Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 02:26 am BST

PDB ID	:	3LH3
Title	:	DFP modified DegS delta PDZ
Authors	:	Sohn, J.; Grant, R.A.; Sauer, R.T.
Deposited on	:	2010-01-21
Resolution	:	2.35 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 following versions of software and data (see references ⓘ) were used in the production of this report:

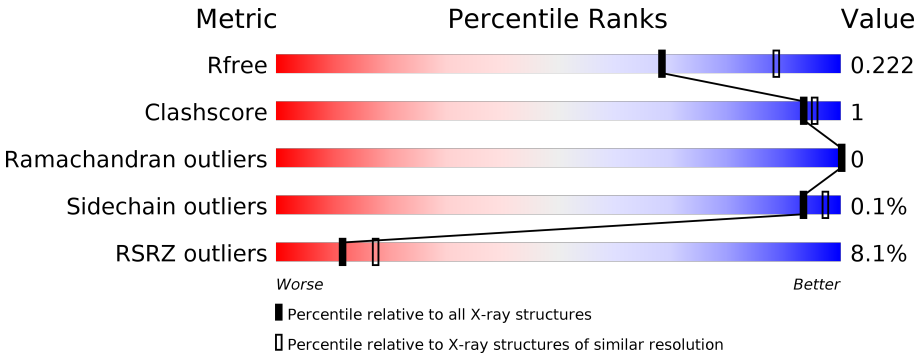
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	5% 82% • 14%
1	B	241	8% 87% • 12%
1	C	241	7% 87% • 11%
1	D	241	6% 84% • 12%
1	E	241	6% 80% • 16%
1	F	241	8% 85% • 12%

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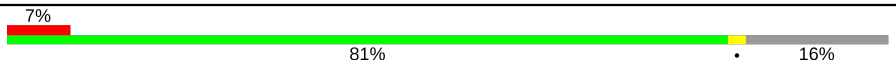
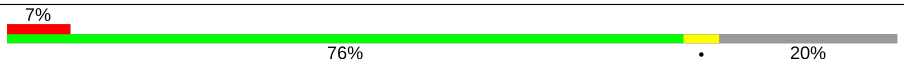
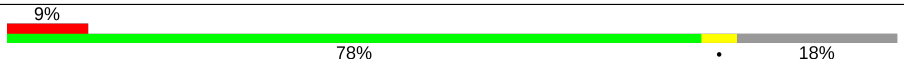
Mol	Chain	Length	Quality of chain
1	G	241	
1	H	241	
1	I	241	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28641 atoms, of which 14016 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	207	Total	C	H	N	O	P	S	0	0	0
			3113	967	1563	276	303	1	3			
1	B	213	Total	C	H	N	O	P	S	0	0	0
			3187	992	1595	285	311	1	3			
1	C	214	Total	C	H	N	O	P	S	0	0	0
			3223	1000	1618	288	313	1	3			
1	D	212	Total	C	H	N	O	P	S	0	0	0
			3203	992	1612	287	308	1	3			
1	E	203	Total	C	H	N	O	P	S	0	0	0
			3056	952	1534	267	299	1	3			
1	F	211	Total	C	H	N	O	P	S	0	0	0
			3180	988	1595	283	310	1	3			
1	G	202	Total	C	H	N	O	P	S	0	0	0
			3053	951	1535	268	295	1	3			
1	H	193	Total	C	H	N	O	P	S	0	0	0
			2898	902	1460	256	276	1	3			
1	I	198	Total	C	H	N	O	P	S	0	0	0
			2992	933	1504	261	290	1	3			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	EXPRESSION TAG	UNP P0AEE3
A	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
A	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
A	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
A	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
A	26	GLY	-	EXPRESSION TAG	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	EXPRESSION TAG	UNP P0AEE3
B	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
B	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
B	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
B	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
B	26	GLY	-	EXPRESSION TAG	UNP P0AEE3
C	16	MET	-	EXPRESSION TAG	UNP P0AEE3
C	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
C	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
C	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
C	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
C	26	GLY	-	EXPRESSION TAG	UNP P0AEE3
D	16	MET	-	EXPRESSION TAG	UNP P0AEE3
D	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
D	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
D	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
D	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
D	26	GLY	-	EXPRESSION TAG	UNP P0AEE3
E	16	MET	-	EXPRESSION TAG	UNP P0AEE3
E	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
E	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
E	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
E	26	GLY	-	EXPRESSION TAG	UNP P0AEE3
F	16	MET	-	EXPRESSION TAG	UNP P0AEE3
F	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
F	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
F	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	26	GLY	-	EXPRESSION TAG	UNP P0AEE3
G	16	MET	-	EXPRESSION TAG	UNP P0AEE3
G	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
G	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
G	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	26	GLY	-	EXPRESSION TAG	UNP P0AEE3
H	16	MET	-	EXPRESSION TAG	UNP P0AEE3
H	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
H	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
H	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	26	GLY	-	EXPRESSION TAG	UNP P0AEE3
I	16	MET	-	EXPRESSION TAG	UNP P0AEE3
I	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
I	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
I	19	SER	-	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	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	25	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	26	GLY	-	EXPRESSION TAG	UNP P0AEE3

