



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 12:30 PM EDT

PDB ID : 2RCE
Title : DFP modified DegS delta PDZ
Authors : Sohn, J.; Grant, R.A.; Sauer, R.T.
Deposited on : unknown
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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

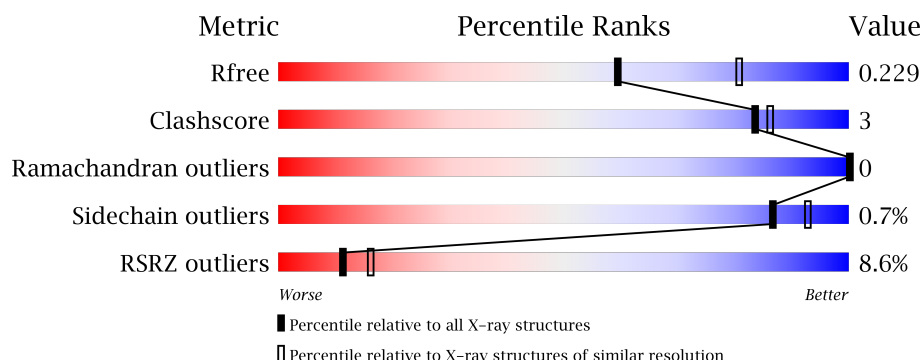
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.






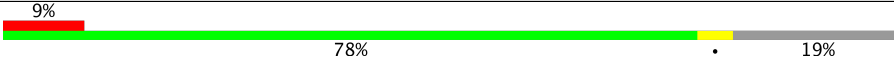
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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>7%</div> <div>79% 5% 16%</div> </div>
1	B	243	<div> <div>7%</div> <div>84% 12%</div> </div>
1	C	243	<div> <div>7%</div> <div>85% 12%</div> </div>
1	D	243	<div> <div>7%</div> <div>79% 7% 15%</div> </div>
1	E	243	<div> <div>7%</div> <div>77% 6% 16%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	243	
1	G	243	
1	H	243	
1	I	243	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14556 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	205	Total	C	N	O	P	S	0	0	0
			1535	954	274	303	1	3			
1	B	213	Total	C	N	O	P	S	0	0	0
			1599	996	286	313	1	3			
1	C	214	Total	C	N	O	P	S	0	0	0
			1611	1003	290	314	1	3			
1	D	207	Total	C	N	O	P	S	0	0	0
			1559	973	281	301	1	3			
1	E	203	Total	C	N	O	P	S	0	0	0
			1526	954	268	300	1	3			
1	F	211	Total	C	N	O	P	S	0	0	0
			1585	988	283	310	1	3			
1	G	205	Total	C	N	O	P	S	0	0	0
			1538	962	272	300	1	3			
1	H	192	Total	C	N	O	P	S	0	0	0
			1436	900	255	277	1	3			
1	I	198	Total	C	N	O	P	S	0	0	0
			1488	933	261	290	1	3			

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	-	expression tag	UNP P0AEE3
A	26	SER	-	expression tag	UNP P0AEE3
B	14	MET	-	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
C	14	MET	-	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
D	14	MET	-	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
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
E	14	MET	-	expression tag	UNP P0AEE3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
F	14	MET	-	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
G	14	MET	-	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
H	14	MET	-	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
I	14	MET	-	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
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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	B	109	Total O 109 109	0	0
2	C	98	Total O 98 98	0	0
2	D	68	Total O 68 68	0	0
2	E	62	Total O 62 62	0	0
2	F	93	Total O 93 93	0	0
2	G	63	Total O 63 63	0	0
2	H	52	Total O 52 52	0	0

Continued on next page...

