



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:22 AM GMT

PDB ID : 2QF0
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

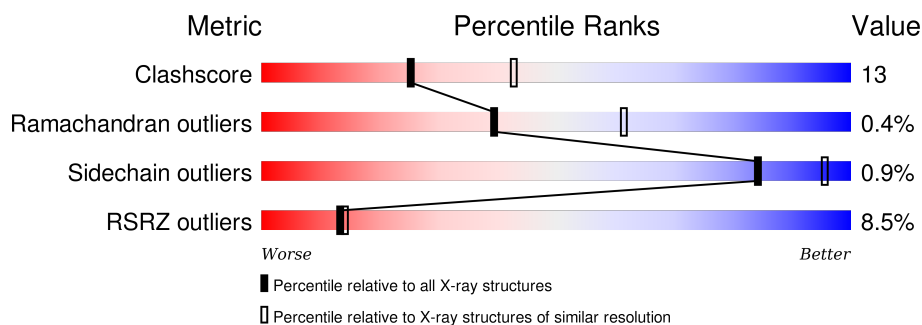
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>4%</div> <div>71%12%17%</div> </div>
1	B	243	<div> <div>3%</div> <div>70%16%13%</div> </div>
1	C	243	<div> <div>6%</div> <div>69%16%15%</div> </div>
1	D	243	<div> <div>5%</div> <div>66%18%16%</div> </div>
1	E	243	<div> <div>7%</div> <div>61%18%21%</div> </div>
1	F	243	<div> <div>3%</div> <div>69%16%14%</div> </div>
1	G	243	<div> <div>4%</div> <div>59%21%19%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	243	<div><div></div><div>14%</div><div>52%</div><div>28%</div><div>19%</div></div>
1	I	243	<div><div></div><div>17%</div><div>47%</div><div>30%</div><div>•</div><div>22%</div></div>

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

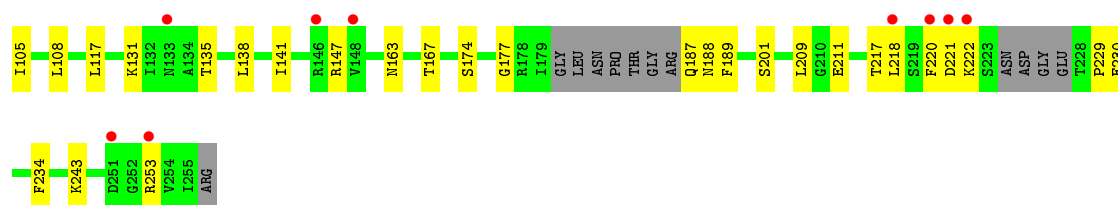
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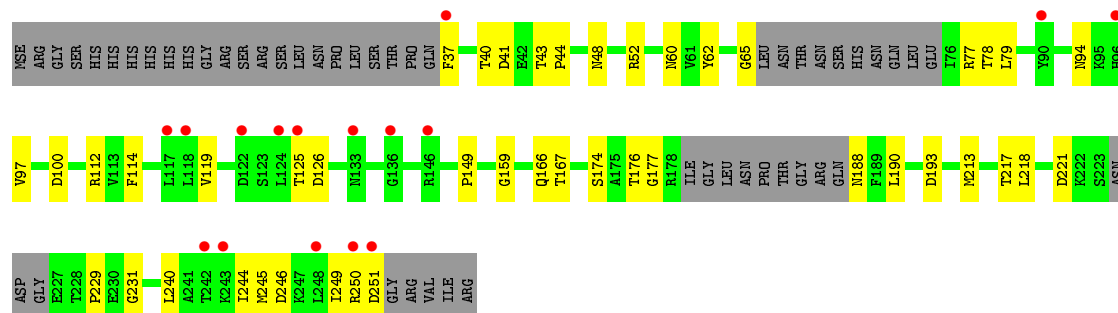
Chain	Residue	Modelled	Actual	Comment	Reference
I	23	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	24	GLY	-	EXPRESSION TAG	UNP P0AEE3
I	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
I	26	SER	-	EXPRESSION TAG	UNP P0AEE3
I	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
I	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
I	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3

- Molecule 2 is water.