- Molecule 2 is water.

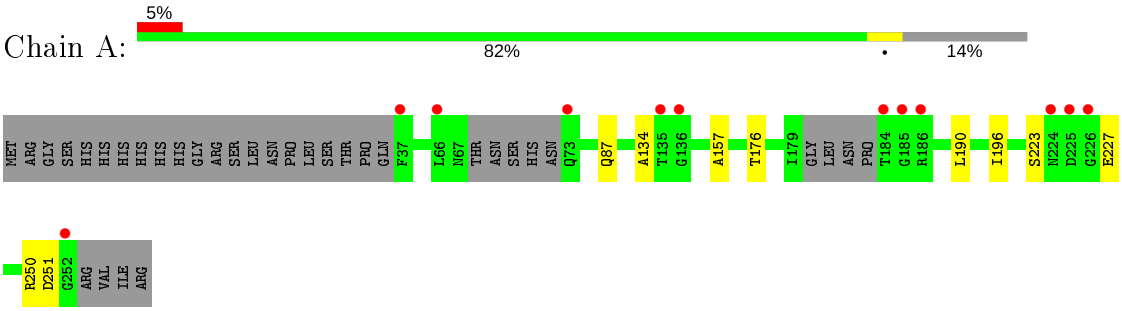
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	103	Total O 103 103	0	0
2	B	121	Total O 121 121	0	0
2	C	103	Total O 103 103	0	0
2	D	81	Total O 81 81	0	0
2	E	71	Total O 71 71	0	0
2	F	86	Total O 86 86	0	0
2	G	66	Total O 66 66	0	0
2	H	59	Total O 59 59	0	0
2	I	46	Total O 46 46	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they 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.

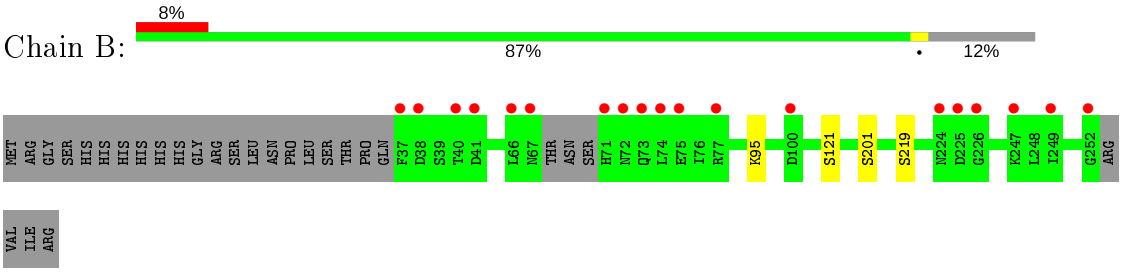
- Molecule 1: Protease degS

Chain A:



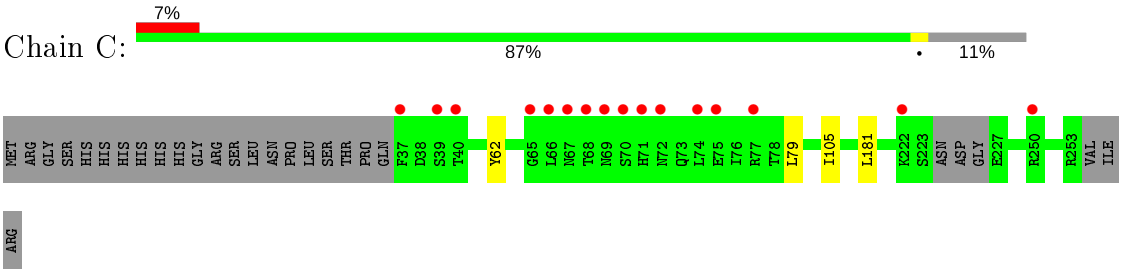
- Molecule 1: Protease degS

Chain B:



