N	2.33	0.44
1:F:332:ASP:HB2	1:F:335:GLU:OE1	2.18	0.44
1:E:332:ASP:O	1:E:336:ILE:HG13	2.18	0.44
1:C:280:ARG:NE	1:C:287:ASP:O	2.45	0.44
1:D:175:SER:O	1:D:176:LEU:C	2.60	0.44
1:F:189:GLY:C	1:F:191:ASP:N	2.75	0.44
1:H:169:MET:O	1:H:170:ALA:C	2.61	0.44
1:H:173:LEU:O	1:H:176:LEU:HD12	2.18	0.44
1:A:217:ASP:OD2	1:A:217:ASP:N	2.51	0.43
1:A:237:ASP:O	1:A:241:PRO:HB3	2.18	0.43
1:D:249:HIS:HE1	1:D:349:THR:O	2.01	0.43
1:E:332:ASP:CG	1:E:334:VAL:HG12	2.43	0.43
1:A:285:TYR:C	1:A:285:TYR:CD2	2.96	0.43
1:B:338:ARG:HG2	1:B:339:ALA:N	2.32	0.43
1:F:273:GLU:HA	1:F:276:SER:HB3	1.99	0.43
1:G:323:VAL:HG12	1:G:325:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:GLN:HE22	1:C:295:ASP:HA	1.83	0.43
1:E:173:LEU:H	1:E:173:LEU:CD1	2.20	0.43
1:H:191:ASP:OD2	1:H:193:MET:N	2.41	0.43
1:H:216:TYR:C	1:H:218:LYS:N	2.77	0.43
1:F:204:THR:O	1:F:208:ARG:HB2	2.18	0.43
1:A:270:LYS:HD3	1:B:193:MET:HE1	2.00	0.43
1:G:188:PRO:HA	1:G:194:LEU:HD23	2.01	0.43
1:H:262:ARG:HA	1:H:293:LEU:HD13	2.01	0.43
1:A:235:TRP:CG	1:A:282:LEU:HD11	2.53	0.43
1:B:185:GLN:NE2	1:B:254:ARG:HH11	2.13	0.43
1:C:208:ARG:HH12	1:C:227:GLU:CD	2.26	0.43
1:H:268:SER:O	1:H:271:GLU:N	2.52	0.43
1:B:320:LYS:HA	1:B:320:LYS:HE2	2.01	0.42
1:E:268:SER:O	1:E:269:LYS:C	2.61	0.42
1:E:300:ALA:HB1	1:E:316:ARG:NH1	2.33	0.42
1:A:231:ARG:NH2	1:A:282:LEU:HD22	2.34	0.42
1:C:275:LEU:O	1:C:276:SER:C	2.62	0.42
1:C:331:LEU:HD23	1:C:335:GLU:HB3	2.01	0.42
1:D:312:LEU:HA	1:D:313:PRO:HD2	1.83	0.42
1:G:304:GLU:O	1:G:305:ALA:C	2.61	0.42
1:B:178:GLY:C	1:B:180:GLU:H	2.27	0.42
1:F:173:LEU:O	1:F:174:ASP:C	2.63	0.42
1:H:307:LEU:HD12	1:H:307:LEU:HA	1.85	0.42
1:B:255:LYS:HE3	1:B:255:LYS:HB2	1.70	0.42
1:F:209:GLN:HE21	1:F:209:GLN:HB2	1.64	0.42
1:C:254:ARG:CG	1:C:254:ARG:NH2	2.70	0.42
1:D:273:GLU:HA	1:D:276:SER:HB3	2.01	0.42
1:A:306:GLY:O	1:A:310:GLN:HB2	2.20	0.42
1:C:209:GLN:HE21	1:C:209:GLN:HB2	1.71	0.42
1:D:193:MET:HE1	1:D:219:ASN:HA	2.02	0.42
1:E:237:ASP:O	1:E:241:PRO:HB3	2.20	0.42
1:F:231:ARG:HH22	1:F:282:LEU:HB3	1.84	0.42
1:B:304:GLU:HG3	1:B:325:PHE:CE2	2.54	0.41
1:D:186:VAL:HG23	1:D:194:LEU:HD22	2.02	0.41
1:F:249:HIS:HE1	1:F:349:THR:O	2.02	0.41
