



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:47 PM UTC

PDB ID : 2W5E / pdb_00002w5e
Title : Structural and biochemical analysis of human pathogenic astrovirus serine protease at 2.0 Angstrom resolution
Authors : Speroni, S.; Rohayem, J.; Nenci, S.; Bonivento, D.; Robel, I.; Barthel, J.; Coutard, B.; Canard, B.; Mattevi, A.
Deposited on : 2008-12-10
Resolution : 2.00 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:

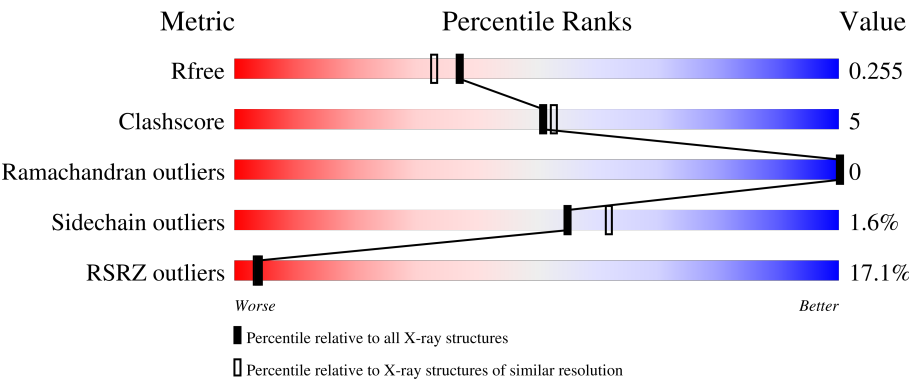
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	163	20% 92% 7% .
1	B	163	14% 91% 8% ..
1	C	163	15% 88% 10% ..
1	D	163	17% 91% 9% .
1	E	163	26% 88% 9% ..

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Mol	Chain	Length	Quality of chain
1	F	163	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1590	-	-	X	-
3	CL	A	1592	-	-	X	-
3	CL	B	1592	-	-	X	-
3	CL	C	1590	-	-	X	-
3	CL	C	1591	-	-	X	-
3	CL	D	1592	-	-	X	-
3	CL	D	1593	-	-	X	-
3	CL	E	1589	-	-	X	-
3	CL	F	1595	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7756 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 PUTATIVE SERINE PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1229	776	212	231	10			
1	B	162	Total	C	N	O	S	0	0	0
			1229	776	212	231	10			
1	C	162	Total	C	N	O	S	0	0	0
			1229	776	212	231	10			
1	D	162	Total	C	N	O	S	0	0	0
			1229	776	212	231	10			
1	E	162	Total	C	N	O	S	0	0	0
			1229	776	212	231	10			
1	F	162	Total	C	N	O	S	0	0	0
			1229	776	212	231	10			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cd	0	0
			4	4		
2	B	2	Total	Cd	0	0
			2	2		
2	C	4	Total	Cd	0	0
			4	4		
2	D	2	Total	Cd	0	0
			2	2		
2	E	3	Total	Cd	0	0
			3	3		
2	F	3	Total	Cd	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Cl 4 4	0	0
3	B	4	Total Cl 4 4	0	0
3	C	5	Total Cl 5 5	0	0
3	D	5	Total Cl 5 5	0	0
3	E	4	Total Cl 4 4	0	0
3	F	6	Total Cl 6 6	0	0

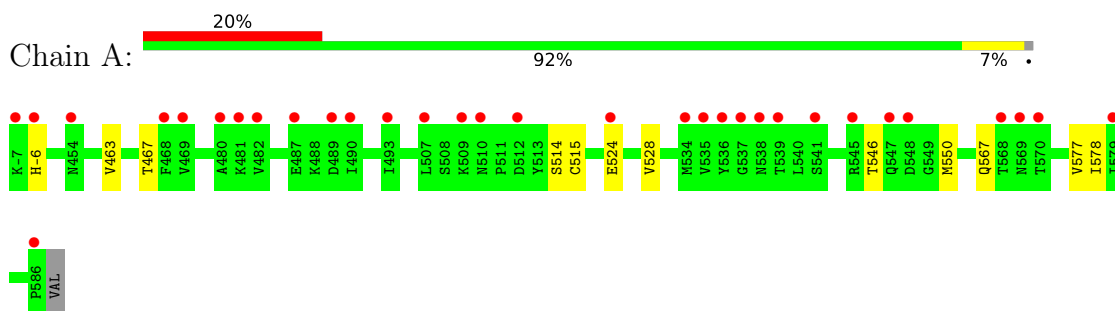
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0
4	B	60	Total O 60 60	0	0
4	C	54	Total O 54 54	0	0
4	D	52	Total O 52 52	0	0
4	E	38	Total O 38 38	0	0
4	F	64	Total O 64 64	0	0

