



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:01 PM UTC

PDB ID : 2QF0 / pdb_00002qf0
Title : Structure of the delta PDZ truncation of the DegS protease
Authors : Sohn, J.; Grant, R.A.; Sauer, R.T.
Deposited on : 2007-06-26
Resolution : 2.50 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
Mogul : 2022.3.0, CSD as543be (2022)
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

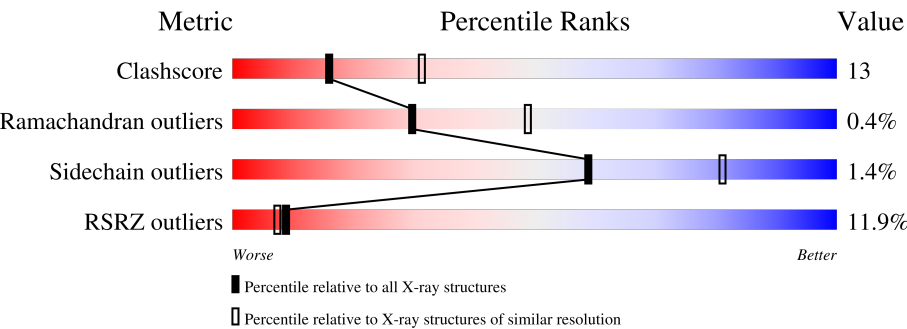
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	243	3% 69% 14% 17%
1	B	243	6% 69% 17% 13%
1	C	243	7% 65% 19% • 15%
1	D	243	10% 65% 17% • 16%
1	E	243	7% 58% 21% 21%
1	F	243	5% 66% 19% • 14%
1	G	243	8% 58% 23% 19%

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Mol	Chain	Length	Quality of chain
1	H	243	17% 52% 28% • 19%
1	I	243	24% 45% 31% • 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13852 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 Protease degS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	Se	0	0	0
			1507	941	267	296	3			
1	B	211	Total	C	N	O	Se	0	0	0
			1570	978	282	307	3			
1	C	206	Total	C	N	O	Se	0	0	0
			1533	959	275	296	3			
1	D	204	Total	C	N	O	Se	0	0	0
			1529	957	276	293	3			
1	E	193	Total	C	N	O	Se	0	0	0
			1442	905	255	279	3			
1	F	208	Total	C	N	O	Se	0	0	0
			1547	966	278	300	3			
1	G	196	Total	C	N	O	Se	0	0	0
			1460	917	260	280	3			
1	H	196	Total	C	N	O	Se	0	0	0
			1455	914	260	278	3			
1	I	189	Total	C	N	O	Se	0	0	0
			1397	877	246	271	3			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MSE	-	expression tag	UNP P0AEE3
A	15	ARG	-	expression tag	UNP P0AEE3
A	16	GLY	-	expression tag	UNP P0AEE3
A	17	SER	-	expression tag	UNP P0AEE3
A	18	HIS	-	expression tag	UNP P0AEE3
A	19	HIS	-	expression tag	UNP P0AEE3
A	20	HIS	-	expression tag	UNP P0AEE3
A	21	HIS	-	expression tag	UNP P0AEE3
A	22	HIS	-	expression tag	UNP P0AEE3
A	23	HIS	-	expression tag	UNP P0AEE3
A	24	GLY	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	-	expression tag	UNP P0AEE3
A	26	SER	-	expression tag	UNP P0AEE3
A	85	MSE	MET	modified residue	UNP P0AEE3
A	213	MSE	MET	modified residue	UNP P0AEE3
A	245	MSE	MET	modified residue	UNP P0AEE3
B	14	MSE	-	expression tag	UNP P0AEE3
B	15	ARG	-	expression tag	UNP P0AEE3
B	16	GLY	-	expression tag	UNP P0AEE3
B	17	SER	-	expression tag	UNP P0AEE3
B	18	HIS	-	expression tag	UNP P0AEE3
B	19	HIS	-	expression tag	UNP P0AEE3
B	20	HIS	-	expression tag	UNP P0AEE3
B	21	HIS	-	expression tag	UNP P0AEE3
B	22	HIS	-	expression tag	UNP P0AEE3
B	23	HIS	-	expression tag	UNP P0AEE3
B	24	GLY	-	expression tag	UNP P0AEE3
B	25	ARG	-	expression tag	UNP P0AEE3
B	26	SER	-	expression tag	UNP P0AEE3
B	85	MSE	MET	modified residue	UNP P0AEE3
B	213	MSE	MET	modified residue	UNP P0AEE3
B	245	MSE	MET	modified residue	UNP P0AEE3
C	14	MSE	-	expression tag	UNP P0AEE3
C	15	ARG	-	expression tag	UNP P0AEE3
C	16	GLY	-	expression tag	UNP P0AEE3
C	17	SER	-	expression tag	UNP P0AEE3
C	18	HIS	-	expression tag	UNP P0AEE3
C	19	HIS	-	expression tag	UNP P0AEE3
C	20	HIS	-	expression tag	UNP P0AEE3
C	21	HIS	-	expression tag	UNP P0AEE3
C	22	HIS	-	expression tag	UNP P0AEE3
C	23	HIS	-	expression tag	UNP P0AEE3
C	24	GLY	-	expression tag	UNP P0AEE3
C	25	ARG	-	expression tag	UNP P0AEE3
C	26	SER	-	expression tag	UNP P0AEE3
C	85	MSE	MET	modified residue	UNP P0AEE3
C	213	MSE	MET	modified residue	UNP P0AEE3
C	245	MSE	MET	modified residue	UNP P0AEE3
D	14	MSE	-	expression tag	UNP P0AEE3
D	15	ARG	-	expression tag	UNP P0AEE3
D	16	GLY	-	expression tag	UNP P0AEE3
D	17	SER	-	expression tag	UNP P0AEE3
D	18	HIS	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	HIS	-	expression tag	UNP P0AEE3
D	20	HIS	-	expression tag	UNP P0AEE3
D	21	HIS	-	expression tag	UNP P0AEE3
D	22	HIS	-	expression tag	UNP P0AEE3
D	23	HIS	-	expression tag	UNP P0AEE3
D	24	GLY	-	expression tag	UNP P0AEE3
D	25	ARG	-	expression tag	UNP P0AEE3
D	26	SER	-	expression tag	UNP P0AEE3
D	85	MSE	MET	modified residue	UNP P0AEE3
D	213	MSE	MET	modified residue	UNP P0AEE3
D	245	MSE	MET	modified residue	UNP P0AEE3
E	14	MSE	-	expression tag	UNP P0AEE3
E	15	ARG	-	expression tag	UNP P0AEE3
E	16	GLY	-	expression tag	UNP P0AEE3
E	17	SER	-	expression tag	UNP P0AEE3
E	18	HIS	-	expression tag	UNP P0AEE3
E	19	HIS	-	expression tag	UNP P0AEE3
E	20	HIS	-	expression tag	UNP P0AEE3
E	21	HIS	-	expression tag	UNP P0AEE3
E	22	HIS	-	expression tag	UNP P0AEE3
E	23	HIS	-	expression tag	UNP P0AEE3
E	24	GLY	-	expression tag	UNP P0AEE3
E	25	ARG	-	expression tag	UNP P0AEE3
E	26	SER	-	expression tag	UNP P0AEE3
E	85	MSE	MET	modified residue	UNP P0AEE3
E	213	MSE	MET	modified residue	UNP P0AEE3
E	245	MSE	MET	modified residue	UNP P0AEE3
F	14	MSE	-	expression tag	UNP P0AEE3
F	15	ARG	-	expression tag	UNP P0AEE3
F	16	GLY	-	expression tag	UNP P0AEE3
F	17	SER	-	expression tag	UNP P0AEE3
F	18	HIS	-	expression tag	UNP P0AEE3
F	19	HIS	-	expression tag	UNP P0AEE3
F	20	HIS	-	expression tag	UNP P0AEE3
F	21	HIS	-	expression tag	UNP P0AEE3
F	22	HIS	-	expression tag	UNP P0AEE3
F	23	HIS	-	expression tag	UNP P0AEE3
F	24	GLY	-	expression tag	UNP P0AEE3
F	25	ARG	-	expression tag	UNP P0AEE3
F	26	SER	-	expression tag	UNP P0AEE3
F	85	MSE	MET	modified residue	UNP P0AEE3
F	213	MSE	MET	modified residue	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	245	MSE	MET	modified residue	UNP P0AEE3
G	14	MSE	-	expression tag	UNP P0AEE3
G	15	ARG	-	expression tag	UNP P0AEE3
G	16	GLY	-	expression tag	UNP P0AEE3
G	17	SER	-	expression tag	UNP P0AEE3
G	18	HIS	-	expression tag	UNP P0AEE3
G	19	HIS	-	expression tag	UNP P0AEE3
G	20	HIS	-	expression tag	UNP P0AEE3
G	21	HIS	-	expression tag	UNP P0AEE3
G	22	HIS	-	expression tag	UNP P0AEE3
G	23	HIS	-	expression tag	UNP P0AEE3
G	24	GLY	-	expression tag	UNP P0AEE3
G	25	ARG	-	expression tag	UNP P0AEE3
G	26	SER	-	expression tag	UNP P0AEE3
G	85	MSE	MET	modified residue	UNP P0AEE3
G	213	MSE	MET	modified residue	UNP P0AEE3
G	245	MSE	MET	modified residue	UNP P0AEE3
H	14	MSE	-	expression tag	UNP P0AEE3
H	15	ARG	-	expression tag	UNP P0AEE3
H	16	GLY	-	expression tag	UNP P0AEE3
H	17	SER	-	expression tag	UNP P0AEE3
H	18	HIS	-	expression tag	UNP P0AEE3
H	19	HIS	-	expression tag	UNP P0AEE3
H	20	HIS	-	expression tag	UNP P0AEE3
H	21	HIS	-	expression tag	UNP P0AEE3
H	22	HIS	-	expression tag	UNP P0AEE3
H	23	HIS	-	expression tag	UNP P0AEE3
H	24	GLY	-	expression tag	UNP P0AEE3
H	25	ARG	-	expression tag	UNP P0AEE3
H	26	SER	-	expression tag	UNP P0AEE3
H	85	MSE	MET	modified residue	UNP P0AEE3
H	213	MSE	MET	modified residue	UNP P0AEE3
H	245	MSE	MET	modified residue	UNP P0AEE3
I	14	MSE	-	expression tag	UNP P0AEE3
I	15	ARG	-	expression tag	UNP P0AEE3
I	16	GLY	-	expression tag	UNP P0AEE3
I	17	SER	-	expression tag	UNP P0AEE3
I	18	HIS	-	expression tag	UNP P0AEE3
I	19	HIS	-	expression tag	UNP P0AEE3
I	20	HIS	-	expression tag	UNP P0AEE3
I	21	HIS	-	expression tag	UNP P0AEE3
I	22	HIS	-	expression tag	UNP P0AEE3

