Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:11 AM GMT

PDB ID	:	2W5E
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

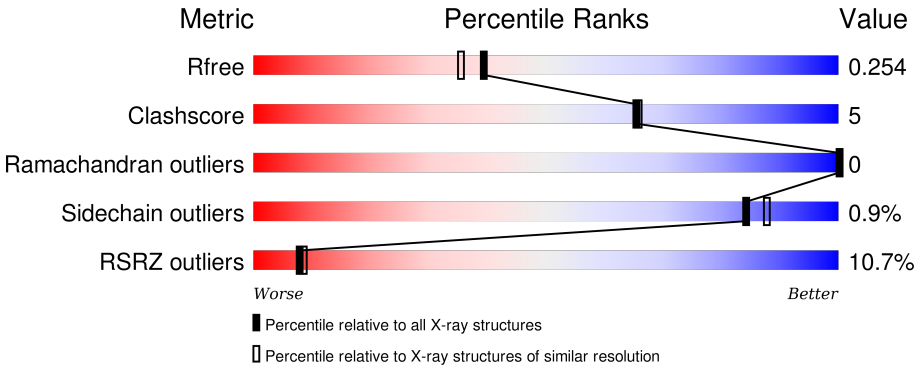
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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 <=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	12% 96%
1	B	163	12% 91% 8%
1	C	163	6% 87% 12%
1	D	163	10% 93% 7%
1	E	163	13% 89% 9%

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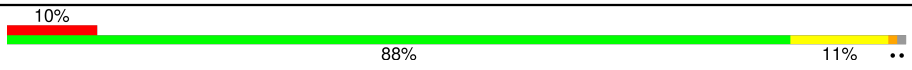
Mol	Chain	Length	Quality of chain
1	F	163	

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

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 (three-letter code: CD) (formula: Cd).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

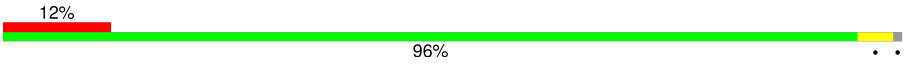
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	68	Total O 68 68	0	0
4	B	60	Total O 60 60	0	0
4	C	54	Total O 54 54	0	0
4	D	52	Total O 52 52	0	0
4	E	38	Total O 38 38	0	0
4	F	64	Total O 64 64	0	0

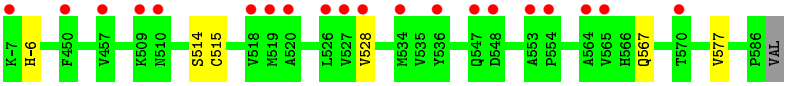
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

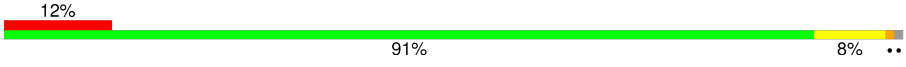
Chain A:

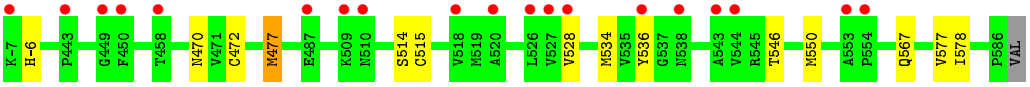




- Molecule 1: PUTATIVE SERINE PROTEASE

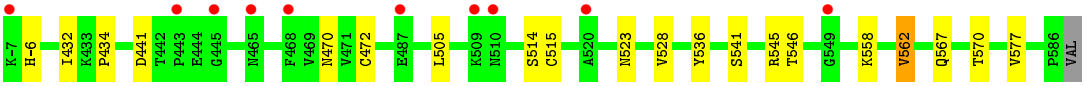
Chain B:





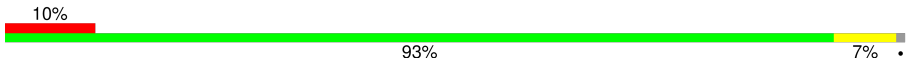
- Molecule 1: PUTATIVE SERINE PROTEASE

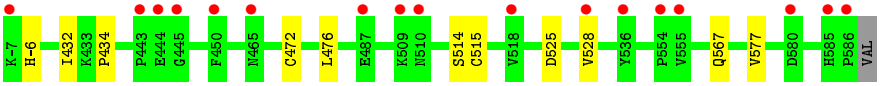
Chain C:



- Molecule 1: PUTATIVE SERINE PROTEASE

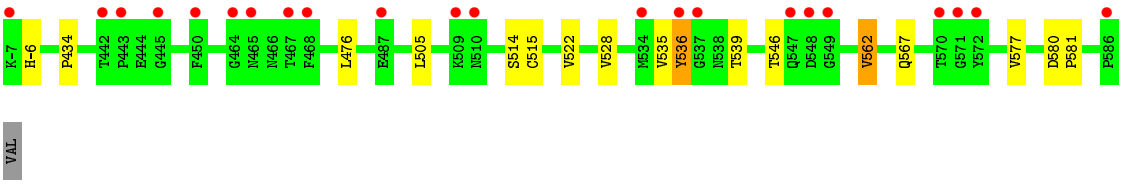
Chain D:





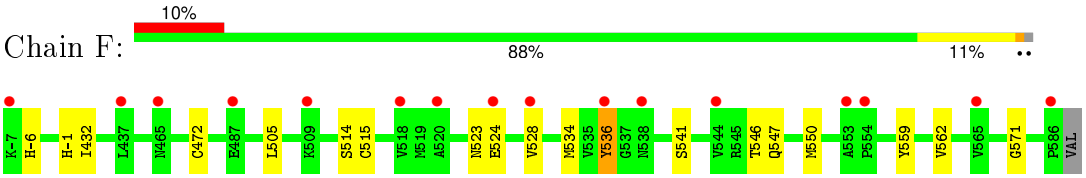
- Molecule 1: PUTATIVE SERINE PROTEASE

Chain E:



- Molecule 1: PUTATIVE SERINE PROTEASE

Chain F:


10%
88%
11%
K-7
H-6
H-1
I432
I437
M465
C472
E487
L505
K509
S514
C515
V518
M519
A520
N523
E524
V528
M534
V535
Y536
G537
N538
S541
V544
R545
T546
Q547
M550
A553
P554
Y559
V562
V565
G571
P586
VAL

4 Data and refinement statistics (i)

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 29.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.00) 97.9 (29.79-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.258 0.232 , 0.254	Depositor DCC
R_{free} test set	1333 reflections (1.02%)	DCC
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.0	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 132317 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, CD

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	0.41	0/1261	0.53	0/1719
1	B	0.44	0/1261	0.54	0/1719
1	C	0.39	0/1261	0.55	0/1719
1	D	0.39	0/1261	0.53	0/1719
1	E	0.44	0/1261	0.60	1/1719 (0.1%)
1	F	0.48	0/1261	0.54	0/1719
All	All	0.43	0/7566	0.55	1/10314 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	536	TYR	N-CA-C	5.23	125.13	111.00