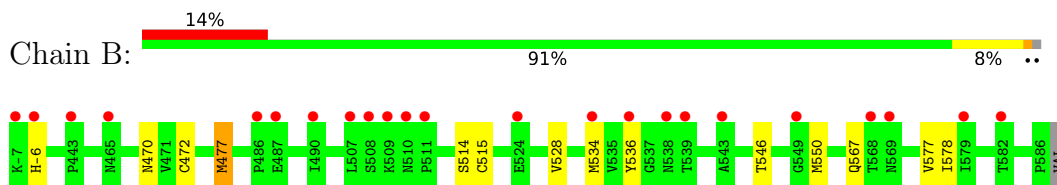
3 Residue-property plots [i](#)

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.

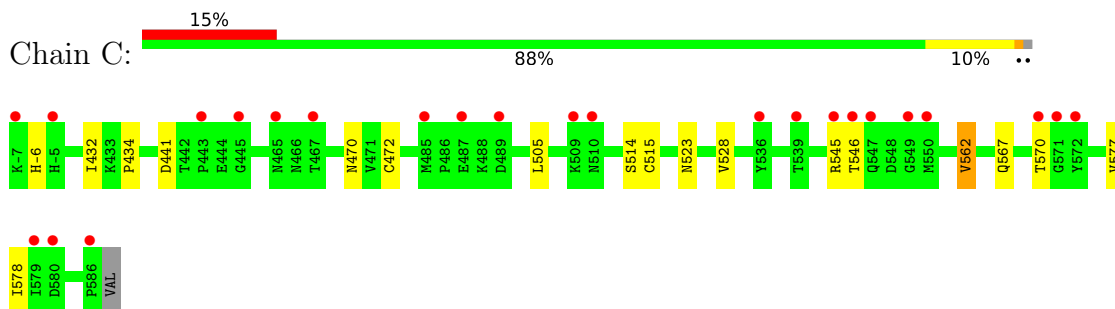
• Molecule 1: PUTATIVE SERINE PROTEASE



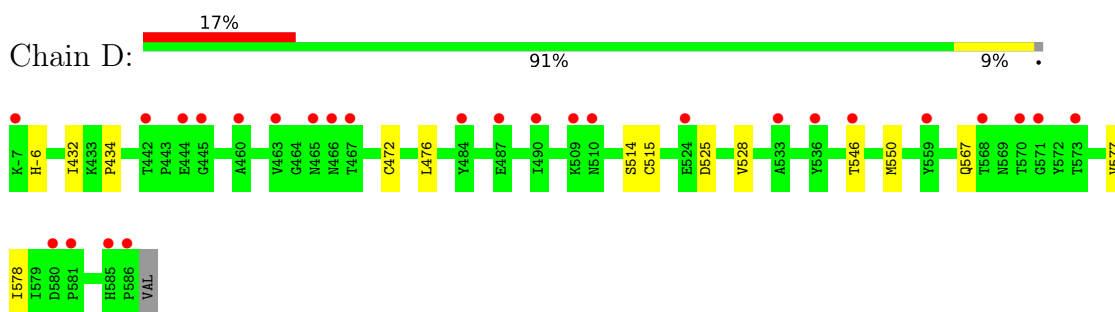
• Molecule 1: PUTATIVE SERINE PROTEASE



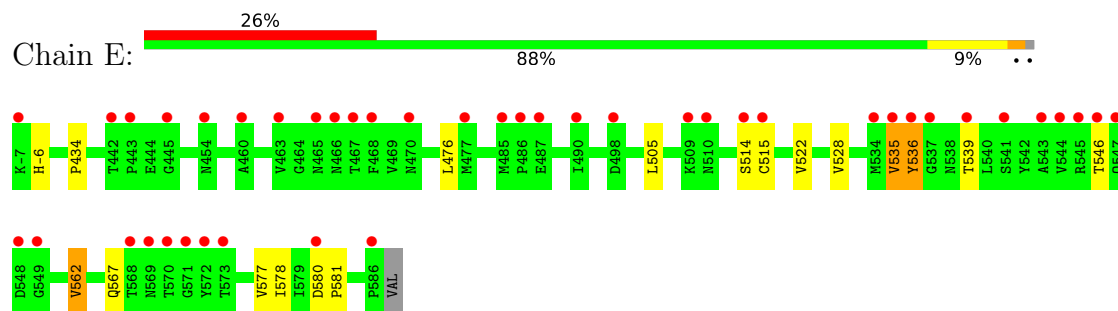
• Molecule 1: PUTATIVE SERINE PROTEASE



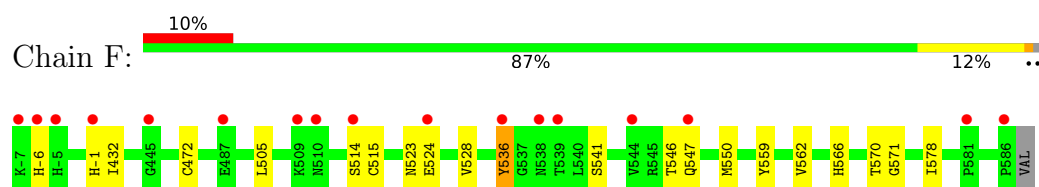
• Molecule 1: PUTATIVE SERINE PROTEASE



- Molecule 1: PUTATIVE SERINE PROTEASE



- Molecule 1: PUTATIVE SERINE PROTEASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.05Å 135.05Å 189.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.00) 97.8 (30.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.258 0.232 , 0.255	Depositor DCC
R_{free} test set	1333 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7756	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: CD, CL

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	0.56	1/1261 (0.1%)	0.70	0/1719
1	B	0.59	0/1261	0.69	0/1719
1	C	0.53	0/1261	0.70	0/1719
1	D	0.52	0/1261	0.69	0/1719
1	E	0.56	0/1261	0.81	5/1719 (0.3%)
1	F	0.64	2/1261 (0.2%)	0.70	0/1719