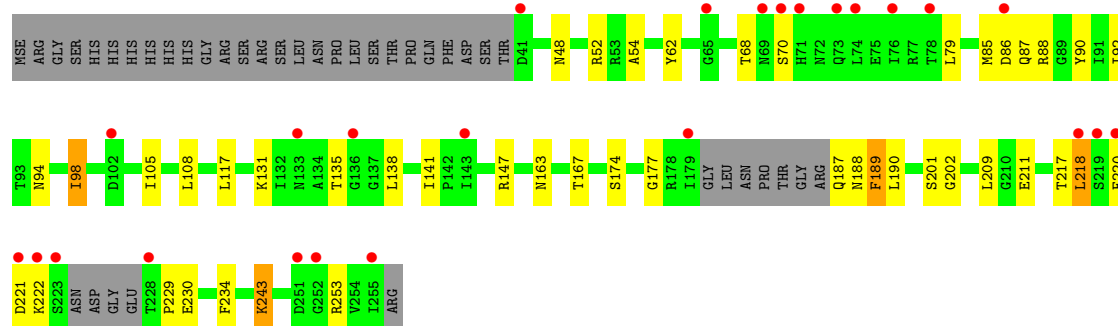
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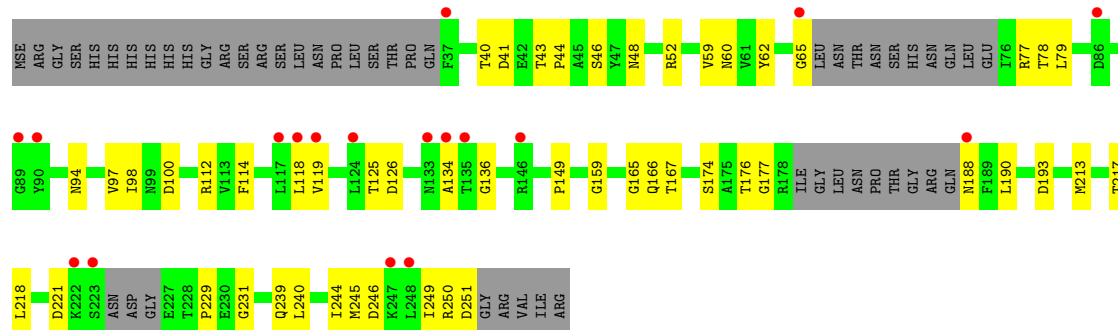
Chain	Residue	Modelled	Actual	Comment	Reference
I	23	HIS	-	expression tag	UNP P0AEE3
I	24	GLY	-	expression tag	UNP P0AEE3
I	25	ARG	-	expression tag	UNP P0AEE3
I	26	SER	-	expression tag	UNP P0AEE3
I	85	MSE	MET	modified residue	UNP P0AEE3
I	213	MSE	MET	modified residue	UNP P0AEE3
I	245	MSE	MET	modified residue	UNP P0AEE3

- Molecule 2 is water.

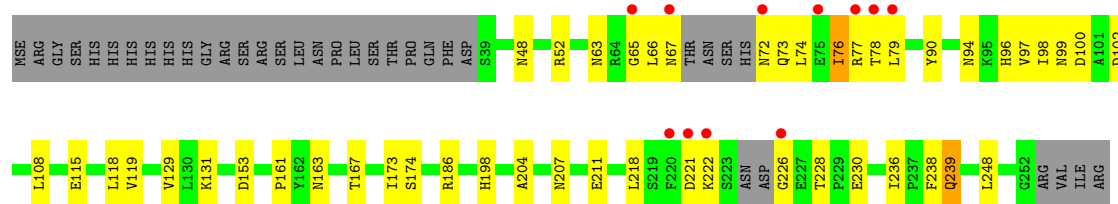
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	70	Total O 70 70	0	0
2	C	63	Total O 63 63	0	0
2	D	48	Total O 48 48	0	0
2	E	39	Total O 39 39	0	0
2	F	70	Total O 70 70	0	0
2	G	30	Total O 30 30	0	0
2	H	21	Total O 21 21	0	0
2	I	14	Total O 14 14	0	0