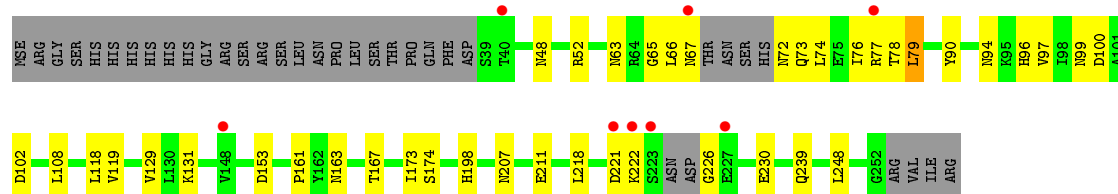
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	70	Total O 70 70	0	0
2	C	63	Total O 63 63	0	0
2	D	48	Total O 48 48	0	0
2	E	39	Total O 39 39	0	0
2	F	70	Total O 70 70	0	0
2	G	30	Total O 30 30	0	0
2	H	21	Total O 21 21	0	0
2	I	14	Total O 14 14	0	0



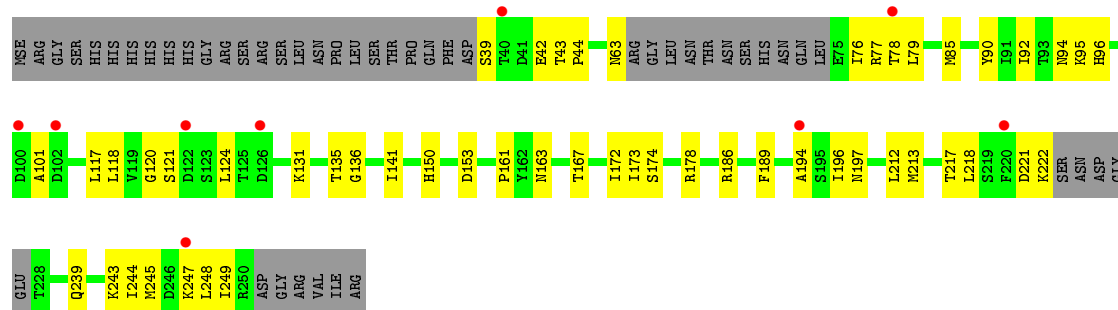
• Molecule 1: Protease degS



• Molecule 1: Protease degS

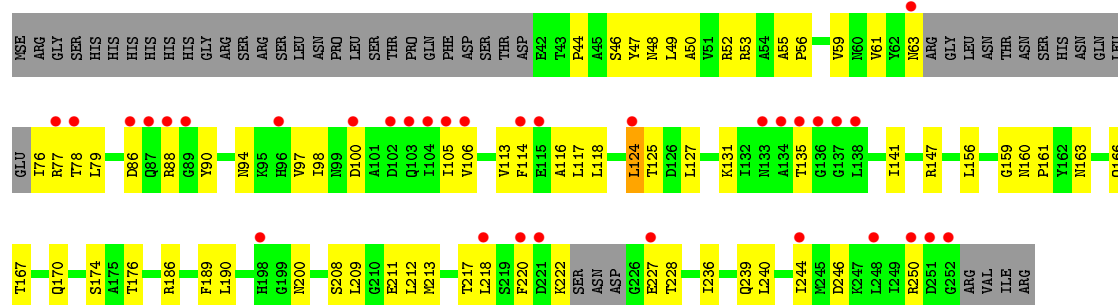


• Molecule 1: Protease degS

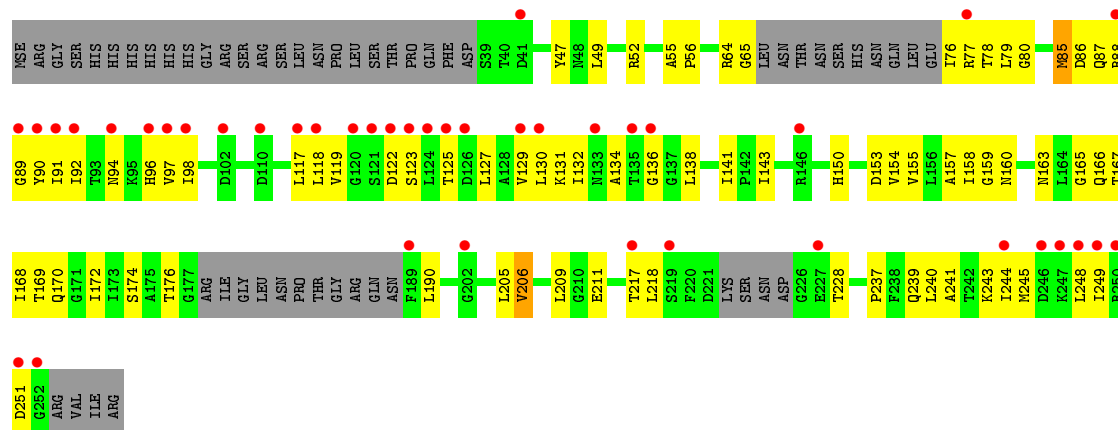


• Molecule 1: Protease degS





• 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 47.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.0 (42.53-2.50) 93.8 (47.82-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.257 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 76039 reflections (0.003%)	Xtriage
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