All	All	0.57	3/7566 (0.0%)	0.72	5/10314 (0.0%)

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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	566	HIS	C-O	-6.49	1.16	1.23
1	F	570	THR	C-O	-5.12	1.18	1.24
1	A	467	THR	C-O	-5.03	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	536	TYR	N-CA-C	9.90	125.13	111.17
1	E	536	TYR	CA-C-N	-5.97	112.70	121.72
1	E	536	TYR	C-N-CA	-5.97	112.70	121.72
1	E	536	TYR	CA-C-O	-5.75	115.60	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	535	VAL	CB-CA-C	-5.40	104.81	111.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	570	THR	Peptide

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	1229	0	1187	7	0
1	B	1229	0	1187	12	0
1	C	1229	0	1187	14	0
1	D	1229	0	1188	14	0
1	E	1229	0	1186	15	0
1	F	1229	0	1188	16	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	2	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	A	4	0	0	6	0
3	B	4	0	0	3	0
3	C	5	0	0	5	0
3	D	5	0	0	5	0
3	E	4	0	0	3	0
3	F	6	0	0	6	0
4	A	68	0	0	3	0
4	B	60	0	0	1	1
4	C	54	0	0	1	0
4	D	52	0	0	1	0
4	E	38	0	0	1	0
4	F	64	0	0	3	1
All	All	7756	0	7123	73	1

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 5.