1:H:249:HIS:HE1	1:H:349:THR:O	2.03	0.41
1:C:187:LEU:HA	1:C:188:PRO:HD2	1.94	0.41
1:D:272:LEU:O	1:D:274:VAL:N	2.53	0.41
1:F:191:ASP:N	1:F:191:ASP:OD2	2.53	0.41
1:F:272:LEU:O	1:F:275:LEU:N	2.53	0.41
1:F:345:SER:O	1:F:346:TYR:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:SER:C	1:C:270:LYS:N	2.78	0.41
1:F:210:VAL:O	1:F:211:LEU:C	2.61	0.41
1:E:255:LYS:HB2	1:E:255:LYS:HE2	1.48	0.41
1:D:228:GLU:OE1	1:D:228:GLU:HA	2.21	0.41
1:D:295:ASP:O	1:D:298:THR:N	2.53	0.41
1:B:185:GLN:HE21	1:B:254:ARG:NH1	2.14	0.41
1:F:173:LEU:HD23	1:F:173:LEU:HA	1.85	0.41
1:G:296:ASP:O	1:G:299:ALA:HB3	2.21	0.41
1:B:307:LEU:HD13	1:B:342:PHE:CE1	2.56	0.41
1:F:328:GLN:HE21	1:F:328:GLN:HB2	1.63	0.41
1:H:248:ILE:HB	1:H:250:PHE:HE1	1.85	0.41
1:H:316:ARG:O	1:H:317:ARG:HG2	2.21	0.41
1:B:209:GLN:NE2	1:C:348:ARG:HH21	2.17	0.41
1:B:360:GLU:HG2	1:B:362:LYS:HD2	2.03	0.41
1:D:310:GLN:HG2	1:D:338:ARG:HG3	2.02	0.41
1:C:251:ASP:O	1:C:253:PRO:HD3	2.21	0.40
1:D:191:ASP:O	1:D:192:LYS:HB2	2.21	0.40
1:G:209:GLN:HE21	1:G:209:GLN:HB2	1.56	0.40
1:G:337:LEU:O	1:G:338:ARG:C	2.62	0.40
1:D:234:ILE:O	1:D:237:ASP:HB2	2.22	0.40
1:G:173:LEU:HD23	1:G:173:LEU:HA	1.91	0.40
1:G:228:GLU:OE1	1:G:228:GLU:HA	2.20	0.40
1:G:315:SER:HB3	1:G:328:GLN:OE1	2.22	0.40
1:G:320:LYS:O	1:G:320:LYS:CG	2.69	0.40
1:A:225:GLU:HG3	1:A:250:PHE:CD1	2.57	0.40
1:C:201:GLU:HA	1:C:201:GLU:OE2	2.22	0.40
1:D:272:LEU:O	1:D:273:GLU:C	2.65	0.40
1:G:170:ALA:O	1:G:174:ASP:HB2	2.21	0.40
1:G:328:GLN:HB3	1:G:329:GLY:H	1.71	0.40
1:H:283:MET:HB3	1:H:285:TYR:CZ	2.57	0.40
1:B:210:VAL:HG11	1:C:177:LEU:CD1	2.51	0.40
1:G:190:ARG:HB2	1:G:190:ARG:NH1	2.36	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	193/227 (85%)	182 (94%)	9 (5%)	2 (1%)	12	38
1	B	191/227 (84%)	178 (93%)	9 (5%)	4 (2%)	5	20
1	C	188/227 (83%)	170 (90%)	15 (8%)	3 (2%)	7	27
1	D	191/227 (84%)	166 (87%)	22 (12%)	3 (2%)	7	27
1	E	190/227 (84%)	170 (90%)	15 (8%)	5 (3%)	4	15
1	F	185/227 (82%)	157 (85%)	23 (12%)	5 (3%)	4	15
1	G	185/227 (82%)	155 (84%)	24 (13%)	6 (3%)	3	11
1	H	187/227 (82%)	164 (88%)	21 (11%)	2 (1%)	11	36
All	All	1510/1816 (83%)	1342 (89%)	138 (9%)	30 (2%)	6	21