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % 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 1.5181e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1522	0.66	0/2061
1	B	0.40	0/1585	0.69	1/2147 (0.0%)
1	C	0.36	0/1548	0.66	0/2096
1	D	0.36	0/1544	0.64	0/2091
1	E	0.33	0/1456	0.62	0/1970
1	F	0.38	0/1562	0.68	1/2115 (0.0%)
1	G	0.33	0/1475	0.61	0/1999
1	H	0.31	0/1470	0.59	0/1991
1	I	0.29	0/1410	0.55	0/1909
All	All	0.35	0/13572	0.63	2/18379 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	79	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	136	GLY	N-CA-C	5.07	125.78	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1507	0	1515	18	0
1	B	1570	0	1588	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1533	0	1560	31	0
1	D	1529	0	1558	39	0
1	E	1442	0	1460	27	0
1	F	1547	0	1571	38	0
1	G	1460	0	1492	36	0
1	H	1455	0	1486	67	0
1	I	1397	0	1416	71	0
2	A	57	0	0	1	0
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	341	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 (341) 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:I:49:LEU:HA	1:I:52:ARG:NH1	1.99	0.76
1:C:217:THR:HG22	1:C:218:LEU:H	1.50	0.76
1:G:186:ARG:HG3	1:G:189:PHE:CE2	2.22	0.73
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: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:O	1:E:240:LEU:HD23	1.90	0.71
1:H:77:ARG:HB2	1:H:77:ARG:NH1	2.05	0.71
1:C:67:ASN:H	1:C:77:ARG:HH21	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:96:HIS:NE2	1:F:218:LEU:HG	2.07	0.69
1:E:48:ASN:OD1	1:E:52:ARG:HD3	1.91	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
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:I:245:MSE:O	1:I:249:ILE:HG13	1.94	0.66
1:E:245:MSE:O	1:E:249:ILE:HG13	1.96	0.66
1:F:76:ILE:H	1:F:76:ILE:HD12	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: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:I:243:LYS:HB2	1:I:243:LYS:NZ	2.17	0.60
1:H:222:LYS:HG2	1:H:222:LYS:O	2.00	0.60
1:I:158:ILE:HG12	1:I:168:ILE:HD12	1.84	0.60
1:A:220:PHE:CZ	1:A:222:LYS:HB2	2.36	0.60
1:H:213:MSE:HE2	1:H:213:MSE:HA	1.84	0.59
1:G:217:THR:HG22	1:G:218:LEU:H	1.68	0.59
1:B:250:ARG:HG3	1:B:251:ASP:OD2	2.03	0.59
1:B:96:HIS:ND1	1:B:218:LEU:HD11	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:217:THR:HG22	1:G:218:LEU:N	2.20	0.56
1:G:135:THR:HG22	1:G:136:GLY: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:98:ILE:C	1:H:100:ASP:H	2.08	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:H:124:LEU:HD23	1:H:124:LEU:O	2.06	0.56
1:G:95:LYS:HD2	1:G:121:SER:HB3	1.87	0.56
1:B:213:MSE:HA	1:B:213:MSE:HE2	1.89	0.55
1:I:239:GLN:C	1:I:241:ALA:H	2.10	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:B:239:GLN:H	1:B:239:GLN:CD	2.09	0.55
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:N	1:D:108:LEU:HD12	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:A:157:ALA:HB3	1:A:169:THR:OG1	2.08	0.53
1:H:228:THR:O	1:H:228:THR:HG23	2.09	0.53
1:H:160:ASN:ND2	1:H:163:ASN:HA	2.23	0.53