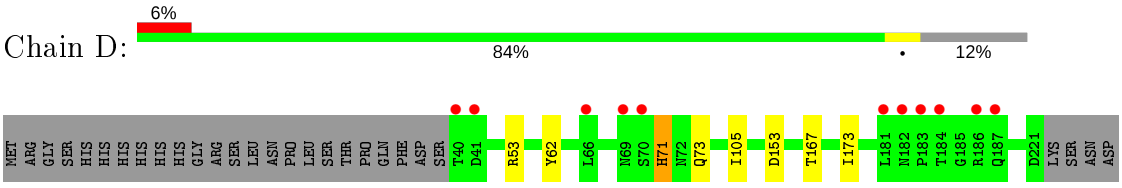
- Molecule 1: Protease degS

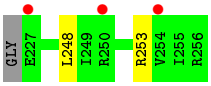
Chain C:



- Molecule 1: Protease degS

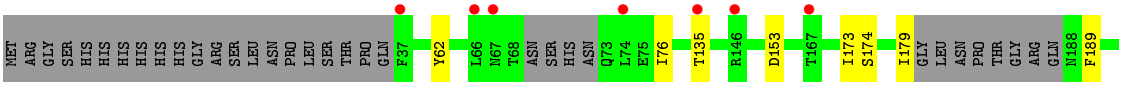
Chain D:

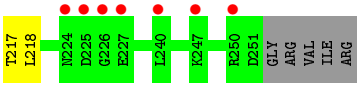




• Molecule 1: Protease degS

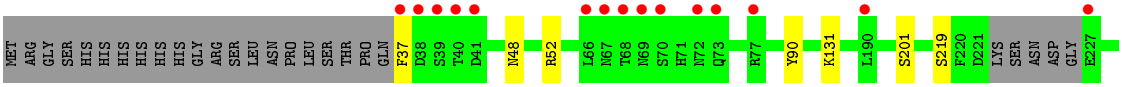
Chain E:

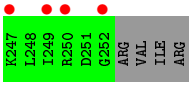




• Molecule 1: Protease degS

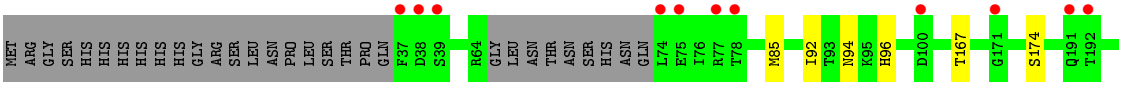
Chain F:

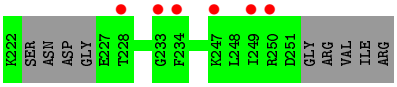




• Molecule 1: Protease degS

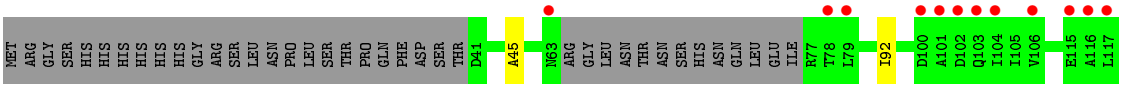
Chain G:

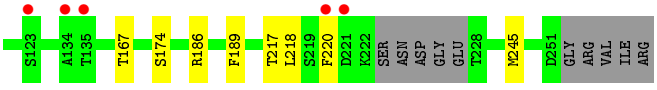




• Molecule 1: Protease degS

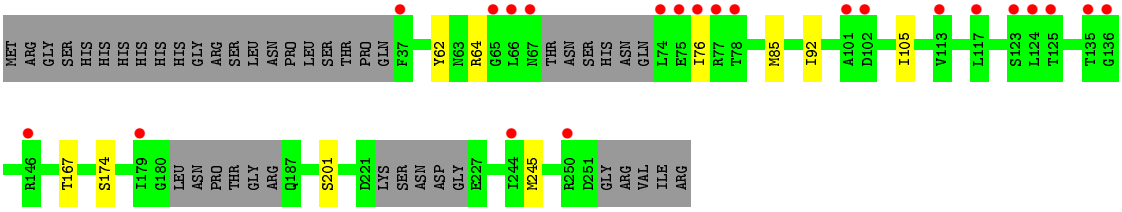
Chain H:





• Molecule 1: Protease degS

Chain I:


MET ARG GLY SER HIS HIS HIS HIS HIS GLY ARG SER LEU ASN PRO LEU SER THR PRO GLN F37 Y62 N63 R64 G65 L66 N67 THR ASN SER HIS ASN GLN L74 E75 I76 R77 T78 M85 I92 A101 D102 I105 V113 L117 S123 L124 T125 T135 G136
R146 T167 S174 I179 G180 LEU ASN PRO THR GLY ARG Q187 S201 D221 LYS SER ASN ASP GLY E227 I244 M245 R250 D251 GLY ARG VAL ILE ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.53Å 132.75Å 231.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.14 – 2.35 37.14 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.0 (37.14-2.35) 91.0 (37.14-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.185 , 0.227 0.180 , 0.222	Depositor DCC
R_{free} test set	4127 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28641	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 38.85 % 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 3.4661e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.28	0/1554	0.48	0/2107
1	B	0.27	0/1599	0.46	0/2172
1	C	0.26	0/1611	0.47	0/2187
1	D	0.26	0/1597	0.47	0/2170
1	E	0.25	0/1526	0.46	0/2071
1	F	0.26	0/1592	0.47	0/2163
1	G	0.26	0/1523	0.47	0/2068
1	H	0.24	0/1442	0.45	0/1959
1	I	0.23	0/1491	0.44	0/2022
All	All	0.26	0/13935	0.47	0/18919

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1550	1563	1563	5	0
1	B	1592	1595	1595	2	0
1	C	1605	1618	1618	4	0
1	D	1591	1612	1612	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1522	1534	1534	6	0
1	F	1585	1595	1595	4	0
1	G	1518	1535	1534	4	0
1	H	1438	1460	1460	6	0
1	I	1488	1504	1504	7	0
2	A	103	0	0	0	0
2	B	121	0	0	0	0
2	C	103	0	0	1	0
2	D	81	0	0	0	0
2	E	71	0	0	0	0
2	F	86	0	0	0	0
2	G	66	0	0	0	0
2	H	59	0	0	0	0
2	I	46	0	0	0	0
All	All	14625	14016	14015	38	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 1.