All (73) 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)
3:C:1591:CL:CL	1:D:472:CYS:SG	2.39	1.17
1:F:514:SER:OG	3:F:1595:CL:CL	2.03	1.12
1:C:472:CYS:SG	3:D:1593:CL:CL	2.54	1.03
1:B:515:CYS:SG	3:B:1592:CL:CL	2.55	1.00
4:E:2010:HOH:O	3:F:1591:CL:CL	2.18	0.97
3:A:1592:CL:CL	1:B:472:CYS:SG	2.63	0.94
1:F:524:GLU:OE1	4:F:2046:HOH:O	1.84	0.93
1:C:515:CYS:SG	3:C:1590:CL:CL	2.63	0.93
1:A:515:CYS:SG	3:A:1590:CL:CL	2.65	0.92
1:D:-6:HIS:ND1	3:D:1593:CL:CL	2.41	0.91
1:E:535:VAL:O	1:E:539:THR:O	1.89	0.89
1:F:546:THR:HG22	1:F:550:MET:HE3	1.57	0.87
1:E:-6:HIS:ND1	3:E:1591:CL:CL	2.44	0.87
1:B:534:MET:SD	1:B:536:TYR:OH	2.36	0.83
1:B:546:THR:HG22	1:B:550:MET:HE3	1.60	0.83
1:A:-6:HIS:ND1	3:A:1592:CL:CL	2.49	0.79
1:A:546:THR:HG22	1:A:550:MET:HE3	1.62	0.79
1:F:472:CYS:SG	3:F:1587:CL:CL	2.79	0.77
1:F:515:CYS:SG	3:F:1595:CL:CL	2.80	0.76
1:D:515:CYS:SG	3:D:1592:CL:CL	2.84	0.73
3:A:1594:CL:CL	4:A:2021:HOH:O	2.44	0.72
1:C:-6:HIS:ND1	3:C:1591:CL:CL	2.57	0.72
1:B:546:THR:CG2	1:B:550:MET:HE3	2.21	0.70
1:C:514:SER:OG	3:C:1590:CL:CL	2.49	0.67
1:A:567:GLN:HG3	1:A:577:VAL:HG23	1.76	0.66
1:E:528:VAL:HB	1:F:528:VAL:HB	1.78	0.66
1:E:514:SER:OG	3:E:1589:CL:CL	2.50	0.65
1:F:547:GLN:NE2	1:F:571:GLY:HA2	2.12	0.64
3:A:1592:CL:CL	4:A:2007:HOH:O	2.52	0.64
1:E:515:CYS:SG	3:E:1589:CL:CL	2.93	0.62
1:D:546:THR:HG22	1:D:550:MET:HE3	1.82	0.61
3:C:1591:CL:CL	4:C:2005:HOH:O	2.53	0.61
1:D:567:GLN:HG3	1:D:577:VAL:HG23	1.84	0.60
1:F:547:GLN:CD	1:F:571:GLY:HA2	2.28	0.58
1:C:528:VAL:HB	1:D:528:VAL:HB	1.86	0.57
1:F:-6:HIS:ND1	3:F:1593:CL:CL	2.74	0.57
1:D:514:SER:OG	3:D:1592:CL:CL	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1593:CL:CL	4:D:2006:HOH:O	2.55	0.56
1:C:567:GLN:HG3	1:C:577:VAL:HG23	1.89	0.55
1:B:550:MET:HE1	4:B:2045:HOH:O	2.05	0.54
1:C:523:ASN:O	1:D:-6:HIS:CD2	2.62	0.52
1:E:567:GLN:HG3	1:E:577:VAL:HG23	1.90	0.52
1:A:514:SER:OG	3:A:1590:CL:CL	2.63	0.52
1:C:545:ARG:HH21	1:D:525:ASP:HB2	1.76	0.51
1:A:550:MET:HE1	4:A:2056:HOH:O	2.10	0.50
1:E:434:PRO:HG2	1:F:432:ILE:HD12	1.94	0.50
1:B:567:GLN:HG3	1:B:577:VAL:HG23	1.94	0.49
1:C:441:ASP:HB3	1:C:470:ASN:HB2	1.94	0.48
1:E:522:VAL:HG21	1:E:546:THR:HG21	1.94	0.48
1:B:-6:HIS:ND1	3:B:1591:CL:CL	2.82	0.48
1:C:434:PRO:HG2	1:D:432:ILE:HD12	1.97	0.46
1:D:476:LEU:HD13	1:E:476:LEU:HD13	1.98	0.46
1:A:528:VAL:HB	1:B:528:VAL:HB	1.96	0.46
1:F:536:TYR:HE2	1:F:541:SER:HB2	1.80	0.46
1:E:-6:HIS:CD2	1:F:523:ASN:O	2.68	0.46
1:E:536:TYR:CD2	1:E:539:THR:HB	2.51	0.45
1:C:505:LEU:HB3	1:C:562:VAL:CG2	2.46	0.45
1:E:505:LEU:HB3	1:E:562:VAL:HG22	1.98	0.45
1:E:505:LEU:HB3	1:E:562:VAL:CG2	2.47	0.45
1:F:505:LEU:HB3	1:F:562:VAL:HG23	1.98	0.44
1:B:470:ASN:HB3	1:B:477:MET:CE	2.48	0.43
1:E:536:TYR:HD2	1:E:539:THR:HB	1.84	0.43
1:C:432:ILE:HD12	1:D:434:PRO:HG2	2.01	0.43
1:B:514:SER:OG	3:B:1592:CL:CL	2.65	0.42
1:D:567:GLN:CG	1:D:577:VAL:HG23	2.49	0.42
1:B:470:ASN:HB3	1:B:477:MET:HE2	2.01	0.42
1:E:580:ASP:OD1	1:E:581:PRO:HD2	2.20	0.42
1:F:550:MET:HE1	4:F:2049:HOH:O	2.18	0.42
1:C:567:GLN:CG	1:C:577:VAL:HG23	2.49	0.42
3:F:1595:CL:CL	4:F:2044:HOH:O	2.58	0.42
1:F:536:TYR:CE2	1:F:541:SER:HB2	2.55	0.41
1:F:-1:HIS:HB2	1:F:559:TYR:O	2.20	0.41
1:C:523:ASN:O	1:D:-6:HIS:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2048:HOH:O	4:F:2063:HOH:O[4_545]	1.83	0.37