1:H:49:LEU:HD21	1:H:53:ARG:NH2	2.24	0.53
1:I:159:GLY:O	1:I:166:GLN:HA	2.09	0.53
1:G:221:ASP:O	1:G:222:LYS:HB2	2.08	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:D:187:GLN:HB2	1:D:189:PHE:HE1	1.69	0.52
1:A:212:LEU:O	1:A:213:MSE:HE2	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:47:TYR:CE2	1:I:154:VAL:HG11	2.45	0.52
1:G:124:LEU:HD23	1:G:124:LEU:O	2.09	0.52
1:F:222:LYS:HE3	1:F:226:GLY:HA2	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:E:167:THR:HG23	1:F:174:SER:HB3	1.92	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: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:A:167:THR:HG23	1:B:174:SER:HB3	1.92	0.51
1:B:67:ASN:CG	1:B:68:THR:H	2.14	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:I:65:GLY:HA3	1:I:77:ARG:CD	2.40	0.51
1:I:55:ALA:HB3	1:I:56:PRO:HD3	1.93	0.51
1:B:223:SER:HB3	1:B:226:GLY:N	2.25	0.51
1:D:147:ARG:NH1	1:D:209:LEU:HD12	2.26	0.50
1:D:54:ALA:HB1	1:D:141:ILE:HD11	1.93	0.50
1:B:240:LEU:O	1:B:244:ILE:HG12	2.12	0.50
1:I:94:ASN:HB2	1:I:97:VAL:HG23	1.94	0.50
1:H:76:ILE:HG13	1:H:77:ARG:H	1.76	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:94:ASN:HB2	1:H:97:VAL:CG2	2.42	0.50
1:F:76:ILE:H	1:F:76:ILE:CD1	2.23	0.50
1:B:48:ASN:OD1	1:B:52:ARG:HD3	2.12	0.50
1:I:86:ASP:C	1:I:88:ARG:H	2.14	0.50
1:D:243:LYS:HB2	1:D:243:LYS:HZ3	1.75	0.50
1:F:65:GLY:HA3	1:F:77:ARG:HH11	1.77	0.50
1:B:85:MSE:HE2	1:B:92:ILE:HD12	1.93	0.50
1:C:65:GLY:HA2	1:C:102:ASP:OD2	2.12	0.50
1:H:117:LEU:CD2	1:H:131:LYS:HB3	2.42	0.49
1:F:67:ASN:O	1:F:72:ASN:HB2	2.12	0.49
1:D:221:ASP:O	1:D:222:LYS:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:HD11	1:D:105:ILE:HD11	1.93	0.49
1:B:64:ARG:NH2	1:B:103:GLN:OE1	2.41	0.49
1:D:217:THR:C	1:D:218:LEU:HD22	2.32	0.49
1:G:63:ASN:OD1	1:G:77:ARG:HD2	2.12	0.49
1:G:39:SER:HB2	1:G:42:GLU:OE2	2.13	0.49
1:B:76:ILE:N	1:B:76:ILE:HD12	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:176:THR:HG22	1:A:190:LEU:HD22	1.94	0.48
1:I:118:LEU:HD23	1:I:118:LEU:C	2.34	0.48
1:A:85:MSE:HE2	1:A:92:ILE:HD12	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:H:239:GLN:CD	1:H:239:GLN:H	2.17	0.48
1:I:87:GLN:C	1:I:89:GLY:H	2.16	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:E:217:THR:O	1:E:218:LEU:HD23	2.13	0.48
1:H:227:GLU:CD	1:H:227:GLU:H	2.17	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:H:79:LEU:HD21	1:H:163:ASN:HB2	1.96	0.48
1:F:221:ASP:O	1:F:222:LYS:HB2	2.13	0.48
1:F:77:ARG:NH1	1:F:100:ASP:O	2.47	0.48
1:I:157:ALA:HB3	1:I:169:THR:OG1	2.14	0.48
1:H:63:ASN:HD22	1:H:78:THR:H	1.61	0.48
1:E:176:THR:HG22	1:E:190:LEU:CD2	2.44	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:205:LEU:HG	1:I:205:LEU:O	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:B:118:LEU:HD13	1:B:118:LEU:C	2.34	0.47
1:F:94:ASN:HB3	1:F:96:HIS:CE1	2.49	0.47
1:I:158:ILE:HG23	1:I:168:ILE:CD1	2.44	0.47
1:I:78:THR:HG22	1:I:79:LEU:N	2.29	0.47
1:H:159:GLY:O	1:H:166:GLN:HA	2.15	0.47
1:A:96:HIS:HA	1:A:99:ASN:ND2	2.29	0.47