All (38) 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:181:LEU:HD11	1:D:105:ILE:HD12	1.92	0.52
1:E:217:THR:HG22	1:E:218:LEU:HG	1.90	0.52
1:I:64:ARG:HG2	1:I:76:ILE:HD13	1.94	0.50
1:D:153:ASP:HB2	1:D:173:ILE:HD12	1.94	0.50
1:F:201:MIS:H31	1:F:219:SER:HB2	1.94	0.49
1:D:167:THR:HG23	1:E:174:SER:HB3	1.96	0.48
1:H:167:THR:HG23	1:I:174:SER:HB3	1.95	0.48
1:E:135:THR:HG21	1:H:45:ALA:HA	1.95	0.47
1:H:92:ILE:HD11	1:H:245:MET:HB2	1.96	0.47
1:D:62:TYR:HB2	1:D:105:ILE:HB	1.97	0.46
1:E:179:ILE:HB	1:E:189:PHE:HD2	1.79	0.46
1:I:201:MIS:OG	1:I:201:MIS:H33	2.16	0.46
1:A:87:GLN:O	1:A:134:ALA:HB1	2.18	0.44
1:D:248:LEU:HD23	1:D:253:ARG:HA	2.00	0.44
1:D:71:HIS:CD2	1:D:73:GLN:HB3	2.52	0.44
1:A:176:THR:HG22	1:A:190:LEU:HD22	1.98	0.44
1:A:157:ALA:HB1	1:A:196:ILE:HD11	1.99	0.44
1:G:174:SER:HB3	1:I:167:THR:HG23	2.00	0.44
1:I:85:MET:HG3	1:I:245:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ASN:HB3	1:G:96:HIS:CE1	2.54	0.43
1:A:223:SER:HB2	1:A:227:GLU:O	2.18	0.43
1:G:167:THR:HG23	1:H:174:SER:HB3	2.00	0.43
1:D:53:ARG:HD3	1:F:37:PHE:CZ	2.54	0.42
1:B:201:MIS:H31	1:B:219:SER:HB3	2.01	0.42
1:G:85:MET:HG3	1:G:92:ILE:HG13	2.02	0.42
1:C:181:LEU:CD1	1:D:105:ILE:HD12	2.50	0.41
1:F:48:ASN:O	1:F:52:ARG:HG3	2.20	0.41
1:C:79:LEU:HD11	2:C:762:HOH:O	2.20	0.41
1:B:95:LYS:HG3	1:B:121:SER:HB2	2.03	0.41
1:E:153:ASP:HB2	1:E:173:ILE:HD12	2.01	0.41
1:H:217:THR:HG22	1:H:218:LEU:HG	2.02	0.41
1:E:62:TYR:CD2	1:E:76:ILE:HD13	2.56	0.41
1:I:62:TYR:HB2	1:I:105:ILE:HB	2.03	0.41
1:I:85:MET:HE2	1:I:92:ILE:HD12	2.03	0.41
1:C:62:TYR:HB2	1:C:105:ILE:HB	2.01	0.41
1:H:186:ARG:HD2	1:H:189:PHE:CE1	2.56	0.41
1:F:90:TYR:CE2	1:F:131:LYS:HD3	2.57	0.40
1:A:250:ARG:O	1:A:251:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/241 (83%)	198 (99%)	2 (1%)	0	100	100
1	B	208/241 (86%)	204 (98%)	4 (2%)	0	100	100
1	C	209/241 (87%)	207 (99%)	2 (1%)	0	100	100
1	D	207/241 (86%)	205 (99%)	2 (1%)	0	100	100
1	E	196/241 (81%)	192 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	206/241 (86%)	202 (98%)	4 (2%)	0	100	100
1	G	195/241 (81%)	193 (99%)	2 (1%)	0	100	100
1	H	186/241 (77%)	182 (98%)	4 (2%)	0	100	100
1	I	189/241 (78%)	188 (100%)	1 (0%)	0	100	100
