



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 4X2V / pdb_00004x2v
Title : Crystal structure of the Murine Norovirus NS6 protease (inactive C139A mutant) with a C-terminal extension to include residue P1 prime of NS7
Authors : Fernandes, H.; Leen, E.N.; Curry, S.
Deposited on : 2014-11-27
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

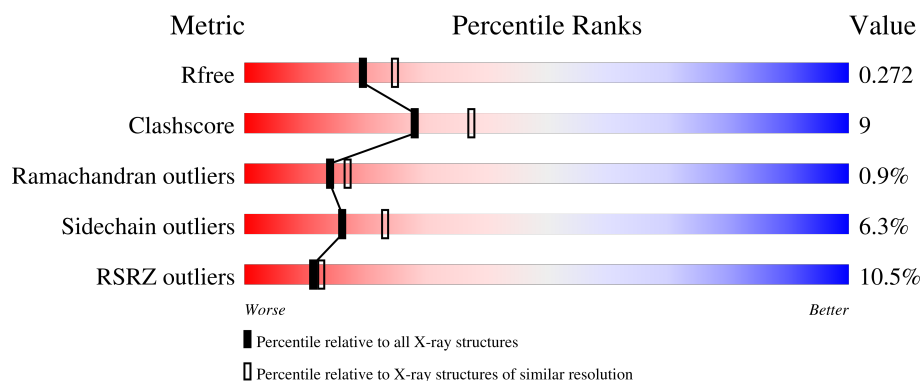
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	185	8% 77% 12% 6%
1	B	185	14% 76% 20% 6%
1	C	185	2% 81% 11% 7%
1	D	185	16% 75% 14% 8%
2	E	5	80% 20%

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Mol	Chain	Length	Quality of chain
3	F	7	86% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5356 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 NS6 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	1	0
			1288	823	227	232	6			
1	B	185	Total	C	N	O	S	0	1	0
			1372	876	239	251	6			
1	C	172	Total	C	N	O	S	0	0	0
			1268	810	222	230	6			
1	D	171	Total	C	N	O	S	0	0	0
			1259	805	221	227	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0FJD7
A	139	ALA	CYS	engineered mutation	UNP A0FJD7
B	0	SER	-	expression tag	UNP A0FJD7
B	139	ALA	CYS	engineered mutation	UNP A0FJD7
C	0	SER	-	expression tag	UNP A0FJD7
C	139	ALA	CYS	engineered mutation	UNP A0FJD7
D	0	SER	-	expression tag	UNP A0FJD7
D	139	ALA	CYS	engineered mutation	UNP A0FJD7

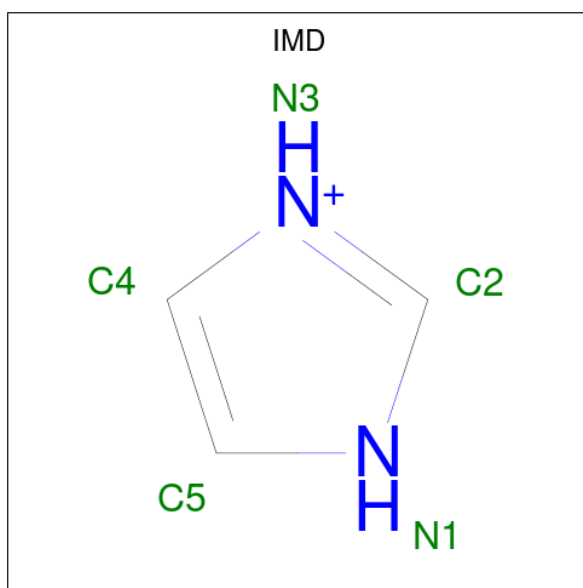
- Molecule 2 is a protein called NS6 Protease.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			41	27	6	8			

- Molecule 3 is a protein called NS6 Protease.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			35	21	7	7			