1:H:105:ILE:HD11	1:H:113:VAL:CG1	2.44	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:I:64:ARG:HA	1:I:76:ILE:HA	1.95	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:I:90:TYR:HE1	1:I:249:ILE:HG12	1.80	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:E:246:ASP:O	1:E:250:ARG:HG2	2.16	0.47
1:H:94:ASN:HB2	1:H:97:VAL:HG23	1.97	0.47
1:F:65:GLY:HA3	1:F:77:ARG:HD3	1.97	0.47
1:F:63:ASN:HB3	1:F:78:THR:HB	1.97	0.46
1:D:217:THR:HG22	1:D:218:LEU:HD23	1.98	0.46
1:F:79:LEU:HD11	1:F:163:ASN:CB	2.39	0.46
1:C:213:MSE:HA	1:C:213:MSE:HE2	1.98	0.46
1:C:219:SER:HA	2:C:282:HOH:O	2.15	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:C:67:ASN:O	1:C:68:THR:C	2.53	0.46
1:H:161:PRO:HG3	1:H:200:ASN:OD1	2.15	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:I:122:ASP:CG	1:I:123:SER:N	2.69	0.46
1:H:63:ASN:HD21	1:H:78:THR:HB	1.81	0.46
1:H:47:TYR:HB3	1:H:156:LEU:HD11	1.97	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:HD22	1:F:66:LEU:N	2.31	0.45
1:B:67:ASN:N	1:B:67:ASN:ND2	2.64	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:C:181:LEU:HD11	1:D:105:ILE:CD1	2.46	0.45
1:C:51:VAL:HG13	1:C:168:ILE:CD1	2.47	0.45
1:H:77:ARG:CB	1:H:77:ARG:HH11	2.29	0.45
1:F:76:ILE:N	1:F:76:ILE:CD1	2.77	0.45
1:I:85:MSE:HE2	1:I:92:ILE:CD1	2.45	0.45
1:I:79:LEU:CD2	1:I:163:ASN:HB2	2.46	0.45
1:A:94:ASN:OD1	1:A:201:SER:HB3	2.17	0.45
1:I:76:ILE:O	1:I:76:ILE:HG23	2.17	0.45
1:D:253:ARG:HG2	2:D:280:HOH:O	2.17	0.45
1:G:96:HIS:CD2	1:G:218:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:ARG:NH1	1:I:165:GLY:HA3	2.32	0.45
1:H:98:ILE:HD12	1:H:118:LEU:HD23	1.98	0.45
1:I:86:ASP:C	1:I:88:ARG:N	2.70	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:I:239:GLN:HG3	1:I:240:LEU:N	2.32	0.45
1:E:119:VAL:HG12	1:E:119:VAL:O	2.16	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: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:D:220:PHE:HB2	1:D:234:PHE:HE1	1.83	0.44
1:H:79:LEU:CD2	1:H:163:ASN:HB2	2.48	0.44
1:C:189:PHE:HE1	1:C:236:ILE:HD13	1.82	0.44
1:D:68:THR:C	1:D:70:SER:H	2.21	0.44
1:I:153:ASP:O	1:I:155:VAL:HG13	2.17	0.44
1:E:193:ASP:HA	1:E:231:GLY:O	2.18	0.44
1:E:43:THR:HA	1:E:44:PRO:HD3	1.89	0.44
1:I:87:GLN:C	1:I:89:GLY:N	2.71	0.44
1:H:170:GLN:HB2	1:I:172:ILE:HD13	1.99	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:E:250:ARG:NH1	1:E:250:ARG:HG3	2.30	0.44
1:I:158:ILE:HG12	1:I:168:ILE:CD1	2.47	0.44
1:C:184:THR:HA	1:D:135:THR:HG22	2.00	0.44
1:I:217:THR:HG22	1:I:218:LEU:HG	1.99	0.44
1:H:160:ASN:HD21	1:H:163:ASN:HA	1.82	0.43
1:G:85:MSE:HE2	1:G:92:ILE:HD12	1.98	0.43
1:I:239:GLN:C	1:I:241:ALA:N	2.71	0.43
1:I:125:THR:O	1:I:127:LEU:HG	2.19	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:158:ILE:HG23	1:I:168:ILE:HD13	1.98	0.43
1:D:79:LEU:CD2	1:D:163:ASN:HB2	2.49	0.43
1:I:98:ILE:C	1:I:98:ILE:HD12	2.38	0.43
1:G:117:LEU:N	1:G:117:LEU:HD22	2.33	0.43
1:A:133:ASN:ND2	2:A:301:HOH:O	2.44	0.43
1:F:67:ASN:HB3	1:F:72:ASN:CB	2.49	0.43
1:E:159:GLY:O	1:E:166:GLN:HA	2.18	0.43
1:G:79:LEU:CD2	1:G:163:ASN:HB2	2.46	0.43