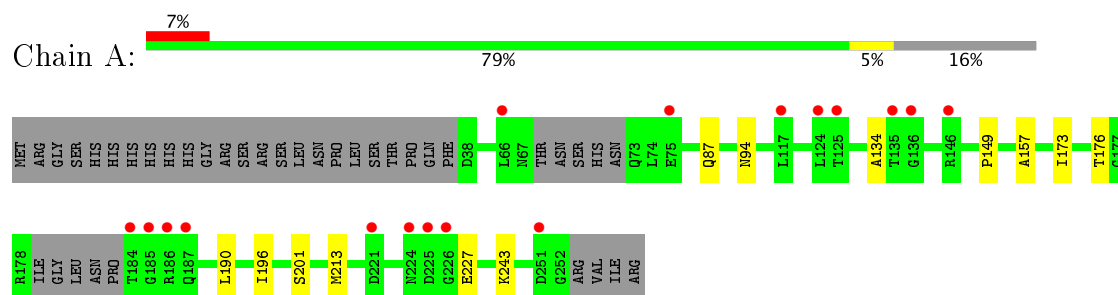
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	42	Total	O	0	0
			42	42		

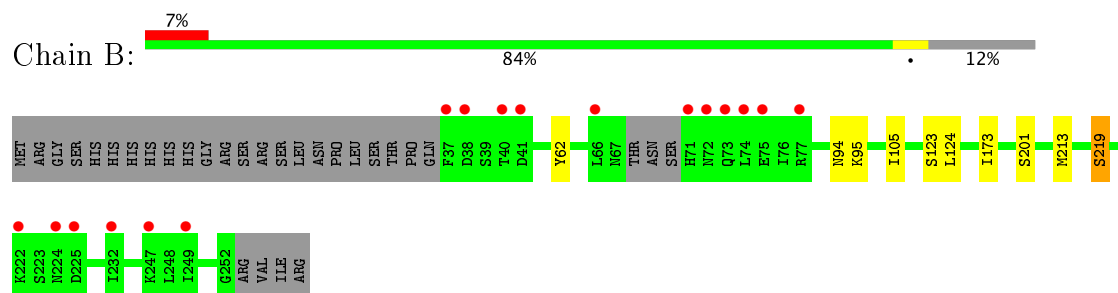
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