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	N	0	0
			5	3	2		

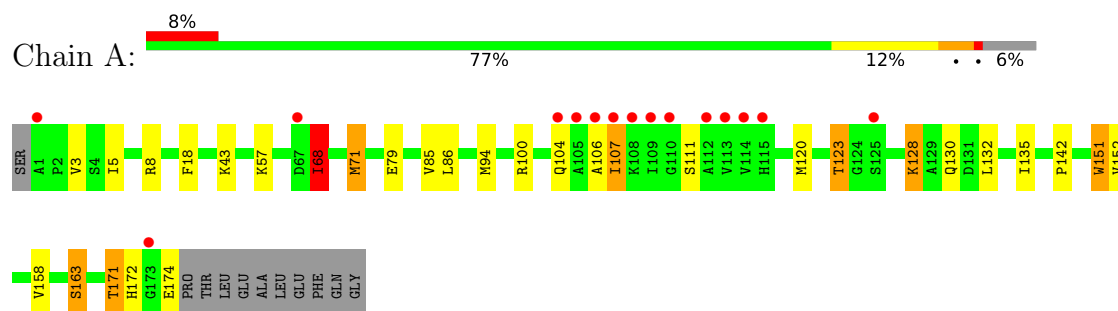
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	24	Total	O	0	0
			24	24		
5	C	22	Total	O	0	0
			22	22		
5	D	2	Total	O	0	0
			2	2		
5	E	1	Total	O	0	0
			1	1		

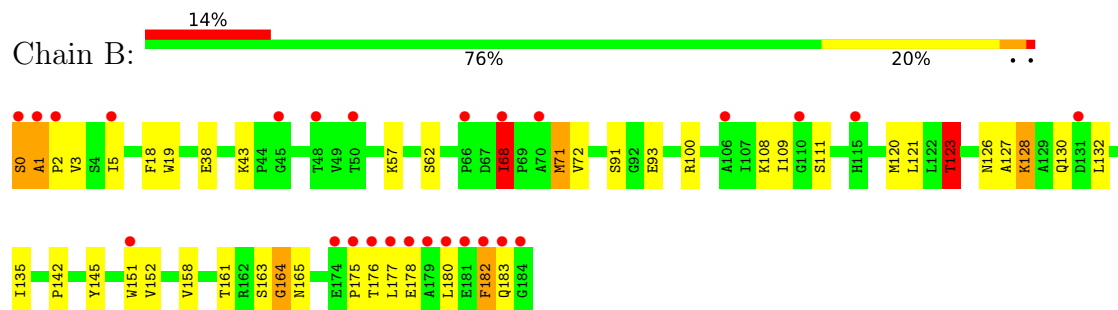
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