1:E:221:ASP:HA	1:E:229:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:VAL:HG23	1:F:248:LEU:HD12	2.00	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:F:108:LEU:N	1:F:108:LEU:HD12	2.34	0.43
1:E:40:THR:HG23	1:E:41:ASP:N	2.33	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:HG23	1:H:141:ILE:O	2.19	0.43
1:F:221:ASP:OD1	1:F:221:ASP:O	2.37	0.43
1:F:119:VAL:O	1:F:119:VAL:HG12	2.19	0.43
1:B:201:SER:OG	1:B:218:LEU:HD23	2.19	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:F:94:ASN:HB2	1:F:97:VAL:HG23	2.00	0.42
1:D:108:LEU:N	1:D:108:LEU:CD1	2.82	0.42
1:I:79:LEU:HD12	1:I:80:GLY:H	1.85	0.42
1:F:48:ASN:OD1	1:F:52:ARG:HD3	2.18	0.42
1:H:176:THR:HG22	1:H:190:LEU:CD2	2.50	0.42
1:H:44:PRO:HG3	1:I:209:LEU:HD12	2.01	0.42
1:C:94:ASN:HB3	1:C:96:HIS:CE1	2.55	0.42
1:H:90:TYR:CE2	1:H:131:LYS:HD3	2.54	0.42
1:H:227:GLU:CD	1:H:227:GLU:N	2.72	0.42
1:E:60:ASN:HB3	1:E:62:TYR:CE1	2.54	0.42
1:A:67:ASN:O	1:A:68:THR:HB	2.19	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:G:213:MSE:HA	1:G:213:MSE:HE2	2.02	0.42
1:F:153:ASP:HB2	1:F:173:ILE:HD12	2.02	0.42
1:F:207:ASN:ND2	1:F:211:GLU:HB2	2.34	0.42
1:D:177:GLY:HA2	1:D:188:ASN:OD1	2.20	0.42
1:C:96:HIS:NE2	1:C:218:LEU:HG	2.35	0.41
1:I:122:ASP:CG	1:I:123:SER:H	2.24	0.41
1:G:150:HIS:HB2	1:G:153:ASP:OD1	2.19	0.41
1:F:207:ASN:HD21	1:F:211:GLU:HB2	1.85	0.41
1:E:79:LEU:C	1:E:79:LEU:HD12	2.40	0.41
1:I:88:ARG:O	1:I:131:LYS:HE2	2.20	0.41
1:G:43:THR:HA	1:G:44:PRO:HD3	1.82	0.41
1:F:90:TYR:CE2	1:F:131:LYS:HD3	2.55	0.41
1:G:141:ILE:HG23	1:G:141:ILE:O	2.20	0.41
1:A:66:LEU:O	1:A:77:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:HIS:NE2	1:C:218:LEU:CD2	2.83	0.41
1:H:98:ILE:C	1:H:100:ASP:N	2.72	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:E:177:GLY:HA2	1:E:188:ASN:CG	2.40	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:D:79:LEU:C	1:D:79:LEU:HD12	2.41	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:H:98:ILE:CD1	1:H:118:LEU:HD23	2.51	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:H:147:ARG:NH1	1:H:209:LEU:HD12	2.36	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:D:62:TYR:HB2	1:D:105:ILE:HB	2.03	0.41
1:D:90:TYR:CE2	1:D:131:LYS:HD2	2.56	0.41
1:D:87:GLN:NE2	1:D:138:LEU:O	2.51	0.41
1:H:50:ALA:HB2	1:H:208:SER:O	2.20	0.41
1:I:237:PRO:HB2	1:I:239:GLN:HG2	2.02	0.41
1:H:63:ASN:ND2	1:H:78:THR:HB	2.36	0.41
1:D:98:ILE:HD12	1:D:98:ILE:C	2.41	0.41
1:D:218:LEU:HA	1:D:218:LEU:HD13	1.94	0.40
1:H:240:LEU:HD23	1:H:240:LEU:C	2.40	0.40
1:I:91:ILE:O	1:I:129:VAL:HA	2.21	0.40
1:I:90:TYR:CD2	1:I:90:TYR:N	2.89	0.40
1:I:217:THR:HG22	1:I:218:LEU:N	2.37	0.40
1:F:161:PRO:HA	1:F:198:HIS:O	2.21	0.40
1:H:240:LEU:O	1:H:244:ILE:HG12	2.21	0.40
1:F:118:LEU:HD13	1:F:118:LEU:C	2.42	0.40
1:H:114:PHE:HE1	1:H:135:THR:HG23	1.86	0.40
1:B:85:MSE:HG3	1:B:92:ILE:HG13	2.02	0.40
1:H:159:GLY:C	1:H:161:PRO:HD3	2.42	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%)	19	34
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%)	6	9
All	All	1747/2187 (80%)	1645 (94%)	95 (5%)	7 (0%)	39	61