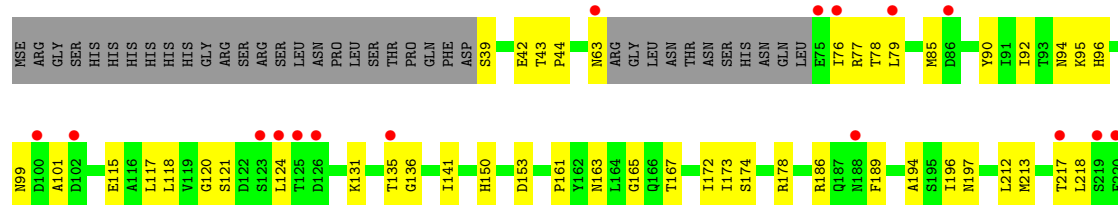
• Molecule 1: Protease degS

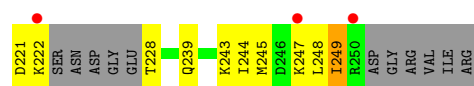


• Molecule 1: Protease degS

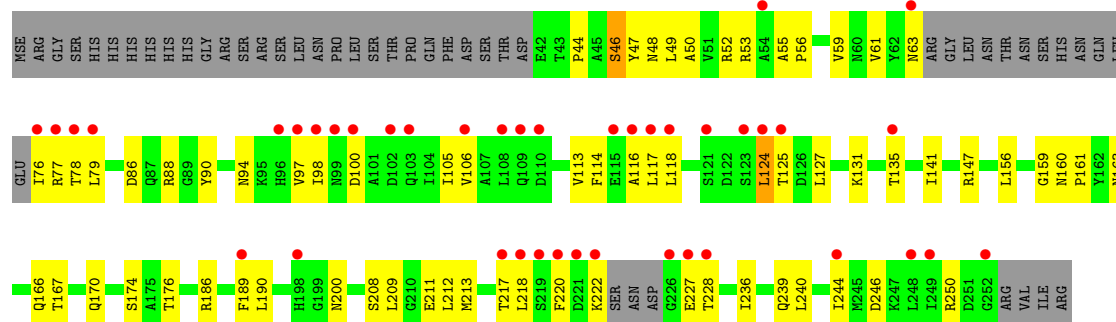


• Molecule 1: Protease degS

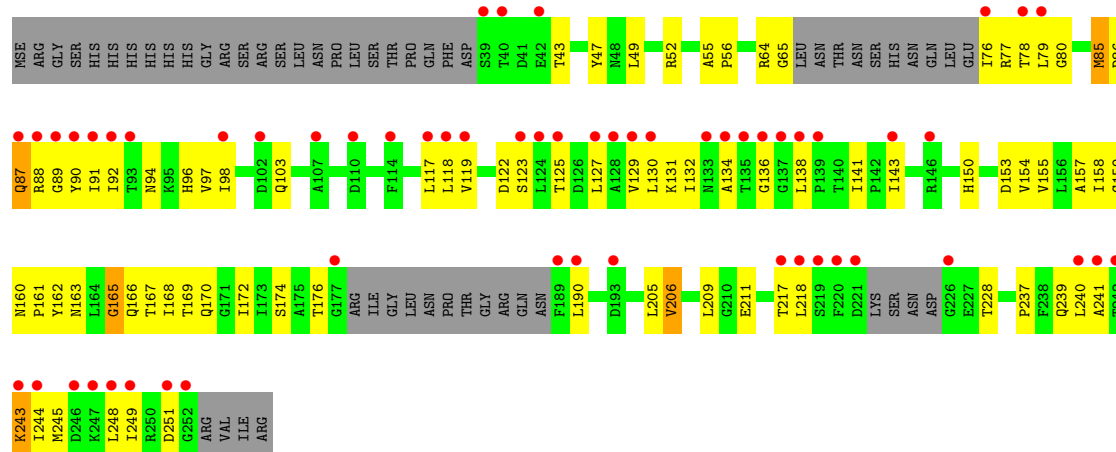
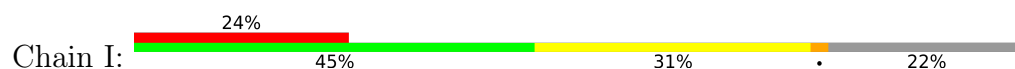




• Molecule 1: Protease degS



• Molecule 1: Protease degS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.17Å 132.97Å 229.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.53 – 2.50 42.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.0 (42.53-2.50) 93.8 (42.53-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.257 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13852	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5099e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.48	0/1522	0.96	3/2061 (0.1%)
1	B	0.50	0/1585	1.01	4/2147 (0.2%)
1	C	0.45	0/1548	0.98	6/2096 (0.3%)
1	D	0.44	0/1544	0.94	4/2091 (0.2%)
1	E	0.41	0/1456	0.92	4/1970 (0.2%)
1	F	0.48	0/1562	1.00	6/2115 (0.3%)
1	G	0.40	0/1475	0.94	5/1999 (0.3%)
1	H	0.38	0/1470	0.88	1/1991 (0.1%)
1	I	0.35	0/1410	0.87	4/1909 (0.2%)
All	All	0.44	0/13572	0.95	37/18379 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	GLY	N-CA-C	9.58	125.78	113.24
1	B	221	ASP	N-CA-C	8.65	122.34	111.69
1	C	221	ASP	N-CA-C	7.58	122.60	113.12
1	C	236	ILE	N-CA-C	-7.33	102.32	108.63
1	B	165	GLY	N-CA-C	-7.07	105.23	111.95
1	I	87	GLN	N-CA-C	-7.02	104.83	113.19
1	F	236	ILE	N-CA-C	-6.97	102.64	108.63
1	E	165	GLY	N-CA-C	-6.94	105.07	112.08
1	A	98	ILE	N-CA-C	6.33	119.10	112.83
1	B	190	LEU	N-CA-C	-6.26	100.37	110.32
1	G	165	GLY	N-CA-C	-6.14	105.77	112.04
1	I	165	GLY	N-CA-C	-6.12	104.50	111.85
1	A	59	VAL	N-CA-C	6.12	118.59	109.17
1	A	204	ALA	N-CA-C	5.66	119.28	110.17
1	F	238	PHE	N-CA-C	5.59	118.14	111.71
1	D	98	ILE	N-CA-C	5.56	118.24	112.90
1	F	115	GLU	N-CA-C	-5.55	100.25	109.46
1	E	46	SER	N-CA-C	5.53	117.49	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	115	GLU	N-CA-C	-5.47	100.26	109.07
1	D	189	PHE	N-CA-C	5.46	118.56	110.48
1	C	59	VAL	N-CA-C	5.35	117.34	108.99
1	C	204	ALA	N-CA-C	5.31	118.72	110.17
1	I	43	THR	CA-C-N	5.22	124.98	119.76
1	I	43	THR	C-N-CA	5.22	124.98	119.76
1	F	204	ALA	N-CA-C	5.21	118.55	110.17
1	D	190	LEU	N-CA-C	-5.20	101.23	109.96
1	H	46	SER	N-CA-C	5.20	116.97	109.07
1	E	98	ILE	N-CA-C	5.17	117.08	112.17
1	G	228	THR	CA-C-N	5.14	125.14	119.90
1	G	228	THR	C-N-CA	5.14	125.14	119.90
1	E	59	VAL	N-CA-C	5.10	116.94	108.99
1	G	249	ILE	N-CA-C	-5.07	106.41	113.00
1	C	115	GLU	N-CA-C	-5.04	101.49	109.96
1	D	202	GLY	N-CA-C	-5.03	109.09	115.08
1	F	228	THR	CA-C-N	5.03	124.96	119.78
1	F	228	THR	C-N-CA	5.03	124.96	119.78
1	C	98	ILE	N-CA-C	5.02	116.94	112.17

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	1507	0	1515	19	0
1	B	1570	0	1588	33	0
1	C	1533	0	1560	34	0
1	D	1529	0	1558	39	0
1	E	1442	0	1460	31	0
1	F	1547	0	1571	40	0
1	G	1460	0	1492	38	0
1	H	1455	0	1486	67	0
1	I	1397	0	1416	74	0
2	A	57	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	70	0	0	1	0
2	C	63	0	0	1	0
2	D	48	0	0	1	0
2	E	39	0	0	0	0
2	F	70	0	0	0	0
2	G	30	0	0	0	0
2	H	21	0	0	0	0
2	I	14	0	0	0	0
All	All	13852	0	13646	357	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 13.