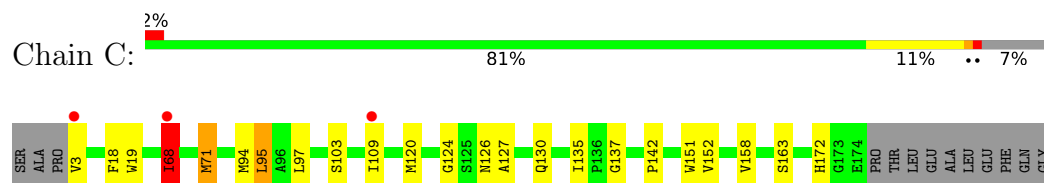
• Molecule 1: NS6 Protease



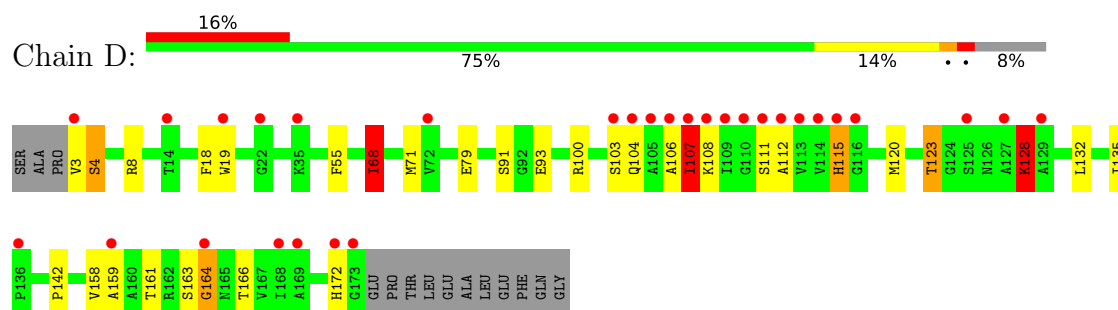
• Molecule 1: NS6 Protease



• Molecule 1: NS6 Protease



• Molecule 1: NS6 Protease



- Molecule 2: NS6 Protease

Chain E:  80% 20%



- Molecule 3: NS6 Protease

Chain F:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.64Å 111.86Å 81.29Å 90.00° 119.24° 90.00°	Depositor
Resolution (Å)	70.89 – 2.30 70.89 – 2.31	Depositor EDS
% Data completeness (in resolution range)	75.6 (70.89-2.30) 75.7 (70.89-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.230 , 0.278 0.227 , 0.272	Depositor DCC
R_{free} test set	860 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.1	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	0.94	EDS
Total number of atoms	5356	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.99	2/1322 (0.2%)	1.10	10/1797 (0.6%)
1	B	0.87	1/1408 (0.1%)	1.06	5/1913 (0.3%)
1	C	0.87	0/1298	1.05	8/1764 (0.5%)
1	D	0.78	0/1289	1.02	5/1752 (0.3%)
2	E	1.10	0/41	0.98	0/53
All	All	0.88	3/5358 (0.1%)	1.06	28/7279 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	SER	CA-C	-6.68	1.44	1.52
1	B	165	ASN	N-CA	-5.72	1.39	1.46
1	A	86	LEU	CA-C	-5.33	1.46	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	VAL	CB-CA-C	-8.87	103.16	111.05
1	A	163	SER	N-CA-C	-8.68	95.15	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	GLY	N-CA-C	7.18	120.89	111.70
1	D	4	SER	N-CA-C	-6.67	98.38	108.52
1	C	172	HIS	N-CA-C	6.60	120.79	112.87
1	C	135	ILE	CA-C-N	-6.47	113.10	119.90
1	C	135	ILE	C-N-CA	-6.47	113.10	119.90
1	A	135	ILE	CA-C-N	-6.29	113.47	119.76
1	A	135	ILE	C-N-CA	-6.29	113.47	119.76
1	D	135	ILE	CA-C-N	-6.05	113.54	119.90
1	D	135	ILE	C-N-CA	-6.05	113.54	119.90
1	B	68	ILE	N-CA-C	5.75	114.20	107.77
1	B	135	ILE	CA-C-N	-5.67	114.09	119.76
1	B	135	ILE	C-N-CA	-5.67	114.09	119.76
1	A	151	TRP	CA-CB-CG	5.59	124.23	113.60
1	A	163	SER	CA-C-O	-5.53	114.24	120.43
1	A	68	ILE	N-CA-C	5.43	113.86	107.77
1	C	68	ILE	N-CA-C	5.35	113.76	107.77
1	D	68	ILE	N-CA-C	5.33	113.74	107.77
1	C	137	GLY	N-CA-C	-5.25	107.75	114.85
1	A	128	LYS	N-CA-C	5.21	117.86	111.82
1	C	163	SER	N-CA-C	5.20	118.72	112.38
1	D	115	HIS	N-CA-C	5.19	117.69	109.50
1	A	85	VAL	CB-CA-C	-5.14	103.93	110.98
1	B	178	GLU	N-CA-C	5.14	116.80	109.14
1	C	126	ASN	N-CA-C	5.10	116.53	109.54
1	A	130	GLN	N-CA-C	5.06	119.33	113.20
1	B	123	THR	N-CA-CB	-5.01	102.58	110.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	THR	Peptide
1	B	164	GLY	Peptide
1	D	164	GLY	Peptide

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	1288	0	1300	19	0
1	B	1372	0	1378	32	0
1	C	1268	0	1272	13	0
1	D	1259	0	1266	43	0
2	E	41	0	36	0	0
3	F	35	0	10	1	0
4	D	5	0	5	3	0
5	A	39	0	0	1	0
5	B	24	0	0	1	0
5	C	22	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
All	All	5356	0	5267	94	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 9.