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
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%)	161 (99%)	2 (1%)	78	93
1	B	170/196 (87%)	168 (99%)	2 (1%)	78	93
1	C	165/196 (84%)	164 (99%)	1 (1%)	90	97
1	D	166/196 (85%)	165 (99%)	1 (1%)	90	97
1	E	156/196 (80%)	152 (97%)	4 (3%)	54	81
1	F	167/196 (85%)	166 (99%)	1 (1%)	90	97
1	G	158/196 (81%)	157 (99%)	1 (1%)	90	97
1	H	156/196 (80%)	155 (99%)	1 (1%)	90	97
1	I	150/196 (76%)	150 (100%)	0	100	100
All	All	1451/1764 (82%)	1438 (99%)	13 (1%)	84	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	224	ASN
1	B	67	ASN
1	B	201	SER
1	C	140	THR
1	D	117	LEU
1	E	37	PHE
1	E	78	THR
1	E	100	ASP
1	E	251	ASP
1	F	239	GLN
1	G	76	ILE
1	H	124	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	150	HIS
1	B	67	ASN
1	B	94	ASN
1	D	69	ASN
1	G	170	GLN
1	G	198	HIS
1	H	63	ASN

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Mol	Chain	Res	Type
1	H	170	GLN
1	I	99	ASN
1	I	170	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	199/243 (81%)	0.30	9 (4%) 37 42	20, 37, 75, 90	0
1	B	208/243 (85%)	0.37	8 (3%) 44 49	17, 32, 76, 107	0
1	C	203/243 (83%)	0.41	14 (6%) 20 22	18, 35, 78, 94	0
1	D	201/243 (82%)	0.38	13 (6%) 22 25	20, 39, 79, 96	1 (0%)
1	E	190/243 (78%)	0.52	16 (8%) 14 14	25, 50, 83, 94	0
1	F	205/243 (84%)	0.21	8 (3%) 43 48	19, 32, 73, 86	0
1	G	193/243 (79%)	0.46	9 (4%) 35 40	29, 47, 84, 92	0
1	H	193/243 (79%)	0.88	33 (17%) 2 2	32, 62, 98, 109	0
1	I	186/243 (76%)	1.28	41 (22%) 1 1	43, 73, 108, 129	0
All	All	1778/2187 (81%)	0.53	151 (8%) 13 14	17, 44, 92, 129	1 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	244	ILE	8.2
1	I	252	GLY	7.7
1	H	135	THR	7.6
1	C	66	LEU	6.9
1	I	251	ASP	5.9
1	B	66	LEU	5.7
1	H	103	GLN	5.7
1	I	124	LEU	5.7
1	I	117	LEU	5.5
1	I	125	THR	5.4
1	I	248	LEU	5.3
1	A	36	GLN	5.3
1	H	220	PHE	5.3
1	I	90	TYR	5.1
1	H	102	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	H	134	ALA	4.9
1	C	74	LEU	4.8
1	G	100	ASP	4.7
1	F	221	ASP	4.6
1	I	120	GLY	4.6
1	H	252	GLY	4.5
1	I	130	LEU	4.5
1	I	123	SER	4.5
1	B	252	GLY	4.5
1	A	75	GLU	4.4
1	I	88	ARG	4.3
1	H	77	ARG	4.3
1	I	136	GLY	4.3
1	H	115	GLU	4.2