All (357) 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:223:SER:HB3	1:C:226:GLY:HA2	1.45	0.98
1:F:79:LEU:HD11	1:F:163:ASN:HB2	1.58	0.86
1:H:167:THR:HG23	1:I:174:SER:HB3	1.58	0.85
1:H:105:ILE:HG13	1:H:114:PHE:O	1.78	0.84
1:D:147:ARG:HD2	1:D:211:GLU:OE2	1.78	0.84
1:B:67:ASN:HD21	1:B:73:GLN:HB3	1.47	0.79
1:D:187:GLN:HB2	1:D:189:PHE:CE1	2.18	0.78
1:C:217:THR:HG22	1:C:218:LEU:H	1.50	0.76
1:I:49:LEU:HA	1:I:52:ARG:NH1	1.99	0.76
1:F:73:GLN:HG2	1:F:74:LEU:H	1.53	0.73
1:G:94:ASN:HB3	1:G:96:HIS:CE1	2.24	0.73
1:G:186:ARG:HG3	1:G:189:PHE:CE2	2.22	0.73
1:I:122:ASP:HB3	1:I:125:THR:OG1	1.89	0.73
1:I:49:LEU:HA	1:I:52:ARG:HH12	1.54	0.72
1:E:240:LEU:HD23	1:E:240:LEU:O	1.90	0.71
1:H:77:ARG:NH1	1:H:77:ARG:HB2	2.05	0.71
1:C:67:ASN:H	1:C:77:ARG:HH21	1.39	0.70
1:C:66:LEU:O	1:C:67:ASN:HB3	1.92	0.70
1:I:65:GLY:HA3	1:I:77:ARG:HD2	1.72	0.69
1:E:48:ASN:OD1	1:E:52:ARG:HD3	1.91	0.69
1:F:96:HIS:NE2	1:F:218:LEU:HG	2.07	0.69
1:E:112:ARG:HD2	1:E:114:PHE:HZ	1.57	0.68
1:F:76:ILE:N	1:F:76:ILE:HD12	2.08	0.68
1:G:79:LEU:HD21	1:G:163:ASN:HB2	1.74	0.68
1:G:172:ILE:HD13	1:I:170:GLN:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ASN:OD1	1:D:52:ARG:HD2	1.94	0.67
1:H:147:ARG:HD2	1:H:211:GLU:OE2	1.94	0.67
1:D:85:MSE:HG3	1:D:92:ILE:HG13	1.75	0.67
1:C:85:MSE:HG3	1:C:92:ILE:HG13	1.75	0.67
1:B:79:LEU:HD11	1:B:160:ASN:HD22	1.59	0.67
1:E:245:MSE:O	1:E:249:ILE:HG13	1.96	0.66
1:I:245:MSE:O	1:I:249:ILE:HG13	1.94	0.66
1:F:76:ILE:HD12	1:F:76:ILE:H	1.61	0.66
1:B:95:LYS:HD2	1:B:121:SER:HB3	1.77	0.65
1:G:153:ASP:HB2	1:G:173:ILE:HD12	1.80	0.64
1:C:124:LEU:HD23	1:C:124:LEU:O	1.98	0.62
1:E:250:ARG:HG3	1:E:250:ARG:HH11	1.63	0.62
1:C:240:LEU:O	1:C:244:ILE:HG12	1.98	0.62
1:B:124:LEU:O	1:B:124:LEU:HD23	1.99	0.62
1:H:59:VAL:HG21	1:H:106:VAL:HG13	1.80	0.62
1:I:237:PRO:HG2	1:I:240:LEU:HB3	1.81	0.61
1:I:85:MSE:HE2	1:I:92:ILE:HD12	1.82	0.61
1:H:98:ILE:C	1:H:100:ASP:H	2.08	0.61
1:A:217:THR:HG22	1:A:218:LEU:HD22	1.83	0.61
1:F:96:HIS:CE1	1:F:218:LEU:HG	2.35	0.61
1:F:96:HIS:HA	1:F:99:ASN:HD22	1.67	0.60
1:H:222:LYS:HG2	1:H:222:LYS:O	2.00	0.60
1:I:243:LYS:HB2	1:I:243:LYS:NZ	2.17	0.60
1:A:220:PHE:CZ	1:A:222:LYS:HB2	2.36	0.60
1:I:158:ILE:HG12	1:I:168:ILE:HD12	1.84	0.60
1:B:239:GLN:H	1:B:239:GLN:CD	2.09	0.59
1:I:239:GLN:C	1:I:241:ALA:H	2.10	0.59
1:H:213:MSE:HE2	1:H:213:MSE:HA	1.84	0.59
1:B:96:HIS:ND1	1:B:218:LEU:HD11	2.18	0.59
1:B:250:ARG:HG3	1:B:251:ASP:OD2	2.03	0.59
1:G:217:THR:HG22	1:G:218:LEU:H	1.68	0.59
1:I:134:ALA:HB2	1:I:138:LEU:HD21	1.83	0.59
1:D:243:LYS:HB2	1:D:243:LYS:NZ	2.17	0.59
1:G:63:ASN:ND2	1:G:101:ALA:HB2	2.19	0.58
1:G:239:GLN:N	1:G:239:GLN:OE1	2.36	0.58
1:H:246:ASP:O	1:H:250:ARG:HG3	2.03	0.58
1:H:220:PHE:CZ	1:H:222:LYS:HB3	2.38	0.58
1:B:79:LEU:HD11	1:B:160:ASN:ND2	2.18	0.57
1:H:55:ALA:HB3	1:H:56:PRO:HD3	1.87	0.57
1:D:217:THR:HG22	1:D:218:LEU:CD2	2.35	0.57
1:H:220:PHE:CE1	1:H:222:LYS:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:THR:HG22	1:G:136:GLY:N	2.20	0.56
1:G:217:THR:HG22	1:G:218:LEU:N	2.20	0.56
1:E:149:PRO:HB3	1:E:213:MSE:SE	2.55	0.56
1:C:94:ASN:HB2	1:C:97:VAL:HG23	1.87	0.56
1:G:243:LYS:HE2	1:G:247:LYS:NZ	2.21	0.56
1:H:117:LEU:H	1:H:117:LEU:HD23	1.70	0.56
1:H:86:ASP:OD1	1:H:88:ARG:HG3	2.06	0.56
1:C:176:THR:HA	1:C:190:LEU:HD23	1.88	0.56
1:G:95:LYS:HD2	1:G:121:SER:HB3	1.87	0.56
1:H:124:LEU:HD23	1:H:124:LEU:O	2.06	0.56
1:B:67:ASN:CG	1:B:68:THR:H	2.14	0.55
1:B:213:MSE:HA	1:B:213:MSE:HE2	1.89	0.55
1:G:90:TYR:CE2	1:G:131:LYS:HD3	2.42	0.55
1:A:176:THR:HG22	1:A:190:LEU:CD2	2.36	0.55
1:I:86:ASP:C	1:I:88:ARG:H	2.14	0.55
1:D:217:THR:C	1:D:218:LEU:HD22	2.32	0.54
1:E:65:GLY:HA3	1:E:77:ARG:HE	1.72	0.54
1:D:79:LEU:HD21	1:D:163:ASN:HB2	1.89	0.54
1:G:118:LEU:HD23	1:G:120:GLY:H	1.71	0.54
1:D:108:LEU:HD12	1:D:108:LEU:N	2.23	0.54
1:B:167:THR:HG23	1:C:174:SER:HB3	1.90	0.54
1:I:94:ASN:HB3	1:I:96:HIS:CE1	2.43	0.54
1:I:243:LYS:HB2	1:I:243:LYS:HZ2	1.74	0.53
1:A:157:ALA:HB3	1:A:169:THR:OG1	2.08	0.53
1:I:118:LEU:C	1:I:118:LEU:HD23	2.34	0.53
1:H:228:THR:HG23	1:H:228:THR:O	2.09	0.53
1:H:239:GLN:CD	1:H:239:GLN:H	2.17	0.53
1:I:87:GLN:C	1:I:89:GLY:H	2.16	0.53
1:H:49:LEU:HD21	1:H:53:ARG:NH2	2.24	0.53
1:H:160:ASN:ND2	1:H:163:ASN:HA	2.23	0.53
1:H:227:GLU:H	1:H:227:GLU:CD	2.17	0.53
1:I:159:GLY:O	1:I:166:GLN:HA	2.09	0.53
1:H:76:ILE:HG13	1:H:77:ARG:N	2.24	0.53
1:I:141:ILE:HG23	1:I:141:ILE:O	2.07	0.53
1:A:212:LEU:O	1:A:213:MSE:HE2	2.08	0.52
1:D:187:GLN:HB2	1:D:189:PHE:HE1	1.69	0.52
1:F:239:GLN:H	1:F:239:GLN:CD	2.17	0.52
1:G:245:MSE:O	1:G:249:ILE:HG13	2.09	0.52
1:I:118:LEU:HD23	1:I:119:VAL:N	2.24	0.52
1:G:221:ASP:O	1:G:222:LYS:HB2	2.08	0.52
1:B:118:LEU:HD13	1:B:118:LEU:C	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:TYR:HA	1:I:130:LEU:O	2.09	0.52
1:I:239:GLN:HG3	1:I:240:LEU:H	1.74	0.52
1:H:186:ARG:HG2	1:H:189:PHE:CE1	2.44	0.52
1:D:167:THR:HG23	1:E:174:SER:HB3	1.92	0.52
1:A:217:THR:HG22	1:A:218:LEU:CD2	2.39	0.52
1:E:112:ARG:HD2	1:E:114:PHE:CZ	2.41	0.52
1:G:124:LEU:O	1:G:124:LEU:HD23	2.09	0.52
1:I:47:TYR:CE2	1:I:154:VAL:HG11	2.45	0.52
1:F:222:LYS:HE3	1:F:226:GLY:HA2	1.92	0.51
1:E:167:THR:HG23	1:F:174:SER:HB3	1.92	0.51
1:H:61:VAL:O	1:H:79:LEU:HA	2.10	0.51
1:I:244:ILE:O	1:I:248:LEU:HG	2.11	0.51
1:H:217:THR:HG22	1:H:218:LEU:H	1.75	0.51
1:C:48:ASN:OD1	1:C:52:ARG:HD3	2.11	0.51
1:A:167:THR:HG23	1:B:174:SER:HB3	1.92	0.51
1:C:223:SER:CB	1:C:226:GLY:HA2	2.30	0.51