All (94) 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:B:120:MET:HE2	1:C:120:MET:HE2	1.32	1.11
1:A:106:ALA:O	1:A:107:ILE:HG12	1.61	0.98
1:D:55:PHE:CE1	1:D:172:HIS:HB2	2.03	0.94
1:A:120:MET:HE2	1:D:120:MET:HE2	1.51	0.92
1:C:94:MET:HE1	1:D:93:GLU:HB3	1.52	0.90
1:B:91:SER:OG	1:B:93:GLU:HG2	1.72	0.89
1:A:71:MET:HE3	1:A:151:TRP:HB3	1.55	0.85
1:A:94:MET:HE1	1:B:93:GLU:HB3	1.60	0.84
1:A:79:GLU:OE2	1:D:166:THR:OG1	1.98	0.81
1:A:163:SER:O	1:A:163:SER:OG	1.98	0.79
1:A:120:MET:HE1	1:D:100:ARG:HG2	1.67	0.77
1:D:55:PHE:CD1	1:D:172:HIS:HB2	2.19	0.76
1:C:95:LEU:HD12	1:C:97:LEU:HD21	1.71	0.72
1:B:71:MET:HE3	1:B:151:TRP:HB3	1.73	0.71
1:C:94:MET:HE1	1:D:93:GLU:CB	2.22	0.70
1:B:100[A]:ARG:HH22	4:D:201:IMD:H2	1.55	0.70
1:D:8:ARG:CZ	1:D:71:MET:HE3	2.23	0.69
1:D:100:ARG:HH12	4:D:201:IMD:H4	1.56	0.69
1:B:72:VAL:HB	1:B:152:VAL:HG12	1.75	0.69
1:D:3:VAL:HG12	1:D:4:SER:N	2.07	0.69
1:D:91:SER:OG	1:D:93:GLU:OE1	2.06	0.68
1:B:108:LYS:O	1:B:109:ILE:HG13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HE2	5:B:214:HOH:O	1.95	0.65
1:D:8:ARG:NE	1:D:71:MET:HE3	2.12	0.65
1:B:126:ASN:OD1	1:B:164:GLY:HA2	1.97	0.64
1:D:106:ALA:HB2	1:D:115:HIS:ND1	2.13	0.64
1:D:108:LYS:NZ	1:D:159:ALA:HB2	2.13	0.63
1:D:106:ALA:CB	1:D:115:HIS:ND1	2.64	0.61
1:D:3:VAL:CG1	1:D:4:SER:N	2.64	0.60
1:D:108:LYS:HZ3	1:D:159:ALA:HB2	1.66	0.60
1:D:128:LYS:HD2	1:D:164:GLY:O	2.01	0.60
1:B:5:ILE:H	1:B:5:ILE:HD12	1.65	0.60
1:D:106:ALA:O	1:D:107:ILE:HG22	2.02	0.60
1:D:100:ARG:HH12	4:D:201:IMD:C4	2.15	0.59
1:C:127:ALA:O	1:C:130:GLN:O	2.23	0.56
1:B:38:GLU:OE2	1:B:43:LYS:NZ	2.23	0.54
1:A:120:MET:CE	1:D:100:ARG:HG2	2.38	0.53
1:A:120:MET:HE1	1:D:100:ARG:CG	2.38	0.52
1:B:100[A]:ARG:HB3	1:C:120:MET:HE1	1.92	0.52
1:B:100[B]:ARG:HB3	1:C:120:MET:HE1	1.92	0.52
1:D:108:LYS:NZ	1:D:159:ALA:CB	2.72	0.51
1:A:123:THR:HG21	1:A:132:LEU:O	2.11	0.51
1:D:123:THR:HG21	1:D:132:LEU:O	2.11	0.51
1:A:171:THR:O	1:A:172:HIS:HB2	2.11	0.50
1:B:126:ASN:OD1	1:B:164:GLY:CA	2.58	0.50
1:B:126:ASN:OD1	1:B:164:GLY:N	2.44	0.50
1:B:121:LEU:HD12	1:B:127:ALA:CB	2.41	0.50
1:D:111:SER:O	1:D:112:ALA:HB2	2.12	0.50
1:B:123:THR:HG21	1:B:132:LEU:O	2.12	0.50
1:B:108:LYS:C	1:B:109:ILE:HG13	2.36	0.50
1:B:176:THR:O	1:B:177:LEU:HD23	2.13	0.48