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	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
1	B	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
1	C	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
1	D	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
1	E	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
1	F	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
All	All	960/978 (98%)	932 (97%)	28 (3%)	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	133/135 (98%)	130 (98%)	3 (2%)	44	49
1	B	133/135 (98%)	131 (98%)	2 (2%)	57	64
1	C	133/135 (98%)	130 (98%)	3 (2%)	44	49
1	D	133/135 (98%)	132 (99%)	1 (1%)	73	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	133/135 (98%)	131 (98%)	2 (2%)	57	64
1	F	133/135 (98%)	131 (98%)	2 (2%)	57	64
All	All	798/810 (98%)	785 (98%)	13 (2%)	55	62

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

Mol	Chain	Res	Type
1	A	463	VAL
1	A	524	GLU
1	A	578	ILE
1	B	477	MET
1	B	578	ILE
1	C	546	THR
1	C	562	VAL
1	C	578	ILE
1	D	578	ILE
1	E	562	VAL
1	E	578	ILE
1	F	536	TYR
1	F	578	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	585	HIS
1	B	585	HIS
1	C	466	ASN
1	C	547	GLN
1	E	510	ASN
1	E	585	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 46 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	162/163 (99%)	1.32	32 (19%) 3 3	22, 31, 44, 46	0
1	B	162/163 (99%)	1.14	23 (14%) 6 5	22, 31, 43, 46	0
1	C	162/163 (99%)	1.11	24 (14%) 5 5	23, 32, 44, 46	0
1	D	162/163 (99%)	1.13	27 (16%) 4 4	23, 32, 44, 47	0
1	E	162/163 (99%)	1.46	43 (26%) 1 1	24, 33, 45, 48	0
1	F	162/163 (99%)	1.04	17 (10%) 11 10	23, 32, 43, 46	0
All	All	972/978 (99%)	1.20	166 (17%) 4 4	22, 32, 44, 48	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-7	LYS	7.2
1	A	510	ASN	7.1
1	E	548	ASP	7.0
1	F	536	TYR	6.9
1	B	487	GLU	6.4
1	E	536	TYR	6.4
1	F	-7	LYS	5.9
1	B	-7	LYS	5.8
1	A	536	TYR	5.8
1	A	569	ASN	5.6
1	D	-7	LYS	5.5
1	F	538	ASN	5.2
1	E	537	GLY	5.1
1	B	538	ASN	5.1
1	A	509	LYS	5.1
1	B	536	TYR	5.0
1	E	543	ALA	5.0
1	D	465	ASN	4.9
1	F	524	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	568	THR	4.8
1	D	580	ASP	4.7
1	C	549	GLY	4.6
1	A	548	ASP	4.6
1	C	-7	LYS	4.6
1	A	547	GLN	4.5
1	A	534	MET	4.4
1	F	487	GLU	4.4