1:H:44:PRO:HG3	1:I:209:LEU:CD1	2.41	0.51
1:C:67:ASN:O	1:C:68:THR:C	2.53	0.51
1:D:217:THR:O	1:D:218:LEU:HD22	2.11	0.51
1:B:67:ASN:ND2	1:B:73:GLN:O	2.44	0.51
1:B:223:SER:HB3	1:B:226:GLY:N	2.25	0.51
1:I:55:ALA:HB3	1:I:56:PRO:HD3	1.93	0.51
1:I:65:GLY:HA3	1:I:77:ARG:CD	2.40	0.51
1:B:240:LEU:O	1:B:244:ILE:HG12	2.12	0.50
1:D:54:ALA:HB1	1:D:141:ILE:HD11	1.93	0.50
1:D:147:ARG:NH1	1:D:209:LEU:HD12	2.26	0.50
1:I:122:ASP:CG	1:I:123:SER:N	2.69	0.50
1:I:94:ASN:HB2	1:I:97:VAL:HG23	1.94	0.50
1:A:220:PHE:CE1	1:A:222:LYS:HB2	2.47	0.50
1:B:189:PHE:HB2	2:B:257:HOH:O	2.12	0.50
1:H:76:ILE:HG13	1:H:77:ARG:H	1.76	0.50
1:H:94:ASN:HB2	1:H:97:VAL:CG2	2.42	0.50
1:B:48:ASN:OD1	1:B:52:ARG:HD3	2.12	0.50
1:F:76:ILE:H	1:F:76:ILE:CD1	2.23	0.50
1:D:243:LYS:HB2	1:D:243:LYS:HZ3	1.75	0.50
1:B:85:MSE:HE2	1:B:92:ILE:HD12	1.93	0.50
1:F:65:GLY:HA3	1:F:77:ARG:HH11	1.77	0.50
1:C:65:GLY:HA2	1:C:102:ASP:OD2	2.12	0.50
1:F:67:ASN:O	1:F:72:ASN:HB2	2.12	0.49
1:H:117:LEU:CD2	1:H:131:LYS:HB3	2.42	0.49
1:D:221:ASP:O	1:D:222:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:ASP:C	1:I:88:ARG:N	2.70	0.49
1:C:181:LEU:HD11	1:D:105:ILE:HD11	1.93	0.49
1:D:217:THR:HG22	1:D:218:LEU:HD22	1.94	0.49
1:G:194:ALA:O	1:G:196:ILE:HG12	2.12	0.49
1:B:64:ARG:NH2	1:B:103:GLN:OE1	2.41	0.49
1:G:63:ASN:OD1	1:G:77:ARG:HD2	2.12	0.49
1:D:68:THR:C	1:D:70:SER:H	2.21	0.49
1:G:39:SER:HB2	1:G:42:GLU:OE2	2.13	0.49
1:B:76:ILE:HD12	1:B:76:ILE:N	2.28	0.49
1:B:86:ASP:OD2	1:B:88:ARG:HB2	2.12	0.49
1:H:59:VAL:CG2	1:H:106:VAL:HG13	2.43	0.48
1:A:85:MSE:HE2	1:A:92:ILE:HD12	1.94	0.48
1:A:176:THR:HG22	1:A:190:LEU:HD22	1.94	0.48
1:B:67:ASN:N	1:B:67:ASN:HD22	2.11	0.48
1:F:77:ARG:HH22	1:F:100:ASP:HB2	1.78	0.48
1:C:96:HIS:NE2	1:C:218:LEU:HD21	2.29	0.48
1:D:94:ASN:OD1	1:D:201:SER:HB3	2.13	0.48
1:I:239:GLN:C	1:I:241:ALA:N	2.71	0.48
1:E:217:THR:O	1:E:218:LEU:HD23	2.13	0.48
1:G:244:ILE:O	1:G:248:LEU:HG	2.13	0.48
1:D:85:MSE:CG	1:D:92:ILE:HG13	2.42	0.48
1:E:213:MSE:HA	1:E:213:MSE:HE2	1.95	0.48
1:F:221:ASP:O	1:F:222:LYS:HB2	2.13	0.48
1:H:79:LEU:HD21	1:H:163:ASN:HB2	1.96	0.48
1:E:176:THR:HG22	1:E:190:LEU:CD2	2.44	0.48
1:F:77:ARG:NH1	1:F:100:ASP:O	2.47	0.48
1:H:63:ASN:HD22	1:H:78:THR:H	1.61	0.48
1:I:157:ALA:HB3	1:I:169:THR:OG1	2.14	0.48
1:D:174:SER:HB3	1:F:167:THR:HG23	1.96	0.48
1:H:77:ARG:HB2	1:H:77:ARG:CZ	2.44	0.48
1:I:98:ILE:C	1:I:98:ILE:HD12	2.38	0.48
1:I:205:LEU:O	1:I:205:LEU:HG	2.14	0.48
1:E:240:LEU:O	1:E:244:ILE:HG12	2.12	0.47
1:E:125:THR:O	1:E:126:ASP:HB3	2.14	0.47
1:F:94:ASN:HB3	1:F:96:HIS:CE1	2.49	0.47
1:I:78:THR:HG22	1:I:79:LEU:N	2.29	0.47
1:I:158:ILE:HG23	1:I:168:ILE:CD1	2.44	0.47
1:A:96:HIS:HA	1:A:99:ASN:ND2	2.29	0.47
1:E:177:GLY:HA2	1:E:188:ASN:CG	2.40	0.47
1:H:159:GLY:O	1:H:166:GLN:HA	2.15	0.47
1:B:240:LEU:O	1:B:240:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ASP:HA	1:D:229:PRO:HG2	1.96	0.47
1:H:105:ILE:HD11	1:H:113:VAL:CG1	2.44	0.47
1:H:227:GLU:CD	1:H:227:GLU:N	2.72	0.47
1:I:64:ARG:HA	1:I:76:ILE:HA	1.95	0.47
1:I:87:GLN:C	1:I:89:GLY:N	2.71	0.47
1:I:117:LEU:N	1:I:117:LEU:HD12	2.29	0.47
1:I:141:ILE:O	1:I:143:ILE:HG13	2.14	0.47
1:G:212:LEU:O	1:G:213:MSE:HE2	2.15	0.47
1:C:239:GLN:HG2	1:C:243:LYS:HE3	1.97	0.47
1:G:167:THR:HG23	1:H:174:SER:HB3	1.96	0.47
1:I:90:TYR:HE1	1:I:249:ILE:HG12	1.80	0.47
1:E:246:ASP:O	1:E:250:ARG:HG2	2.16	0.47
1:F:65:GLY:HA3	1:F:77:ARG:HD3	1.97	0.47
1:H:94:ASN:HB2	1:H:97:VAL:HG23	1.97	0.47
1:F:63:ASN:HB3	1:F:78:THR:HB	1.97	0.46
1:E:239:GLN:H	1:E:239:GLN:CD	2.24	0.46
1:D:217:THR:HG22	1:D:218:LEU:HD23	1.98	0.46
1:E:79:LEU:C	1:E:79:LEU:HD12	2.40	0.46
1:I:122:ASP:CG	1:I:123:SER:H	2.24	0.46
1:C:213:MSE:HE2	1:C:213:MSE:HA	1.98	0.46
1:C:219:SER:HA	2:C:282:HOH:O	2.15	0.46
1:F:79:LEU:HD11	1:F:163:ASN:CB	2.39	0.46
1:C:96:HIS:HA	1:C:99:ASN:HD22	1.81	0.46
1:H:212:LEU:O	1:H:213:MSE:HE2	2.16	0.46
1:H:161:PRO:HG3	1:H:200:ASN:OD1	2.15	0.46
1:D:79:LEU:HD12	1:D:79:LEU:C	2.41	0.46
1:I:176:THR:HG22	1:I:190:LEU:CD2	2.46	0.46
1:C:96:HIS:CD2	1:C:218:LEU:HD21	2.50	0.46
1:H:47:TYR:HB3	1:H:156:LEU:HD11	1.97	0.46
1:H:63:ASN:HD21	1:H:78:THR:HB	1.81	0.46
1:B:108:LEU:HD12	1:B:108:LEU:N	2.31	0.46
1:B:196:ILE:HG22	1:B:219:SER:HB3	1.97	0.45
1:F:66:LEU:N	1:F:66:LEU:HD22	2.31	0.45
1:B:67:ASN:ND2	1:B:67:ASN:N	2.64	0.45
1:C:51:VAL:HG13	1:C:168:ILE:CD1	2.47	0.45
1:C:181:LEU:HD11	1:D:105:ILE:CD1	2.46	0.45
1:G:186:ARG:HG3	1:G:189:PHE:HE2	1.77	0.45
1:I:90:TYR:CE1	1:I:249:ILE:HG12	2.51	0.45
1:D:98:ILE:HD12	1:D:98:ILE:C	2.41	0.45
1:H:240:LEU:C	1:H:240:LEU:HD23	2.40	0.45
1:H:77:ARG:CB	1:H:77:ARG:HH11	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:OD1	1:A:201:SER:HB3	2.17	0.45
1:F:76:ILE:N	1:F:76:ILE:CD1	2.77	0.45
1:I:79:LEU:CD2	1:I:163:ASN:HB2	2.46	0.45
1:I:85:MSE:HE2	1:I:92:ILE:CD1	2.45	0.45
1:D:253:ARG:HG2	2:D:280:HOH:O	2.17	0.45
1:F:118:LEU:HD13	1:F:118:LEU:C	2.42	0.45
1:I:76:ILE:O	1:I:76:ILE:HG23	2.17	0.45
1:G:96:HIS:CD2	1:G:218:LEU:HD21	2.51	0.45
1:G:178:ARG:NH1	1:I:165:GLY:HA3	2.32	0.45
1:H:159:GLY:C	1:H:161:PRO:HD3	2.42	0.45
1:H:98:ILE:HD12	1:H:118:LEU:HD23	1.98	0.45
1:H:127:LEU:HD21	1:H:236:ILE:HG13	1.99	0.45
1:E:94:ASN:HB2	1:E:97:VAL:HG23	1.99	0.45
1:E:119:VAL:HG12	1:E:119:VAL:O	2.16	0.45
1:I:239:GLN:HG3	1:I:240:LEU:N	2.32	0.45
1:I:176:THR:HG22	1:I:190:LEU:HD23	1.99	0.44
1:I:132:ILE:HD11	1:I:138:LEU:HD13	2.00	0.44
1:D:220:PHE:HB2	1:D:234:PHE:HE1	1.83	0.44