1:B:1:ALA:HB1	1:B:2:PRO:HD2	1.95	0.48
1:D:55:PHE:CZ	1:D:172:HIS:HB2	2.45	0.48
1:D:128:LYS:CE	1:D:164:GLY:O	2.62	0.47
1:D:106:ALA:HB1	1:D:115:HIS:CE1	2.49	0.47
1:B:127:ALA:O	1:B:130:GLN:O	2.33	0.47
1:C:94:MET:CE	1:D:93:GLU:HB3	2.37	0.47
1:D:8:ARG:CD	1:D:71:MET:HE3	2.44	0.47
1:B:18:PHE:CD1	1:B:142:PRO:HG3	2.51	0.46
1:C:19:TRP:HB3	1:C:68:ILE:HD12	1.97	0.46
1:D:123:THR:HG23	1:D:132:LEU:HB3	1.97	0.45
1:A:3:VAL:HG11	1:A:68:ILE:CG2	2.47	0.45
1:B:123:THR:HG23	1:B:132:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ILE:O	1:D:107:ILE:HG23	2.16	0.45
1:A:57:LYS:HE3	1:A:174:GLU:HB3	1.98	0.45
1:A:57:LYS:HE3	1:A:174:GLU:CB	2.47	0.45
1:D:18:PHE:HZ	1:D:71:MET:HE1	1.80	0.45
1:D:123:THR:CG2	1:D:132:LEU:HB3	2.46	0.45
1:B:19:TRP:HB3	1:B:68:ILE:HD12	1.99	0.44
1:A:5:ILE:HA	1:A:8[B]:ARG:HH11	1.81	0.44
1:D:55:PHE:CE1	1:D:172:HIS:CB	2.89	0.44
1:A:43:LYS:NZ	5:A:201:HOH:O	2.48	0.44
1:D:128:LYS:HD3	1:D:161:THR:O	2.18	0.43
1:B:0:SER:O	1:B:0:SER:OG	2.32	0.43
1:D:128:LYS:CD	1:D:164:GLY:O	2.66	0.43
1:B:128:LYS:HD2	1:B:128:LYS:HA	1.61	0.43
1:C:3:VAL:HG11	1:C:68:ILE:CG2	2.48	0.43
1:D:107:ILE:O	1:D:107:ILE:CG2	2.67	0.43
1:B:3:VAL:HG11	1:B:68:ILE:CG2	2.49	0.43
1:A:107:ILE:HG13	3:F:5:UNK:HA	2.00	0.43
1:B:161:THR:HG21	1:C:103:SER:OG	2.19	0.43
1:D:18:PHE:CD1	1:D:142:PRO:HG3	2.54	0.43
1:C:71:MET:HE3	1:C:151:TRP:HB3	2.01	0.42
1:B:123:THR:CG2	1:B:132:LEU:HB3	2.49	0.42
1:D:19:TRP:HB3	1:D:68:ILE:HD12	2.01	0.42
1:A:106:ALA:C	1:A:107:ILE:HG12	2.36	0.42
1:B:145:TYR:CE1	1:B:152:VAL:CG2	3.03	0.42
1:D:8:ARG:CD	1:D:71:MET:CE	2.98	0.42
1:A:18:PHE:CD1	1:A:142:PRO:HG3	2.54	0.42
1:D:106:ALA:HB1	1:D:115:HIS:ND1	2.34	0.41
1:D:106:ALA:CB	1:D:115:HIS:CE1	3.04	0.41
1:C:18:PHE:CD1	1:C:142:PRO:HG3	2.55	0.41
1:B:91:SER:OG	1:B:93:GLU:CG	2.58	0.41
1:B:182:PHE:C	1:B:183:GLN:HG3	2.46	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	173/185 (94%)	165 (95%)	7 (4%)	1 (1%)	21	27
1	B	184/185 (100%)	178 (97%)	4 (2%)	2 (1%)	11	13
1	C	170/185 (92%)	163 (96%)	6 (4%)	1 (1%)	21	27
1	D	169/185 (91%)	158 (94%)	9 (5%)	2 (1%)	10	12
2	E	3/5 (60%)	3 (100%)	0	0	100	100
All	All	699/745 (94%)	667 (95%)	26 (4%)	6 (1%)	14	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	128	LYS
1	D	107	ILE
1	B	175	PRO
1	A	111	SER
1	C	109	ILE
1	B	1	ALA