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	175	SER
1	C	176	LEU
1	D	272	LEU
1	D	273	GLU
1	E	331	LEU
1	E	332	ASP
1	F	190	ARG
1	F	235	TRP
1	F	236	LEU
1	G	190	ARG
1	A	170	ALA
1	A	190	ARG
1	B	183	ARG
1	B	309	GLN
1	B	332	ASP
1	C	270	LYS
1	E	183	ARG
1	H	217	ASP
1	G	217	ASP
1	G	237	ASP
1	G	297	VAL
1	B	179	GLN
1	F	296	ASP

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Mol	Chain	Res	Type
1	G	320	LYS
1	E	181	LYS
1	E	269	LYS
1	F	276	SER
1	D	329	GLY
1	G	284	PRO
1	H	240	TYR

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	166/193 (86%)	142 (86%)	24 (14%)	3	11
1	B	165/193 (86%)	141 (86%)	24 (14%)	3	11
1	C	164/193 (85%)	139 (85%)	25 (15%)	3	10
1	D	165/193 (86%)	142 (86%)	23 (14%)	3	12
1	E	165/193 (86%)	135 (82%)	30 (18%)	2	6
1	F	161/193 (83%)	136 (84%)	25 (16%)	2	9
1	G	161/193 (83%)	133 (83%)	28 (17%)	2	7
1	H	163/193 (84%)	135 (83%)	28 (17%)	2	7
All	All	1310/1544 (85%)	1103 (84%)	207 (16%)	2	9

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	MET
1	A	173	LEU
1	A	183	ARG
1	A	186	VAL
1	A	187	LEU
1	A	196	VAL
1	A	208	ARG
1	A	209	GLN

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Mol	Chain	Res	Type
1	A	217	ASP
1	A	218	LYS
1	A	219	ASN
1	A	251	ASP
1	A	252	GLU
1	A	263	GLN
1	A	270	LYS
1	A	273	GLU
1	A	282	LEU
1	A	293	LEU
1	A	307	LEU
1	A	310	GLN
1	A	320	LYS
1	A	338	ARG
1	A	348	ARG
1	A	362	LYS
1	B	175	SER
1	B	176	LEU
1	B	177	LEU
1	B	179	GLN
1	B	181	LYS
1	B	186	VAL
1	B	196	VAL
1	B	208	ARG
1	B	209	GLN
1	B	221	ARG
1	B	260	LEU
1	B	263	GLN
1	B	269	LYS
1	B	270	LYS
1	B	282	LEU
1	B	291	ILE
1	B	307	LEU
1	B	310	GLN
1	B	316	ARG
1	B	324	THR
1	B	333	ASP
1	B	338	ARG
1	B	345	SER
1	B	362	LYS
1	C	173	LEU
1	C	176	LEU

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Mol	Chain	Res	Type
1	C	180	GLU
1	C	196	VAL
1	C	205	LEU
1	C	208	ARG
1	C	209	GLN
1	C	217	ASP
1	C	221	ARG
1	C	254	ARG
1	C	263	GLN
1	C	265	ASN
1	C	269	LYS
1	C	270	LYS
1	C	291	ILE
1	C	297	VAL
1	C	307	LEU
1	C	310	GLN
1	C	324	THR
1	C	334	VAL
1	C	338	ARG
1	C	348	ARG
1	C	356	GLN
1	C	359	ILE
1	C	362	LYS
1	D	176	LEU
1	D	177	LEU
1	D	182	GLU
1	D	183	ARG
1	D	186	VAL
1	D	196	VAL
1	D	205	LEU
1	D	208	ARG
1	D	215	ASP
1	D	217	ASP
1	D	254	ARG
1	D	255	LYS
1	D	260	LEU
1	D	263	GLN
1	D	269	LYS
1	D	270	LYS
1	D	274	VAL
1	D	291	ILE
1	D	307	LEU

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Mol	Chain	Res	Type
1	D	310	GLN
1	D	338	ARG
1	D	348	ARG
1	D	362	LYS
1	E	172	GLU
1	E	173	LEU
1	E	176	LEU
1	E	177	LEU
1	E	180	GLU
1	E	183	ARG
1	E	186	VAL
1	E	196	VAL
1	E	208	ARG
1	E	209	GLN
1	E	217	ASP
1	E	218	LYS
1	E	254	ARG
1	E	255	LYS
1	E	263	GLN
1	E	270	LYS
1	E	271	GLU
1	E	273	GLU
1	E	297	VAL
1	E	298	THR
1	E	307	LEU
1	E	315	SER
1	E	316	ARG
1	E	320	LYS
1	E	331	LEU
1	E	332	ASP
1	E	333	ASP
1	E	334	VAL
1	E	359	ILE
1	E	362	LYS
1	F	183	ARG
1	F	186	VAL
1	F	194	LEU
1	F	196	VAL
1	F	205	LEU
1	F	208	ARG
1	F	252	GLU
1	F	254	ARG