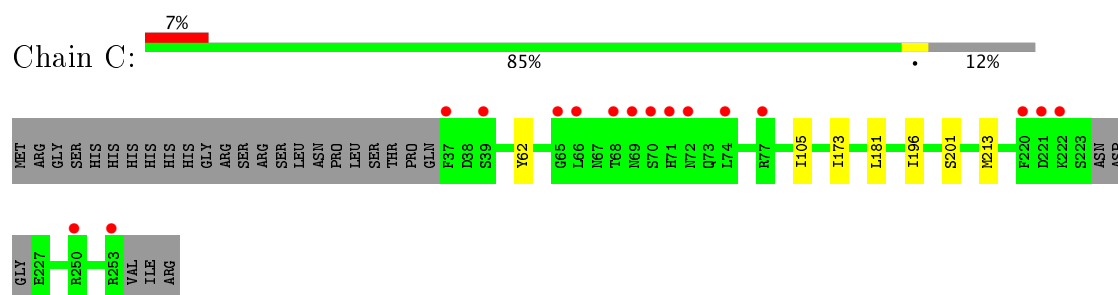
- Molecule 1: Protease degS



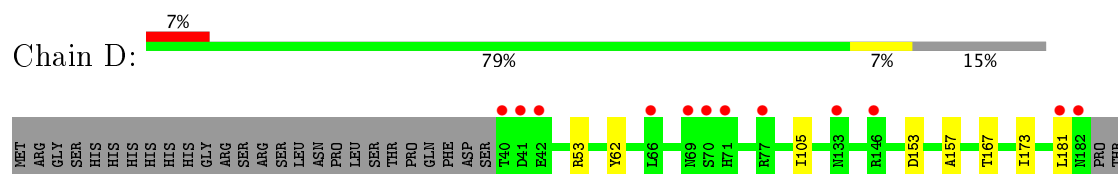
- Molecule 1: Protease degS

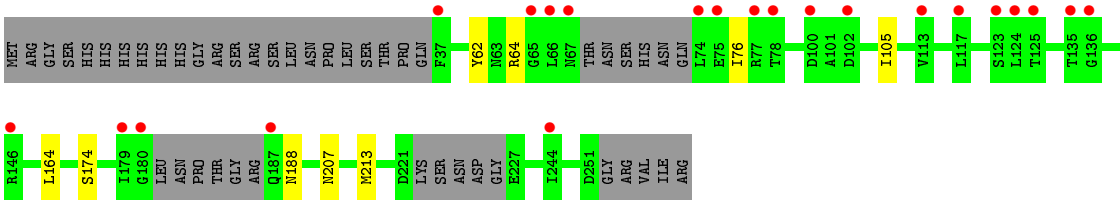


- Molecule 1: Protease degS



- 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	71.53Å 132.75Å 231.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.22 – 2.35 37.14 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.0 (37.22-2.35) 91.0 (37.14-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.236 0.190 , 0.229	Depositor DCC
R_{free} test set	4127 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14556	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.44	0/1538	0.58	0/2085
1	B	0.40	0/1606	0.56	0/2180
1	C	0.40	0/1618	0.56	0/2196
1	D	0.41	0/1563	0.54	0/2121
1	E	0.37	0/1530	0.53	0/2076
1	F	0.41	0/1592	0.56	0/2163
1	G	0.38	0/1543	0.55	0/2093
1	H	0.36	0/1440	0.53	0/1956
1	I	0.36	0/1491	0.51	0/2022
All	All	0.39	0/13921	0.55	0/18892

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	1535	0	1547	11	0
1	B	1599	0	1608	7	0
1	C	1611	0	1626	9	0
1	D	1559	0	1584	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1526	0	1540	10	0
1	F	1585	0	1595	7	0
1	G	1538	0	1555	10	0
1	H	1436	0	1460	9	0
1	I	1488	0	1504	5	0
2	A	92	0	0	2	0
2	B	109	0	0	2	0
2	C	98	0	0	2	0
2	D	68	0	0	1	0
2	E	62	0	0	2	0
2	F	93	0	0	1	0
2	G	63	0	0	1	0
2	H	52	0	0	1	0
2	I	42	0	0	0	0
All	All	14556	0	14019	77	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 3.