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	133/141 (94%)	125 (94%)	8 (6%)	17	25
1	B	142/141 (101%)	131 (92%)	11 (8%)	12	16
1	C	131/141 (93%)	126 (96%)	5 (4%)	29	44
1	D	130/141 (92%)	121 (93%)	9 (7%)	14	20
2	E	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	540/568 (95%)	506 (94%)	34 (6%)	16	23

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ILE
1	A	71	MET
1	A	100	ARG
1	A	104	GLN
1	A	107	ILE
1	A	123	THR
1	A	128	LYS
1	A	152	VAL
1	B	0	SER
1	B	62	SER
1	B	68	ILE
1	B	71	MET
1	B	111	SER
1	B	123	THR
1	B	128	LYS
1	B	158	VAL
1	B	163	SER
1	B	180	LEU
1	B	182	PHE
1	C	68	ILE
1	C	71	MET
1	C	95	LEU
1	C	152	VAL
1	C	158	VAL
1	D	68	ILE
1	D	79	GLU
1	D	103	SER
1	D	104	GLN
1	D	107	ILE
1	D	123	THR
1	D	128	LYS
1	D	158	VAL
1	D	163	SER
2	E	183	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	B	130	GLN
1	B	165	ASN
1	C	78	GLN
1	C	165	ASN

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Mol	Chain	Res	Type
1	D	130	GLN
1	D	165	ASN
1	D	172	HIS
2	E	183	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	IMD	D	201	-	5,5,5	0.70	0	5,5,5	0.75	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
4	IMD	D	201	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	201	IMD	3	0

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	174/185 (94%)	0.52	15 (8%) 16 17	19, 54, 116, 161	1 (0%)
1	B	185/185 (100%)	0.87	26 (14%) 6 7	26, 71, 131, 167	1 (0%)
1	C	172/185 (92%)	0.43	3 (1%) 69 70	35, 59, 104, 140	0
1	D	171/185 (92%)	1.28	30 (17%) 4 4	48, 103, 179, 202	0
2	E	5/5 (100%)	0.29	0 100 100	36, 45, 49, 58	0
3	F	0/7	-	-	-	-
All	All	707/752 (94%)	0.77	74 (10%) 11 13	19, 70, 148, 202	2 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	ILE	4.6
1	B	180	LEU	4.6
1	B	179	ALA	4.5
1	D	105	ALA	4.4
1	A	106	ALA	4.2
1	D	108	LYS	4.1
1	A	112	ALA	4.1
1	D	3	VAL	3.8
1	B	182	PHE	3.8
1	D	116	GLY	3.8
1	B	175	PRO	3.7
1	D	109	ILE	3.7
1	A	104	GLN	3.7
1	A	108	LYS	3.6
1	A	105	ALA	3.6
1	B	184	GLY	3.4
1	B	110	GLY	3.3
1	A	109	ILE	3.3
1	B	106	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	176	THR	3.2
1	D	173	GLY	3.2
1	D	172	HIS	3.2
1	B	115	HIS	3.1
1	A	1	ALA	3.1
1	D	103	SER	3.0
1	D	112	ALA	3.0
1	D	107	ILE	3.0
1	D	72	VAL	3.0
1	D	129	ALA	2.9
1	B	131	ASP	2.9
1	B	181	GLU	2.9
1	D	106	ALA	2.9
1	A	173	GLY	2.9
1	B	183	GLN	2.9
1	C	109	ILE	2.9
1	D	127	ALA	2.8
1	A	110	GLY	2.7
1	D	114	VAL	2.7
1	D	113	VAL	2.7
1	D	159	ALA	2.7
1	D	136	PRO	2.7
1	D	104	GLN	2.6
1	D	35	LYS	2.6
1	B	174	GLU	2.6
1	B	151	TRP	2.6
1	B	70	ALA	2.6
1	D	164	GLY	2.6
1	D	168	ILE	2.6
1	B	66	PRO	2.6
1	B	177	LEU	2.5
1	D	169	ALA	2.5
1	D	110	GLY	2.5
1	B	5	ILE	2.4
1	D	111	SER	2.4
1	B	45	GLY	2.3
1	A	113	VAL	2.3
1	A	67	ASP	2.3
1	B	50	THR	2.3
1	B	48	THR	2.3
1	A	114	VAL	2.3
1	D	125	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	3	VAL	2.2
1	B	1	ALA	2.2
1	B	2	PRO	2.1
1	B	178	GLU	2.1
1	D	14	THR	2.1
1	A	125	SER	2.1
1	B	0	SER	2.1
1	A	115	HIS	2.1
1	D	115	HIS	2.1
1	C	68	ILE	2.1
1	D	22	GLY	2.1
1	D	19	TRP	2.1
1	B	68	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
4	IMD	D	201	5/5	0.91	0.12	32,35,38,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.