1:F:77:ARG:HH22	1:F:100:ASP:CB	2.30	0.44
1:I:160:ASN:ND2	1:I:163:ASN:HA	2.32	0.44
1:C:189:PHE:HE1	1:C:236:ILE:HD13	1.82	0.44
1:H:79:LEU:CD2	1:H:163:ASN:HB2	2.48	0.44
1:I:118:LEU:HD23	1:I:119:VAL:C	2.42	0.44
1:E:43:THR:HA	1:E:44:PRO:HD3	1.89	0.44
1:E:193:ASP:HA	1:E:231:GLY:O	2.18	0.44
1:I:153:ASP:O	1:I:155:VAL:HG13	2.17	0.44
1:G:174:SER:HB3	1:I:167:THR:HG23	2.00	0.44
1:H:125:THR:HG21	1:H:240:LEU:HD21	2.00	0.44
1:H:170:GLN:HB2	1:I:172:ILE:HD13	1.99	0.44
1:C:184:THR:HA	1:D:135:THR:HG22	2.00	0.44
1:E:250:ARG:HG3	1:E:250:ARG:NH1	2.30	0.44
1:I:158:ILE:HG12	1:I:168:ILE:CD1	2.47	0.44
1:I:217:THR:HG22	1:I:218:LEU:HG	1.99	0.44
1:G:85:MSE:HE2	1:G:92:ILE:HD12	1.98	0.43
1:H:160:ASN:HD21	1:H:163:ASN:HA	1.82	0.43
1:A:40:THR:HG23	1:A:41:ASP:N	2.33	0.43
1:A:125:THR:O	1:A:126:ASP:HB3	2.17	0.43
1:I:125:THR:O	1:I:127:LEU:HG	2.19	0.43
1:D:79:LEU:CD2	1:D:163:ASN:HB2	2.49	0.43
1:I:158:ILE:HG23	1:I:168:ILE:HD13	1.98	0.43
1:A:133:ASN:ND2	2:A:301:HOH:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:LEU:HD22	1:G:117:LEU:N	2.33	0.43
1:E:159:GLY:O	1:E:166:GLN:HA	2.18	0.43
1:F:67:ASN:HB3	1:F:72:ASN:CB	2.49	0.43
1:H:98:ILE:C	1:H:100:ASP:N	2.72	0.43
1:E:134:ALA:C	1:E:136:GLY:H	2.27	0.43
1:E:221:ASP:HA	1:E:229:PRO:HG3	2.01	0.43
1:F:129:VAL:HG23	1:F:248:LEU:HD12	2.00	0.43
1:G:79:LEU:CD2	1:G:163:ASN:HB2	2.46	0.43
1:E:40:THR:HG23	1:E:41:ASP:N	2.33	0.43
1:F:108:LEU:HD12	1:F:108:LEU:N	2.34	0.43
1:I:64:ARG:HH21	1:I:103:GLN:CD	2.26	0.43
1:I:98:ILE:HD13	1:I:118:LEU:HD12	1.99	0.43
1:I:150:HIS:HB2	1:I:153:ASP:OD2	2.18	0.43
1:G:161:PRO:HB3	1:G:197:ASN:HB2	2.01	0.43
1:H:48:ASN:OD1	1:H:52:ARG:HD3	2.18	0.43
1:H:141:ILE:O	1:H:141:ILE:HG23	2.19	0.43
1:F:119:VAL:O	1:F:119:VAL:HG12	2.19	0.43
1:F:221:ASP:O	1:F:221:ASP:OD1	2.37	0.43
1:B:201:SER:OG	1:B:218:LEU:HD23	2.19	0.42
1:F:98:ILE:HD12	1:F:98:ILE:C	2.44	0.42
1:G:63:ASN:HB3	1:G:78:THR:O	2.18	0.42
1:H:217:THR:HG22	1:H:218:LEU:N	2.34	0.42
1:D:108:LEU:N	1:D:108:LEU:CD1	2.82	0.42
1:F:48:ASN:OD1	1:F:52:ARG:HD3	2.18	0.42
1:F:94:ASN:HB2	1:F:97:VAL:HG23	2.00	0.42
1:H:176:THR:HG22	1:H:190:LEU:CD2	2.50	0.42
1:I:79:LEU:HD12	1:I:80:GLY:H	1.85	0.42
1:H:44:PRO:HG3	1:I:209:LEU:HD12	2.01	0.42
1:A:67:ASN:O	1:A:68:THR:HB	2.19	0.42
1:C:94:ASN:HB3	1:C:96:HIS:CE1	2.55	0.42
1:E:60:ASN:HB3	1:E:62:TYR:CE1	2.54	0.42
1:H:90:TYR:CE2	1:H:131:LYS:HD3	2.54	0.42
1:C:222:LYS:O	1:C:223:SER:C	2.62	0.42
1:G:124:LEU:HD23	1:G:124:LEU:C	2.45	0.42
1:H:46:SER:HB2	1:I:153:ASP:OD1	2.19	0.42
1:I:206:VAL:HA	1:I:211:GLU:O	2.20	0.42
1:F:65:GLY:HA2	1:F:102:ASP:HB2	2.02	0.42
1:F:153:ASP:HB2	1:F:173:ILE:HD12	2.02	0.42
1:G:213:MSE:HE2	1:G:213:MSE:HA	2.02	0.42
1:D:177:GLY:HA2	1:D:188:ASN:OD1	2.20	0.42
1:E:240:LEU:HD23	1:E:240:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ASN:ND2	1:F:211:GLU:HB2	2.34	0.42
1:I:161:PRO:O	1:I:162:TYR:C	2.63	0.42
1:A:227:GLU:H	1:A:227:GLU:CD	2.28	0.41
1:C:96:HIS:NE2	1:C:218:LEU:HG	2.35	0.41
1:F:207:ASN:HD21	1:F:211:GLU:HB2	1.85	0.41
1:G:150:HIS:HB2	1:G:153:ASP:OD1	2.19	0.41
1:A:66:LEU:O	1:A:77:ARG:NH2	2.53	0.41
1:F:90:TYR:CE2	1:F:131:LYS:HD3	2.55	0.41
1:G:43:THR:HA	1:G:44:PRO:HD3	1.82	0.41
1:G:141:ILE:O	1:G:141:ILE:HG23	2.20	0.41
1:I:88:ARG:O	1:I:131:LYS:HE2	2.20	0.41
1:C:96:HIS:NE2	1:C:218:LEU:CD2	2.83	0.41
1:G:217:THR:O	1:G:218:LEU:C	2.63	0.41
1:B:86:ASP:OD2	1:B:88:ARG:N	2.40	0.41
1:B:94:ASN:HA	1:B:126:ASP:O	2.21	0.41
1:C:221:ASP:O	1:C:229:PRO:HD2	2.19	0.41
1:H:117:LEU:HD23	1:H:117:LEU:N	2.35	0.41
1:I:122:ASP:OD2	1:I:125:THR:HG23	2.20	0.41
1:B:194:ALA:O	1:B:196:ILE:HG12	2.21	0.41
1:A:133:ASN:HD21	1:A:135:THR:HB	1.86	0.41
1:C:47:TYR:HB3	1:C:156:LEU:HD11	2.02	0.41
1:C:63:ASN:CG	1:C:101:ALA:HB2	2.46	0.41
1:E:118:LEU:HD13	1:E:118:LEU:C	2.46	0.41
1:H:98:ILE:CD1	1:H:118:LEU:HD23	2.51	0.41
1:B:96:HIS:HD1	1:B:218:LEU:HD11	1.84	0.41
1:D:62:TYR:HB2	1:D:105:ILE:HB	2.03	0.41
1:D:87:GLN:NE2	1:D:138:LEU:O	2.51	0.41
1:D:90:TYR:CE2	1:D:131:LYS:HD2	2.56	0.41
1:H:50:ALA:HB2	1:H:208:SER:O	2.20	0.41
1:H:116:ALA:HA	1:H:131:LYS:O	2.21	0.41
1:H:117:LEU:HD21	1:H:131:LYS:HB3	2.03	0.41
1:H:147:ARG:NH1	1:H:209:LEU:HD12	2.36	0.41
1:H:63:ASN:ND2	1:H:78:THR:HB	2.36	0.41
1:I:237:PRO:HB2	1:I:239:GLN:HG2	2.02	0.41
1:D:218:LEU:HD13	1:D:218:LEU:HA	1.94	0.40
1:I:91:ILE:O	1:I:129:VAL:HA	2.21	0.40
1:F:161:PRO:HA	1:F:198:HIS:O	2.21	0.40
1:I:90:TYR:CD2	1:I:90:TYR:N	2.89	0.40
1:H:240:LEU:O	1:H:244:ILE:HG12	2.21	0.40
1:B:85:MSE:HG3	1:B:92:ILE:HG13	2.02	0.40
1:C:79:LEU:HD11	1:C:163:ASN:CG	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:PHE:HE1	1:H:135:THR:HG23	1.86	0.40
1:C:189:PHE:CE1	1:C:236:ILE:HD13	2.56	0.40
1:D:86:ASP:OD2	1:D:88:ARG:HB2	2.21	0.40
1:D:230:GLU:OE2	1:F:230:GLU:HA	2.22	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	196/243 (81%)	190 (97%)	6 (3%)	0	100	100
1	B	205/243 (84%)	196 (96%)	7 (3%)	2 (1%)	12	24
1	C	200/243 (82%)	193 (96%)	7 (4%)	0	100	100
1	D	198/243 (82%)	187 (94%)	11 (6%)	0	100	100
1	E	185/243 (76%)	177 (96%)	8 (4%)	0	100	100
1	F	202/243 (83%)	195 (96%)	7 (4%)	0	100	100
1	G	190/243 (78%)	184 (97%)	6 (3%)	0	100	100
1	H	190/243 (78%)	168 (88%)	22 (12%)	0	100	100
1	I	181/243 (74%)	155 (86%)	21 (12%)	5 (3%)	4	6
All	All	1747/2187 (80%)	1645 (94%)	95 (5%)	7 (0%)	30	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	251	ASP
1	B	40	THR
1	I	206	VAL
1	I	136	GLY