All (77) 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:F:173:ILE:HD11	1:F:213:MET:HE3	1.49	0.93
1:H:173:ILE:HD11	1:H:213:MET:HE3	1.74	0.68
1:E:213:MET:HE1	2:E:273:HOH:O	1.95	0.66
1:F:173:ILE:CD1	1:F:213:MET:HE3	2.26	0.66
1:B:173:ILE:HD11	1:B:213:MET:HE3	1.78	0.65
1:B:213:MET:HE2	2:B:298:HOH:O	1.96	0.65
1:G:173:ILE:HD11	1:G:213:MET:HE3	1.78	0.64
1:E:213:MET:CE	2:E:273:HOH:O	2.48	0.62
1:A:213:MET:CE	2:A:292:HOH:O	2.46	0.61
1:A:213:MET:HE1	2:A:292:HOH:O	1.99	0.61
1:C:173:ILE:HD11	1:C:213:MET:HE3	1.81	0.60
1:I:207:ASN:HB3	1:I:213:MET:HE2	1.84	0.60
1:A:176:THR:HG22	1:A:190:LEU:HD22	1.82	0.60
1:C:213:MET:HE2	2:C:276:HOH:O	2.02	0.60
1:C:196:ILE:CG2	1:C:201:MIS:H31	2.32	0.59
1:D:173:ILE:HD11	1:D:213:MET:HE3	1.84	0.58
1:E:153:ASP:HB2	1:E:173:ILE:HD12	1.86	0.58
1:H:95:LYS:NZ	1:H:123:SER:HB3	2.21	0.56
1:G:62:TYR:HB2	1:G:105:ILE:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HD11	1:A:213:MET:HE3	1.88	0.54
1:A:149:PRO:HB3	1:A:213:MET:HE3	1.89	0.54
1:B:201:MIS:H31	1:B:219:SER:HB2	1.91	0.53
1:H:213:MET:HE2	2:H:279:HOH:O	2.10	0.52
1:C:181:LEU:HD11	1:D:105:ILE:HD12	1.90	0.52
1:B:62:TYR:HB2	1:B:105:ILE:HB	1.92	0.52
1:F:196:ILE:HG22	1:F:201:MIS:H31	1.92	0.52
1:A:173:ILE:CD1	1:A:213:MET:HE3	2.41	0.51
1:D:153:ASP:HB2	1:D:173:ILE:HD12	1.93	0.51
1:D:181:LEU:HD21	1:D:220:PHE:HA	1.94	0.50
1:F:196:ILE:CG2	1:F:201:MIS:H31	2.43	0.49
1:D:157:ALA:HB1	1:D:196:ILE:HD11	1.93	0.49
1:G:173:ILE:CD1	1:G:213:MET:HE3	2.43	0.49
1:E:127:LEU:HD11	1:E:236:ILE:HG21	1.95	0.49
1:D:157:ALA:CB	1:D:196:ILE:HD11	2.42	0.48
1:G:213:MET:HE1	2:G:294:HOH:O	2.13	0.48
1:H:95:LYS:HZ3	1:H:123:SER:HB3	1.77	0.48
1:E:179:ILE:HB	1:E:189:PHE:HD2	1.79	0.48
1:E:173:ILE:HD11	1:E:213:MET:HE3	1.95	0.47
1:H:196:ILE:HG22	1:H:201:MIS:H31	1.97	0.47
1:A:149:PRO:HA	1:A:213:MET:HE1	1.97	0.47
1:D:167:THR:HG23	1:E:174:SER:HB3	1.96	0.47
1:C:181:LEU:CD1	1:D:105:ILE:HD12	2.44	0.47
1:H:196:ILE:CG2	1:H:201:MIS:H31	2.45	0.47
1:A:196:ILE:CG2	1:A:201:MIS:H31	2.45	0.46
1:D:248:LEU:HD23	1:D:253:ARG:HA	1.98	0.46
1:G:157:ALA:HB1	1:G:196:ILE:HD11	1.97	0.45
1:I:64:ARG:HG2	1:I:76:ILE:HD13	1.98	0.45
1:D:213:MET:HE2	2:D:292:HOH:O	2.15	0.45
1:D:62:TYR:HB2	1:D:105:ILE:HB	1.99	0.45
1:A:157:ALA:HB1	1:A:196:ILE:HD11	1.99	0.45
1:A:243:LYS:HB3	1:A:243:LYS:HE2	1.69	0.45
1:C:196:ILE:HG22	1:C:201:MIS:H31	1.98	0.44
1:H:173:ILE:HD11	1:H:213:MET:CE	2.47	0.44
1:G:220:PHE:HE2	1:I:164:LEU:HD21	1.83	0.44