1	C	487	GLU	4.3
1	C	570	THR	4.3
1	E	510	ASN	4.1
1	C	580	ASP	4.1
1	E	549	GLY	4.0
1	B	534	MET	4.0
1	B	510	ASN	4.0
1	C	510	ASN	4.0
1	E	572	TYR	3.9
1	E	570	THR	3.9
1	D	536	TYR	3.8
1	E	547	GLN	3.8
1	D	445	GLY	3.8
1	E	534	MET	3.8
1	D	509	LYS	3.7
1	E	509	LYS	3.7
1	C	536	TYR	3.6
1	E	465	ASN	3.6
1	C	546	THR	3.5
1	A	480	ALA	3.5
1	C	586	PRO	3.5
1	C	571	GLY	3.4
1	B	509	LYS	3.4
1	B	511	PRO	3.4
1	E	-7	LYS	3.4
1	B	-6	HIS	3.3
1	A	570	THR	3.3
1	B	465	ASN	3.3
1	F	586	PRO	3.3
1	D	570	THR	3.2
1	A	538	ASN	3.2
1	E	571	GLY	3.2
1	E	586	PRO	3.2
1	E	546	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	443	PRO	3.1
1	E	487	GLU	3.1
1	B	539	THR	3.1
1	B	549	GLY	3.0
1	C	445	GLY	3.0
1	C	465	ASN	3.0
1	D	546	THR	3.0
1	E	535	VAL	3.0
1	A	454	ASN	3.0
1	E	573	THR	3.0
1	E	580	ASP	3.0
1	A	487	GLU	3.0
1	D	586	PRO	3.0
1	E	541	SER	3.0
1	D	487	GLU	3.0
1	F	-6	HIS	3.0
1	A	586	PRO	2.9
1	A	482	VAL	2.9
1	A	541	SER	2.9
1	C	509	LYS	2.9
1	E	539	THR	2.9
1	A	512	ASP	2.8
1	A	539	THR	2.8
1	C	572	TYR	2.8
1	C	545	ARG	2.8
1	E	460	ALA	2.8
1	E	454	ASN	2.8
1	E	467	THR	2.8
1	A	535	VAL	2.8
1	B	579	ILE	2.8
1	F	514	SER	2.7
1	A	524	GLU	2.7
1	A	490	ILE	2.7
1	F	547	GLN	2.7
1	D	466	ASN	2.7
1	B	568	THR	2.7
1	A	-6	HIS	2.7
1	D	568	THR	2.6
1	F	544	VAL	2.6
1	E	445	GLY	2.6
1	A	537	GLY	2.6
1	C	-5	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	585	HIS	2.5
1	D	484	TYR	2.5
1	E	515	CYS	2.5
1	E	568	THR	2.5
1	D	581	PRO	2.5
1	B	524	GLU	2.4
1	A	468	PHE	2.4
1	E	466	ASN	2.4
1	E	463	VAL	2.4
1	E	545	ARG	2.4
1	D	571	GLY	2.4
1	E	569	ASN	2.3
1	F	510	ASN	2.3
1	F	-5	HIS	2.3
1	A	489	ASP	2.3
1	E	544	VAL	2.3
1	F	509	LYS	2.3
1	E	485	MET	2.3
1	D	490	ILE	2.3
1	F	539	THR	2.3
1	A	493	ILE	2.2
1	A	579	ILE	2.2
1	E	490	ILE	2.2
1	C	443	PRO	2.2
1	C	467	THR	2.2
1	E	442	THR	2.2
1	E	498	ASP	2.2
1	C	579	ILE	2.2
1	E	486	PRO	2.2
1	E	477	MET	2.2
1	B	507	LEU	2.2
1	C	547	GLN	2.2
1	B	508	SER	2.2
1	C	550	MET	2.2
1	E	514	SER	2.2
1	D	559	TYR	2.2
1	A	481	LYS	2.2
1	D	510	ASN	2.2
1	C	485	MET	2.2
1	D	467	THR	2.2
1	F	581	PRO	2.1
1	E	468	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	533	ALA	2.1
1	E	470	ASN	2.1
1	C	489	ASP	2.1
1	B	443	PRO	2.1
1	B	490	ILE	2.1
1	A	469	VAL	2.1
1	D	573	THR	2.1
1	F	-1	HIS	2.1
1	A	507	LEU	2.1
1	B	486	PRO	2.1