1	H	63	ASN	4.2
1	A	225	ASP	4.2
1	I	122	ASP	4.1
1	I	219	SER	4.1
1	B	69	ASN	4.1
1	D	69	ASN	4.1
1	I	217	THR	4.0
1	C	65	GLY	4.0
1	D	222	LYS	3.9
1	H	100	ASP	3.9
1	B	68	THR	3.9
1	I	89	GLY	3.8
1	I	146	ARG	3.8
1	I	102	ASP	3.7
1	B	38	ASP	3.7
1	H	138	LEU	3.7
1	A	37	PHE	3.6
1	I	94	ASN	3.6
1	I	189	PHE	3.6
1	I	126	ASP	3.6
1	B	67	ASN	3.5
1	H	78	THR	3.4
1	H	133	ASN	3.4
1	D	251	ASP	3.2
1	H	198	HIS	3.2
1	I	135	THR	3.2
1	H	251	ASP	3.2
1	H	96	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	244	ILE	3.1
1	C	250	ARG	3.1
1	E	124	LEU	3.1
1	C	221	ASP	3.1
1	H	137	GLY	3.1
1	D	70	SER	3.0
1	I	249	ILE	3.0
1	E	133	ASN	2.9
1	G	40	THR	2.9
1	E	146	ARG	2.9
1	C	251	ASP	2.9
1	H	105	ILE	2.9
1	E	117	LEU	2.9
1	E	248	LEU	2.9
1	H	136	GLY	2.9
1	I	247	LYS	2.8
1	D	133	ASN	2.8
1	C	102	ASP	2.7
1	C	67	ASN	2.7
1	H	221	ASP	2.7
1	I	118	LEU	2.7
1	H	114	PHE	2.7
1	H	87	GLN	2.6
1	C	120	GLY	2.6
1	E	37	PHE	2.6
1	D	221	ASP	2.6
1	F	67	ASN	2.6
1	C	78	THR	2.6
1	G	102	ASP	2.6
1	F	77	ARG	2.5
1	I	129	VAL	2.5
1	D	77	ARG	2.5
1	H	104	ILE	2.5
1	E	250	ARG	2.5
1	B	41	ASP	2.4
1	E	96	HIS	2.4
1	I	77	ARG	2.4
1	H	106	VAL	2.4
1	H	248	LEU	2.4
1	G	126	ASP	2.4
1	I	96	HIS	2.4
1	G	247	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	220	PHE	2.4
1	H	89	GLY	2.4
1	E	118	LEU	2.4
1	H	227	GLU	2.4
1	D	253	ARG	2.4
1	A	96	HIS	2.4
1	I	246	ASP	2.3
1	F	223	SER	2.3
1	H	88	ARG	2.3
1	I	133	ASN	2.3
1	C	136	GLY	2.3
1	G	122	ASP	2.3
1	H	250	ARG	2.3
1	G	78	THR	2.3
1	H	218	LEU	2.2
1	I	41	ASP	2.2
1	C	219	SER	2.2
1	E	125	THR	2.2
1	I	97	VAL	2.2
1	I	121	SER	2.2
1	F	148	VAL	2.2
1	G	194	ALA	2.2
1	H	86	ASP	2.2
1	E	136	GLY	2.2
1	C	68	THR	2.2
1	F	222	LYS	2.2
1	C	252	GLY	2.1
1	A	188	ASN	2.1
1	I	227	GLU	2.1
1	E	90	TYR	2.1
1	B	40	THR	2.1
1	E	251	ASP	2.1
1	A	67	ASN	2.1
1	F	227	GLU	2.1
1	I	202	GLY	2.1
1	D	148	VAL	2.1
1	I	250	ARG	2.1
1	I	91	ILE	2.1
1	I	98	ILE	2.1
1	D	66	LEU	2.1
1	A	121	SER	2.1
1	D	146	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	243	LYS	2.0
1	I	92	ILE	2.0
1	G	220	PHE	2.0
1	E	122	ASP	2.0
1	D	218	LEU	2.0
1	H	124	LEU	2.0
1	E	242	THR	2.0
1	I	110	ASP	2.0
1	A	68	THR	2.0
1	F	40	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.