1:E:196:ILE:CG2	1:E:201:MIS:H31	2.47	0.44
1:G:94:ASN:HB3	1:G:96:HIS:CE1	2.53	0.43
1:B:213:MET:CE	2:B:298:HOH:O	2.60	0.43
1:H:167:THR:HG23	1:I:174:SER:HB3	2.01	0.43
1:A:87:GLN:O	1:A:134:ALA:HB1	2.19	0.43
1:B:94:ASN:HD22	1:B:94:ASN:HA	1.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ALA:HB1	1:E:196:ILE:HD11	2.01	0.42
1:H:236:ILE:CG2	1:H:240:LEU:HD22	2.49	0.42
1:C:62:TYR:HB2	1:C:105:ILE:HB	2.01	0.42
1:D:250:ARG:HG2	1:D:251:ASP:OD1	2.20	0.42
1:C:173:ILE:HD11	1:C:213:MET:CE	2.47	0.41
1:C:213:MET:CE	2:C:276:HOH:O	2.65	0.41
1:E:250:ARG:O	1:E:251:ASP:HB2	2.19	0.41
1:G:182:ASN:HB2	1:G:183:PRO:CD	2.49	0.41
1:D:53:ARG:HD3	1:F:37:PHE:CZ	2.55	0.41
1:I:62:TYR:HB2	1:I:105:ILE:HB	2.03	0.41
1:D:173:ILE:HD11	1:D:213:MET:CE	2.50	0.41
1:F:213:MET:CE	2:F:266:HOH:O	2.68	0.41
1:B:95:LYS:NZ	1:B:123:SER:HB3	2.36	0.41
1:G:228:THR:HA	1:G:229:PRO:HD3	1.82	0.41
1:F:157:ALA:HB1	1:F:196:ILE:HD11	2.03	0.40
1:D:196:ILE:CG2	1:D:201:MIS:H31	2.51	0.40
1:G:236:ILE:HG23	1:G:240:LEU:HD23	2.03	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	198/243 (82%)	192 (97%)	6 (3%)	0	100	100
1	B	208/243 (86%)	204 (98%)	4 (2%)	0	100	100
1	C	209/243 (86%)	205 (98%)	4 (2%)	0	100	100
1	D	200/243 (82%)	196 (98%)	4 (2%)	0	100	100
1	E	196/243 (81%)	186 (95%)	10 (5%)	0	100	100
1	F	206/243 (85%)	201 (98%)	5 (2%)	0	100	100
1	G	198/243 (82%)	192 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	185/243 (76%)	183 (99%)	2 (1%)	0	100	100
1	I	189/243 (78%)	187 (99%)	2 (1%)	0	100	100
All	All	1789/2187 (82%)	1746 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	164/199 (82%)	162 (99%)	2 (1%)	75	86
1	B	171/199 (86%)	169 (99%)	2 (1%)	75	86
1	C	173/199 (87%)	173 (100%)	0	100	100
1	D	167/199 (84%)	167 (100%)	0	100	100
1	E	164/199 (82%)	162 (99%)	2 (1%)	75	86
1	F	170/199 (85%)	169 (99%)	1 (1%)	89	94
1	G	164/199 (82%)	164 (100%)	0	100	100
1	H	153/199 (77%)	150 (98%)	3 (2%)	60	73
1	I	159/199 (80%)	158 (99%)	1 (1%)	89	94
All	All	1485/1791 (83%)	1474 (99%)	11 (1%)	87	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	227	GLU
1	B	124	LEU
1	B	219	SER
1	E	78	THR
1	E	221	ASP
1	F	94	ASN
1	H	189	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	219	SER
1	H	228	THR
1	I	188	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	201	1	12,12,13	0.60	0	10,16,18	1.00	0
1	MIS	B	201	1	12,12,13	0.61	0	10,16,18	1.13	1 (10%)
1	MIS	C	201	1	12,12,13	0.64	0	10,16,18	0.89	0