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Mol	Chain	Res	Type
1	F	255	LYS
1	F	263	GLN
1	F	270	LYS
1	F	278	LYS
1	F	290	ASN
1	F	291	ILE
1	F	298	THR
1	F	307	LEU
1	F	310	GLN
1	F	316	ARG
1	F	320	LYS
1	F	328	GLN
1	F	338	ARG
1	F	344	ASP
1	F	345	SER
1	F	348	ARG
1	F	362	LYS
1	G	172	GLU
1	G	176	LEU
1	G	183	ARG
1	G	187	LEU
1	G	192	LYS
1	G	196	VAL
1	G	205	LEU
1	G	208	ARG
1	G	209	GLN
1	G	215	ASP
1	G	217	ASP
1	G	218	LYS
1	G	254	ARG
1	G	260	LEU
1	G	263	GLN
1	G	270	LYS
1	G	291	ILE
1	G	307	LEU
1	G	315	SER
1	G	316	ARG
1	G	320	LYS
1	G	331	LEU
1	G	334	VAL
1	G	338	ARG
1	G	344	ASP

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Mol	Chain	Res	Type
1	G	356	GLN
1	G	359	ILE
1	G	362	LYS
1	H	169	MET
1	H	176	LEU
1	H	186	VAL
1	H	187	LEU
1	H	196	VAL
1	H	205	LEU
1	H	208	ARG
1	H	209	GLN
1	H	210	VAL
1	H	217	ASP
1	H	248	ILE
1	H	254	ARG
1	H	255	LYS
1	H	260	LEU
1	H	263	GLN
1	H	270	LYS
1	H	273	GLU
1	H	293	LEU
1	H	298	THR
1	H	307	LEU
1	H	320	LYS
1	H	332	ASP
1	H	333	ASP
1	H	334	VAL
1	H	338	ARG
1	H	341	GLN
1	H	356	GLN
1	H	362	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	249	HIS
1	A	263	GLN
1	A	341	GLN
1	B	179	GLN
1	B	185	GLN
1	B	249	HIS

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Mol	Chain	Res	Type
1	B	263	GLN
1	B	328	GLN
1	B	341	GLN
1	C	199	GLN
1	C	249	HIS
1	C	263	GLN
1	C	328	GLN
1	D	185	GLN
1	D	209	GLN
1	D	219	ASN
1	D	249	HIS
1	D	263	GLN
1	D	341	GLN
1	E	185	GLN
1	E	249	HIS
1	E	263	GLN
1	E	265	ASN
1	E	302	GLN
1	E	328	GLN
1	E	341	GLN
1	F	185	GLN
1	F	249	HIS
1	F	263	GLN
1	F	265	ASN
1	F	341	GLN
1	G	249	HIS
1	G	263	GLN
1	G	265	ASN
1	G	319	HIS
1	G	328	GLN
1	G	341	GLN
1	H	249	HIS
1	H	263	GLN
1	H	319	HIS
1	H	328	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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(Å ²)	Q<0.9
1	A	195/227 (85%)	-0.08	3 (1%) 72 63	17, 40, 62, 73	0
1	B	193/227 (85%)	-0.09	1 (0%) 87 82	18, 40, 64, 70	0
1	C	190/227 (83%)	0.06	1 (0%) 87 82	20, 45, 69, 78	0
1	D	193/227 (85%)	0.24	1 (0%) 87 82	25, 49, 74, 83	0
1	E	192/227 (84%)	0.19	9 (4%) 36 29	23, 47, 74, 89	0
1	F	189/227 (83%)	0.23	6 (3%) 50 40	20, 47, 81, 94	0
1	G	189/227 (83%)	0.44	6 (3%) 50 40	31, 53, 76, 80	0
1	H	191/227 (84%)	0.45	8 (4%) 40 32	32, 51, 76, 83	0
All	All	1532/1816 (84%)	0.18	35 (2%) 61 51	17, 47, 74, 94	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	171	ALA	6.0
1	G	169	MET	5.2
1	A	168	HIS	4.5
1	B	170	ALA	3.5
1	F	270	LYS	3.4
1	F	272	LEU	3.4
1	E	178	GLY	3.3
1	D	170	ALA	3.2
1	E	183	ARG	3.2
1	A	180	GLU	3.0
1	E	173	LEU	2.9
1	E	331	LEU	2.9
1	H	330	ALA	2.7
1	E	176	LEU	2.7
1	H	168	HIS	2.7
1	E	330	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	178	GLY	2.6
1	G	362	LYS	2.6
1	G	177	LEU	2.6
1	F	269	LYS	2.5
1	H	218	LYS	2.3
1	F	287	ASP	2.3
1	E	362	LYS	2.3
1	F	274	VAL	2.2
1	H	362	LYS	2.2
1	H	214	GLY	2.2
1	E	177	LEU	2.2
1	A	334	VAL	2.2
1	F	278	LYS	2.2
1	H	325	PHE	2.1
1	H	348	ARG	2.1
1	C	274	VAL	2.1
1	G	183	ARG	2.0
1	G	270	LYS	2.0
1	G	338	ARG	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.