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Mol	Chain	Res	Type
1	B	67	ASN
1	I	85	MSE
1	I	228	THR

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	163/196 (83%)	160 (98%)	3 (2%)	51	77
1	B	170/196 (87%)	167 (98%)	3 (2%)	51	77
1	C	165/196 (84%)	164 (99%)	1 (1%)	78	91
1	D	166/196 (85%)	163 (98%)	3 (2%)	51	77
1	E	156/196 (80%)	153 (98%)	3 (2%)	50	76
1	F	167/196 (85%)	164 (98%)	3 (2%)	51	77
1	G	158/196 (81%)	156 (99%)	2 (1%)	61	82
1	H	156/196 (80%)	155 (99%)	1 (1%)	78	91
1	I	150/196 (76%)	149 (99%)	1 (1%)	76	89
All	All	1451/1764 (82%)	1431 (99%)	20 (1%)	59	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	148	VAL
1	A	224	ASN
1	B	67	ASN
1	B	79	LEU
1	B	146	ARG
1	C	140	THR
1	D	117	LEU
1	D	218	LEU
1	D	243	LYS
1	E	78	THR

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Mol	Chain	Res	Type
1	E	100	ASP
1	E	251	ASP
1	F	76	ILE
1	F	186	ARG
1	F	239	GLN
1	G	76	ILE
1	G	99	ASN
1	H	124	LEU
1	I	243	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	133	ASN
1	A	216	ASN
1	B	67	ASN
1	B	94	ASN
1	B	133	ASN
1	B	187	GLN
1	D	69	ASN
1	E	96	HIS
1	G	187	GLN
1	G	216	ASN
1	H	63	ASN
1	H	99	ASN
1	H	103	GLN
1	H	187	GLN
1	I	99	ASN