1	MIS	D	201	1	12,12,13	0.61	0	10,16,18	0.80	0
1	MIS	E	201	1	12,12,13	0.60	0	10,16,18	0.90	0
1	MIS	F	201	1	12,12,13	0.62	0	10,16,18	1.21	1 (10%)
1	MIS	G	201	1	12,12,13	0.65	0	10,16,18	1.35	1 (10%)
1	MIS	H	201	1	12,12,13	0.61	0	10,16,18	0.93	0
1	MIS	I	201	1	12,12,13	0.61	0	10,16,18	0.85	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	A	201	1	-	0/10/13/15	0/0/0/0
1	MIS	B	201	1	-	0/10/13/15	0/0/0/0
1	MIS	C	201	1	-	0/10/13/15	0/0/0/0
1	MIS	D	201	1	-	0/10/13/15	0/0/0/0
1	MIS	E	201	1	-	0/10/13/15	0/0/0/0
1	MIS	F	201	1	-	0/10/13/15	0/0/0/0
1	MIS	G	201	1	-	0/10/13/15	0/0/0/0
1	MIS	H	201	1	-	0/10/13/15	0/0/0/0
1	MIS	I	201	1	-	0/10/13/15	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	MIS	OG-CB-CA	2.32	110.46	108.17
1	F	201	MIS	OG-CB-CA	2.51	110.64	108.17
1	G	201	MIS	OG-CB-CA	3.69	111.80	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	201	MIS	1	0
1	B	201	MIS	1	0
1	C	201	MIS	2	0
1	D	201	MIS	1	0
1	E	201	MIS	1	0
1	F	201	MIS	2	0
1	H	201	MIS	2	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	204/243 (83%)	0.40	17 (8%)	12 17	20, 33, 68, 99	0
1	B	212/243 (87%)	0.47	17 (8%)	13 19	21, 33, 76, 113	0
1	C	213/243 (87%)	0.17	16 (7%)	15 22	20, 32, 69, 93	0
1	D	206/243 (84%)	-0.04	16 (7%)	14 20	21, 33, 71, 83	1 (0%)
1	E	202/243 (83%)	0.46	18 (8%)	10 15	20, 33, 62, 73	0
1	F	210/243 (86%)	0.52	19 (9%)	10 15	21, 32, 67, 92	0
1	G	204/243 (83%)	0.49	19 (9%)	9 15	23, 32, 72, 102	0
1	H	191/243 (78%)	0.27	14 (7%)	16 23	20, 31, 55, 69	0
1	I	197/243 (81%)	0.65	22 (11%)	6 9	21, 33, 62, 74	0
All	All	1839/2187 (84%)	0.38	158 (8%)	11 16	20, 33, 67, 113	1 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	68	THR	7.7
1	G	225	ASP	7.2
1	G	252	GLY	6.9
1	A	184	THR	6.8
1	F	37	PHE	6.7
1	B	37	PHE	6.2
1	B	66	LEU	6.1
1	I	37	PHE	5.4
1	D	181	LEU	5.3
1	I	66	LEU	5.3
1	B	74	LEU	5.3
1	A	225	ASP	5.2
1	F	69	ASN	5.2
1	B	72	ASN	5.2
1	G	100	ASP	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	71	HIS	4.8
1	G	253	ARG	4.7
1	C	68	THR	4.6
1	H	78	THR	4.6
1	E	225	ASP	4.5
1	B	225	ASP	4.4
1	C	66	LEU	4.3
1	H	100	ASP	4.3
1	I	67	ASN	4.3
1	I	117	LEU	4.3
1	E	226	GLY	4.2
1	G	37	PHE	4.2
1	I	124	LEU	4.2
1	G	78	THR	4.1
1	G	38	ASP	4.1
1	F	38	ASP	4.0
1	C	71	HIS	4.0
1	A	226	GLY	3.9
1	D	40	THR	3.9
1	I	65	GLY	3.9
1	I	77	ARG	3.9
1	F	67	ASN	3.9
1	G	250	ARG	3.9
1	E	66	LEU	3.9
1	C	74	LEU	3.8
1	B	224	ASN	3.6
1	H	102	ASP	3.6
1	D	77	ARG	3.6
1	F	39	SER	3.6
1	G	226	GLY	3.6
1	F	66	LEU	3.6
1	B	38	ASP	3.5