All	All	1796/2169 (83%)	1771 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/197 (84%)	165 (100%)	0	100	100
1	B	169/197 (86%)	169 (100%)	0	100	100
1	C	171/197 (87%)	171 (100%)	0	100	100
1	D	170/197 (86%)	169 (99%)	1 (1%)	86	93
1	E	163/197 (83%)	163 (100%)	0	100	100
1	F	170/197 (86%)	170 (100%)	0	100	100
1	G	162/197 (82%)	162 (100%)	0	100	100
1	H	152/197 (77%)	151 (99%)	1 (1%)	84	91
1	I	159/197 (81%)	159 (100%)	0	100	100
All	All	1481/1773 (84%)	1479 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	71	HIS
1	H	220	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	69	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MIS	H	201	1	11,12,13	0.70	0	10,16,18	0.58	0
1	MIS	E	201	1	11,12,13	0.70	0	10,16,18	0.58	0
1	MIS	I	201	1	11,12,13	0.63	0	10,16,18	0.87	0
1	MIS	C	201	1	11,12,13	0.75	0	10,16,18	0.59	0
1	MIS	B	201	1	11,12,13	0.72	0	10,16,18	0.55	0
1	MIS	G	201	1	11,12,13	0.69	0	10,16,18	0.57	0
1	MIS	D	201	1	11,12,13	0.72	0	10,16,18	0.60	0
1	MIS	A	201	1	11,12,13	0.73	0	10,16,18	0.69	0
1	MIS	F	201	1	11,12,13	0.74	0	10,16,18	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MIS	H	201	1	-	3/10/13/15	-
1	MIS	E	201	1	-	3/10/13/15	-
1	MIS	I	201	1	-	4/10/13/15	-
1	MIS	C	201	1	-	3/10/13/15	-
1	MIS	B	201	1	-	3/10/13/15	-
1	MIS	G	201	1	-	4/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MIS	D	201	1	-	3/10/13/15	-
1	MIS	A	201	1	-	2/10/13/15	-
1	MIS	F	201	1	-	3/10/13/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	201	MIS	CB-OG-P-O1P
1	G	201	MIS	CB-OG-P-O2P
1	G	201	MIS	CB-OG-P-O3P
1	H	201	MIS	CB-OG-P-O3P
1	E	201	MIS	CB-OG-P-O3P
1	I	201	MIS	CB-OG-P-O3P
1	C	201	MIS	CB-OG-P-O3P
1	B	201	MIS	CB-OG-P-O3P
1	D	201	MIS	CB-OG-P-O3P
1	A	201	MIS	CB-OG-P-O3P
1	F	201	MIS	CB-OG-P-O3P
1	B	201	MIS	CA-CB-OG-P
1	G	201	MIS	CA-CB-OG-P
1	D	201	MIS	CA-CB-OG-P
1	F	201	MIS	CA-CB-OG-P
1	I	201	MIS	C3-C1-O3P-P
1	H	201	MIS	CB-OG-P-O2P
1	E	201	MIS	CB-OG-P-O2P
1	I	201	MIS	CB-OG-P-O2P
1	C	201	MIS	CB-OG-P-O2P
1	B	201	MIS	CB-OG-P-O2P
1	D	201	MIS	CB-OG-P-O2P
1	A	201	MIS	CB-OG-P-O2P
1	F	201	MIS	CB-OG-P-O2P
1	I	201	MIS	C1-O3P-P-OG
1	H	201	MIS	CA-CB-OG-P
1	E	201	MIS	CA-CB-OG-P
1	C	201	MIS	CA-CB-OG-P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	201	MIS	1	0
1	B	201	MIS	1	0
1	F	201	MIS	1	0