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 [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	199/243 (81%)	0.22	7 (3%) 47 42	20, 37, 75, 90	0
1	B	208/243 (85%)	0.31	14 (6%) 24 21	17, 32, 76, 107	0
1	C	203/243 (83%)	0.40	18 (8%) 15 13	18, 35, 78, 94	0
1	D	201/243 (82%)	0.54	25 (12%) 8 6	18, 39, 79, 96	1 (0%)
1	E	190/243 (78%)	0.68	18 (9%) 14 12	25, 50, 83, 94	0
1	F	205/243 (84%)	0.19	11 (5%) 31 27	19, 32, 73, 86	0
1	G	193/243 (79%)	0.70	19 (9%) 13 11	29, 47, 84, 92	0
1	H	193/243 (79%)	1.21	41 (21%) 2 2	32, 62, 98, 109	0
1	I	186/243 (76%)	1.63	58 (31%) 1 1	43, 73, 108, 129	0
All	All	1778/2187 (81%)	0.64	211 (11%) 9 7	17, 44, 92, 129	1 (0%)

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	ASN	8.1
1	C	66	LEU	6.1
1	D	255	ILE	5.4
1	C	252	GLY	5.4
1	F	221	ASP	5.1
1	I	137	GLY	5.0
1	A	68	THR	4.9
1	H	218	LEU	4.9
1	H	220	PHE	4.8
1	B	226	GLY	4.6
1	D	223	SER	4.6
1	G	222	LYS	4.6
1	E	37	PHE	4.6
1	I	226	GLY	4.5
1	C	65	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	252	GLY	4.5
1	I	252	GLY	4.5
1	I	218	LEU	4.5
1	H	252	GLY	4.3
1	A	75	GLU	4.3
1	H	76	ILE	4.2
1	C	102	ASP	4.2
1	D	218	LEU	4.1
1	A	37	PHE	4.1
1	H	103	GLN	4.0
1	H	244	ILE	4.0
1	H	102	ASP	4.0
1	I	124	LEU	4.0
1	C	74	LEU	4.0
1	I	219	SER	3.9
1	E	223	SER	3.9
1	I	193	ASP	3.8
1	I	177	GLY	3.8
1	H	63	ASN	3.7
1	H	78	THR	3.7
1	I	39	SER	3.7
1	B	66	LEU	3.6
1	I	79	LEU	3.6
1	G	76	ILE	3.6
1	I	119	VAL	3.5
1	I	118	LEU	3.5
1	C	221	ASP	3.4
1	H	96	HIS	3.4
1	D	220	PHE	3.3
1	I	90	TYR	3.3
1	H	118	LEU	3.3
1	E	134	ALA	3.3
1	I	92	ILE	3.3
1	I	88	ARG	3.3
1	H	106	VAL	3.3
1	I	117	LEU	3.3
1	I	130	LEU	3.3
1	I	139	PRO	3.3
1	B	67	ASN	3.2
1	G	220	PHE	3.2
1	I	189	PHE	3.2
1	H	221	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	219	SER	3.2
1	I	76	ILE	3.2
1	G	100	ASP	3.1
1	D	70	SER	3.1
1	E	86	ASP	3.1
1	H	124	LEU	3.1
1	C	78	THR	3.1
1	H	135	THR	3.1
1	D	86	ASP	3.1
1	H	249	ILE	3.1
1	H	222	LYS	3.0
1	E	146	ARG	3.0
1	E	65	GLY	3.0
1	I	138	LEU	3.0
1	C	251	ASP	3.0
1	I	102	ASP	3.0
1	I	244	ILE	2.9
1	I	220	PHE	2.9
1	C	226	GLY	2.9
1	D	71	HIS	2.9
1	E	117	LEU	2.9
1	G	126	ASP	2.9
1	B	220	PHE	2.9
1	I	136	GLY	2.9
1	F	75	GLU	2.8
1	F	65	GLY	2.8
1	D	69	ASN	2.8
1	C	79	LEU	2.8
1	D	252	GLY	2.8
1	H	219	SER	2.8
1	I	133	ASN	2.8
1	H	116	ALA	2.8
1	E	135	THR	2.7
1	I	89	GLY	2.7
1	H	98	ILE	2.7
1	G	219	SER	2.7
1	G	217	THR	2.7
1	I	247	LYS	2.7
1	H	115	GLU	2.7
1	A	252	GLY	2.7
1	E	89	GLY	2.7
1	D	179	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	68	THR	2.7
1	I	125	THR	2.7
1	H	198	HIS	2.7
1	H	226	GLY	2.6
1	D	143	ILE	2.6
1	F	220	PHE	2.6
1	D	102	ASP	2.6
1	E	118	LEU	2.6
1	I	134	ALA	2.6
1	I	190	LEU	2.6
1	H	99	ASN	2.6
1	I	78	THR	2.6
1	G	250	ARG	2.6
1	H	100	ASP	2.6
1	G	75	GLU	2.6
1	I	248	LEU	2.6
1	E	119	VAL	2.6
1	E	133	ASN	2.6
1	E	188	ASN	2.6
1	I	87	GLN	2.6
1	D	228	THR	2.6
1	G	125	THR	2.6
1	H	228	THR	2.6
1	I	242	THR	2.6
1	C	76	ILE	2.5
1	I	123	SER	2.5
1	D	222	LYS	2.5
1	I	135	THR	2.5
1	B	41	ASP	2.5
1	I	93	THR	2.5
1	C	136	GLY	2.5
1	I	240	LEU	2.5
1	H	189	PHE	2.5
1	B	69	ASN	2.5
1	E	124	LEU	2.4
1	C	73	GLN	2.4
1	G	135	THR	2.4
1	I	128	ALA	2.4
1	I	91	ILE	2.4
1	H	79	LEU	2.4
1	E	247	LYS	2.4
1	F	78	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	73	GLN	2.4
1	C	220	PHE	2.4
1	I	129	VAL	2.4
1	F	67	ASN	2.4
1	I	107	ALA	2.4
1	B	79	LEU	2.3
1	G	79	LEU	2.3
1	H	117	LEU	2.3
1	I	241	ALA	2.3
1	D	74	LEU	2.3
1	I	246	ASP	2.3
1	G	188	ASN	2.3
1	H	217	THR	2.3
1	I	127	LEU	2.3
1	I	114	PHE	2.3
1	H	97	VAL	2.3
1	H	125	THR	2.3
1	D	219	SER	2.3
1	H	248	LEU	2.3
1	C	86	ASP	2.3
1	B	136	GLY	2.2
1	H	108	LEU	2.2
1	D	41	ASP	2.2
1	G	63	ASN	2.2
1	D	136	GLY	2.2
1	E	222	LYS	2.2
1	D	221	ASP	2.2
1	H	227	GLU	2.2
1	E	90	TYR	2.2
1	F	79	LEU	2.2
1	D	76	ILE	2.2
1	I	143	ILE	2.2
1	G	86	ASP	2.2
1	I	110	ASP	2.2
1	I	251	ASP	2.2
1	H	77	ARG	2.2
1	F	222	LYS	2.2
1	I	40	THR	2.2
1	E	248	LEU	2.2
1	I	98	ILE	2.2
1	B	221	ASP	2.2
1	G	247	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	188	ASN	2.1
1	F	72	ASN	2.1
1	G	124	LEU	2.1
1	F	77	ARG	2.1
1	A	222	LYS	2.1
1	B	179	ILE	2.1
1	H	110	ASP	2.1
1	F	226	GLY	2.1
1	I	217	THR	2.1
1	I	146	ARG	2.1
1	B	227	GLU	2.1
1	G	102	ASP	2.1
1	G	123	SER	2.1
1	I	221	ASP	2.1
1	I	243	LYS	2.1
1	H	121	SER	2.1
1	D	65	GLY	2.1
1	I	42	GLU	2.1
1	D	78	THR	2.0
1	A	110	ASP	2.0
1	D	251	ASP	2.0
1	H	109	GLN	2.0
1	H	54	ALA	2.0
1	C	68	THR	2.0
1	C	143	ILE	2.0
1	I	249	ILE	2.0
1	B	96	HIS	2.0
1	H	123	SER	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.