1	H	103	GLN	3.5
1	C	77	ARG	3.5
1	I	179	ILE	3.5
1	G	74	LEU	3.4
1	C	250	ARG	3.4
1	B	77	ARG	3.4
1	G	39	SER	3.3
1	E	135	THR	3.3
1	H	221	ASP	3.3
1	G	227	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	41	ASP	3.2
1	H	134	ALA	3.2
1	A	136	GLY	3.2
1	H	123	SER	3.2
1	A	224	ASN	3.1
1	I	74	LEU	3.1
1	C	70	SER	3.0
1	E	37	PHE	3.0
1	H	63	ASN	3.0
1	I	75	GLU	2.9
1	H	135	THR	2.9
1	A	66	LEU	2.9
1	F	252	GLY	2.9
1	G	247	LYS	2.9
1	I	136	GLY	2.9
1	C	39	SER	2.9
1	A	185	GLY	2.9
1	A	186	ARG	2.9
1	E	224	ASN	2.8
1	E	65	GLY	2.8
1	F	41	ASP	2.8
1	I	102	ASP	2.8
1	H	117	LEU	2.8
1	D	227	GLU	2.8
1	E	73	GLN	2.8
1	C	72	ASN	2.8
1	F	72	ASN	2.8
1	C	221	ASP	2.8
1	I	113	VAL	2.7
1	F	40	THR	2.7
1	A	75	GLU	2.7
1	I	146	ARG	2.6
1	E	75	GLU	2.6
1	E	68	THR	2.6
1	H	116	ALA	2.6
1	I	244	ILE	2.6
1	B	222	LYS	2.6
1	E	247	LYS	2.6
1	I	123	SER	2.6
1	C	65	GLY	2.6
1	D	69	ASN	2.6
1	H	220	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	100	ASP	2.6
1	H	115	GLU	2.6
1	B	247	LYS	2.6
1	E	240	LEU	2.5
1	C	69	ASN	2.5
1	D	146	ARG	2.5
1	G	228	THR	2.5
1	E	119	VAL	2.5
1	E	146	ARG	2.5
1	F	190	LEU	2.5
1	D	133	ASN	2.5
1	E	67	ASN	2.5
1	B	249	ILE	2.5
1	D	70	SER	2.5
1	I	125	THR	2.4
1	D	42	GLU	2.4
1	C	37	PHE	2.4
1	G	192	THR	2.4
1	G	249	ILE	2.4
1	A	135	THR	2.4
1	I	135	THR	2.4
1	B	75	GLU	2.4
1	F	250	ARG	2.4
1	D	228	THR	2.4
1	I	78	THR	2.3
1	D	182	ASN	2.3
1	F	227	GLU	2.3
1	I	180	GLY	2.3
1	A	187	GLN	2.3
1	D	250	ARG	2.3
1	G	173	ILE	2.3
1	B	41	ASP	2.3
1	G	41	ASP	2.3
1	B	73	GLN	2.3
1	B	232	ILE	2.3
1	I	187	GLN	2.3
1	B	40	THR	2.2
1	D	71	HIS	2.2
1	A	221	ASP	2.2
1	G	75	GLU	2.2
1	E	100	ASP	2.2
1	A	117	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	220	PHE	2.2
1	F	192	THR	2.2
1	D	66	LEU	2.2
1	C	222	LYS	2.1
1	F	249	ILE	2.1
1	C	253	ARG	2.1
1	H	96	HIS	2.1
1	F	136	GLY	2.1
1	F	172	ILE	2.1
1	A	146	ARG	2.1
1	E	136	GLY	2.1
1	A	124	LEU	2.1
1	F	73	GLN	2.0
1	A	125	THR	2.0
1	A	251	ASP	2.0
1	D	254	VAL	2.0
1	E	111	GLY	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	MIS	C	201	13/14	0.98	0.10	-	23,34,41,41	0
1	MIS	I	201	13/14	0.95	0.11	-	23,34,41,41	0
1	MIS	H	201	13/14	0.97	0.10	-	23,34,40,40	0
1	MIS	E	201	13/14	0.98	0.15	-	23,33,40,40	0
1	MIS	F	201	13/14	0.99	0.12	-	23,33,41,41	0
1	MIS	D	201	13/14	0.98	0.08	-	23,33,40,41	0
1	MIS	A	201	13/14	0.98	0.15	-	23,33,40,41	0
1	MIS	B	201	13/14	0.98	0.15	-	23,34,40,42	0
1	MIS	G	201	13/14	0.98	0.12	-	26,35,42,43	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.