1	B	582	THR	2.1
1	D	463	VAL	2.1
1	D	444	GLU	2.0
1	B	569	ASN	2.0
1	C	539	THR	2.0
1	D	442	THR	2.0
1	D	524	GLU	2.0
1	B	543	ALA	2.0
1	D	460	ALA	2.0
1	A	545	ARG	2.0
1	F	445	GLY	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
2	CD	C	1592	1/1	0.87	0.10	68,68,68,68	0
3	CL	E	1589	1/1	0.89	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	A	1591	1/1	0.90	0.12	58,58,58,58	0
3	CL	E	1593	1/1	0.91	0.19	50,50,50,50	0
3	CL	B	1587	1/1	0.92	0.11	39,39,39,39	0
3	CL	D	1593	1/1	0.93	0.09	38,38,38,38	0
2	CD	F	1594	1/1	0.93	0.09	67,67,67,67	0
3	CL	D	1588	1/1	0.93	0.15	42,42,42,42	0
3	CL	F	1588	1/1	0.93	0.12	40,40,40,40	0
3	CL	D	1587	1/1	0.94	0.15	52,52,52,52	0
2	CD	C	1594	1/1	0.95	0.07	55,55,55,55	0
3	CL	C	1595	1/1	0.95	0.15	41,41,41,41	0
3	CL	A	1592	1/1	0.96	0.08	19,19,19,19	0
3	CL	D	1590	1/1	0.96	0.08	31,31,31,31	0
3	CL	A	1590	1/1	0.96	0.15	26,26,26,26	0
3	CL	F	1591	1/1	0.96	0.08	36,36,36,36	0
3	CL	F	1593	1/1	0.96	0.06	37,37,37,37	0
3	CL	E	1588	1/1	0.97	0.11	32,32,32,32	0
2	CD	A	1593	1/1	0.97	0.07	58,58,58,58	0
3	CL	C	1590	1/1	0.97	0.12	28,28,28,28	0
3	CL	C	1591	1/1	0.97	0.06	33,33,33,33	0
3	CL	F	1589	1/1	0.97	0.08	32,32,32,32	0
3	CL	D	1592	1/1	0.97	0.07	26,26,26,26	0
3	CL	A	1594	1/1	0.97	0.05	29,29,29,29	0
2	CD	E	1592	1/1	0.98	0.06	55,55,55,55	0
2	CD	C	1589	1/1	0.98	0.03	29,29,29,29	0
3	CL	C	1593	1/1	0.98	0.09	41,41,41,41	0
3	CL	E	1591	1/1	0.98	0.04	29,29,29,29	0
2	CD	E	1590	1/1	0.98	0.03	30,30,30,30	0
3	CL	F	1587	1/1	0.98	0.07	35,35,35,35	0
3	CL	B	1589	1/1	0.98	0.06	28,28,28,28	0
3	CL	B	1591	1/1	0.98	0.08	36,36,36,36	0
3	CL	B	1592	1/1	0.98	0.18	17,17,17,17	0
3	CL	C	1588	1/1	0.98	0.06	34,34,34,34	0
3	CL	F	1595	1/1	0.98	0.18	11,11,11,11	0
2	CD	F	1592	1/1	0.99	0.02	28,28,28,28	0
2	CD	A	1589	1/1	0.99	0.02	23,23,23,23	0
3	CL	A	1588	1/1	0.99	0.06	32,32,32,32	0
2	CD	B	1588	1/1	0.99	0.02	26,26,26,26	0
2	CD	D	1589	1/1	0.99	0.02	23,23,23,23	0
2	CD	D	1591	1/1	0.99	0.02	24,24,24,24	0
2	CD	E	1587	1/1	0.99	0.02	24,24,24,24	0
2	CD	C	1587	1/1	0.99	0.02	26,26,26,26	0
2	CD	A	1587	1/1	0.99	0.02	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	F	1590	1/1	0.99	0.03	26,26,26,26	0
2	CD	B	1590	1/1	1.00	0.02	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.