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, 95^{th} 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	206/241 (85%)	0.33	12 (5%)	23	33	18, 32, 76, 121	0
1	B	212/241 (87%)	0.49	19 (8%)	9	14	17, 33, 80, 127	0
1	C	213/241 (88%)	0.18	16 (7%)	14	21	16, 33, 84, 108	0
1	D	211/241 (87%)	0.21	14 (6%)	18	26	24, 38, 84, 92	0
1	E	202/241 (83%)	0.54	14 (6%)	16	24	25, 46, 86, 102	0
1	F	210/241 (87%)	0.46	19 (9%)	9	14	19, 33, 78, 121	0
1	G	201/241 (83%)	0.45	17 (8%)	10	16	24, 40, 83, 100	0
1	H	192/241 (79%)	0.35	17 (8%)	9	14	25, 47, 84, 96	0
1	I	197/241 (81%)	0.75	22 (11%)	5	8	30, 57, 96, 113	0
All	All	1844/2169 (85%)	0.41	150 (8%)	12	17	16, 40, 86, 127	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	68	THR	10.7
1	A	184	THR	7.0
1	D	183	PRO	7.0
1	B	66	LEU	6.3
1	I	66	LEU	6.3
1	B	37	PHE	6.2
1	A	225	ASP	6.2
1	B	72	ASN	6.1
1	E	66	LEU	6.1
1	F	37	PHE	6.0
1	E	225	ASP	5.9
1	D	181	LEU	5.9
1	A	226	GLY	5.3
1	C	66	LEU	5.2
1	B	71	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	74	LEU	5.0
1	B	224	ASN	4.9
1	I	77	ARG	4.8
1	B	225	ASP	4.7
1	F	69	ASN	4.7
1	E	135	THR	4.7
1	I	67	ASN	4.7
1	H	103	GLN	4.7
1	G	100	ASP	4.6
1	A	37	PHE	4.5
1	G	247	LYS	4.5
1	F	38	ASP	4.5
1	G	250	ARG	4.3
1	D	182	ASN	4.3
1	D	40	THR	4.3
1	H	78	THR	4.3
1	H	102	ASP	4.3
1	E	224	ASN	4.2
1	I	65	GLY	4.2
1	B	77	ARG	4.1
1	I	37	PHE	4.1
1	C	74	LEU	4.0
1	I	74	LEU	4.0
1	C	77	ARG	3.9
1	C	68	THR	3.9
1	F	70	SER	3.8
1	E	226	GLY	3.8
1	I	244	ILE	3.7
1	A	186	ARG	3.7
1	G	37	PHE	3.7
1	I	124	LEU	3.7
1	E	37	PHE	3.7
1	A	66	LEU	3.6
1	I	179	ILE	3.6
1	H	63	ASN	3.5
1	I	117	LEU	3.5
1	I	75	GLU	3.5
1	G	38	ASP	3.5
1	G	78	THR	3.4
1	D	187	GLN	3.4
1	C	69	ASN	3.3
1	F	39	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	67	ASN	3.3
1	B	73	GLN	3.2
1	D	186	ARG	3.2
1	C	250	ARG	3.1
1	F	66	LEU	3.1
1	D	66	LEU	3.1
1	B	249	ILE	3.1
1	B	247	LYS	3.1
1	C	70	SER	3.1
1	A	136	GLY	3.1
1	A	185	GLY	3.0
1	I	146	ARG	3.0
1	I	250	ARG	3.0
1	G	39	SER	3.0
1	A	224	ASN	3.0
1	C	65	GLY	3.0
1	A	73	GLN	3.0
1	F	40	THR	3.0
1	C	39	SER	3.0
1	F	252	GLY	3.0
1	F	250	ARG	3.0
1	I	76	ILE	3.0
1	E	67	ASN	3.0
1	D	69	ASN	2.9
1	F	72	ASN	2.9
1	D	184	THR	2.9
1	H	220	PHE	2.9
1	B	38	ASP	2.9
1	G	249	ILE	2.8
1	D	41	ASP	2.8
1	H	117	LEU	2.8
1	H	123	SER	2.8
1	D	250	ARG	2.8
1	G	233	GLY	2.8
1	C	222	LYS	2.8
1	A	135	THR	2.7
1	I	78	THR	2.7
1	F	249	ILE	2.7
1	H	79	LEU	2.7
1	I	125	THR	2.7
1	B	226	GLY	2.7
1	G	74	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	247	LYS	2.7
1	I	113	VAL	2.7
1	C	37	PHE	2.6
1	F	77	ARG	2.6
1	H	221	ASP	2.6
1	D	70	SER	2.6
1	D	254	VAL	2.5
1	G	75	GLU	2.5
1	H	116	ALA	2.5
1	G	192	THR	2.5
1	B	100	ASP	2.5
1	F	73	GLN	2.5
1	B	75	GLU	2.4
1	B	67	ASN	2.4
1	G	77	ARG	2.4
1	H	101	ALA	2.4
1	G	228	THR	2.3
1	C	67	ASN	2.3
1	I	135	THR	2.3
1	F	41	ASP	2.3
1	B	40	THR	2.3
1	B	252	GLY	2.3
1	G	171	GLY	2.3
1	G	234	PHE	2.3
1	B	41	ASP	2.3
1	I	102	ASP	2.3
1	H	104	ILE	2.3
1	H	134	ALA	2.3
1	D	227	GLU	2.2
1	E	167	THR	2.2
1	E	146	ARG	2.2
1	A	252	GLY	2.2
1	E	227	GLU	2.2
1	E	240	LEU	2.2
1	E	250	ARG	2.2
1	F	247	LYS	2.2
1	C	75	GLU	2.1
1	C	72	ASN	2.1
1	F	190	LEU	2.1
1	H	100	ASP	2.1
1	C	40	THR	2.1
1	H	135	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	106	VAL	2.1
1	F	227	GLU	2.1
1	H	115	GLU	2.0
1	E	74	LEU	2.0
1	I	136	GLY	2.0
1	G	191	GLN	2.0
1	C	71	HIS	2.0
1	I	123	SER	2.0
1	I	101	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MIS	I	201	13/14	0.96	0.14	39,56,71,71	0
1	MIS	H	201	13/14	0.97	0.14	34,57,74,74	0
1	MIS	E	201	13/14	0.98	0.19	27,43,56,63	0
1	MIS	C	201	13/14	0.98	0.14	18,38,48,52	0
1	MIS	B	201	13/14	0.98	0.16	21,36,47,57	0
1	MIS	G	201	13/14	0.98	0.16	29,42,56,60	0
1	MIS	D	201	13/14	0.98	0.14	21,44,63,63	0
1	MIS	A	201	13/14	0.98	0.18	19,34,52,52	0
1	MIS	F	201	13/14	0.98	0.15	20,36,57,62	0

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.