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	5	0
1	B	1229	0	1187	11	0
1	C	1229	0	1187	15	0
1	D	1229	0	1188	13	0
1	E	1229	0	1186	15	0
1	F	1229	0	1188	17	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	2	0
4	B	60	0	0	0	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	2	1
All	All	7756	0	7123	71	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 (71) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:-6:HIS:ND1	3:A:1592:CL:CL	2.49	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:C:514:SER:OG	3:C:1590:CL:CL	2.49	0.67
1:E:528:VAL:HB	1:F:528:VAL:HB	1.78	0.66
1:A:567:GLN:HG3	1:A:577:VAL:HG23	1.76	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
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:D:514:SER:OG	3:D:1592:CL:CL	2.57	0.59
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
3:D:1593:CL:CL	4:D:2006:HOH:O	2.55	0.56
1:B:470:ASN:HB3	1:B:477:MET:HE2	1.87	0.56
1:F:534:MET:SD	1:F:536:TYR:OH	2.60	0.55
1:C:536:TYR:HE1	1:C:541:SER:HG	1.52	0.55
1:C:567:GLN:HG3	1:C:577:VAL:HG23	1.89	0.55
1:F:547:GLN:CD	1:F:571:GLY:HA2	2.28	0.53
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: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:E:522:VAL:HG21	1:E:546:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ASP:HB3	1:C:470:ASN:HB2	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:B:546:THR:HG22	1:B:550:MET:HE3	1.97	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:F:546:THR:HG22	1:F:550:MET:CE	2.46	0.45
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:F:546:THR:HG22	1:F:550:MET:HE2	1.98	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:E:536:TYR:HD2	1:E:539:THR:HB	1.84	0.43
1:B:470:ASN:HB3	1:B:477:MET:CE	2.48	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:E:580:ASP:OD1	1:E:581:PRO:HD2	2.20	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:B:546:THR:HG22	1:B:550:MET:CE	2.50	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%)	133 (100%)	0	100	100
1	B	133/135 (98%)	131 (98%)	2 (2%)	72	75
1	C	133/135 (98%)	130 (98%)	3 (2%)	58	60
1	D	133/135 (98%)	133 (100%)	0	100	100
1	E	133/135 (98%)	132 (99%)	1 (1%)	86	89
1	F	133/135 (98%)	132 (99%)	1 (1%)	86	89
All	All	798/810 (98%)	791 (99%)	7 (1%)	84	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	477	MET
1	B	578	ILE
1	C	546	THR

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Mol	Chain	Res	Type
1	C	558	LYS
1	C	562	VAL
1	E	562	VAL
1	F	536	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	466	ASN
1	B	466	ASN
1	D	466	ASN
1	E	466	ASN
1	F	466	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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, 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	162/163 (99%)	0.60	20 (12%) 5 6	22, 31, 44, 46	0
1	B	162/163 (99%)	0.58	19 (11%) 6 7	22, 31, 43, 46	0
1	C	162/163 (99%)	0.43	10 (6%) 24 25	23, 32, 44, 47	0
1	D	162/163 (99%)	0.55	17 (10%) 8 9	23, 32, 44, 47	0
1	E	162/163 (99%)	0.74	22 (13%) 4 4	24, 33, 45, 48	0
1	F	162/163 (99%)	0.49	16 (9%) 9 10	23, 32, 43, 46	0
All	All	972/978 (99%)	0.57	104 (10%) 8 8	22, 32, 44, 48	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	572	TYR	5.5
1	F	-7	LYS	5.5
1	A	-7	LYS	4.8
1	E	536	TYR	4.5
1	E	465	ASN	4.5
1	E	548	ASP	4.5
1	B	-7	LYS	4.4
1	E	547	GLN	4.4
1	A	536	TYR	4.3
1	B	528	VAL	4.3
1	D	509	LYS	4.3
1	A	510	ASN	4.3
1	D	465	ASN	4.1
1	A	528	VAL	4.0
1	E	510	ASN	4.0
1	E	509	LYS	4.0
1	E	571	GLY	3.8
1	E	443	PRO	3.6
1	C	509	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	527	VAL	3.5
1	F	528	VAL	3.5
1	E	570	THR	3.5
1	C	-7	LYS	3.5
1	A	509	LYS	3.5
1	D	487	GLU	3.5
1	A	526	LEU	3.3
1	F	509	LYS	3.3
1	B	487	GLU	3.3
1	B	509	LYS	3.2
1	C	445	GLY	3.2
1	E	464	GLY	3.2
1	B	520	ALA	3.2
1	C	487	GLU	3.1
1	D	518	VAL	3.0
1	E	537	GLY	3.0
1	A	520	ALA	3.0
1	A	534	MET	3.0
1	C	465	ASN	3.0
1	E	586	PRO	3.0
1	B	518	VAL	3.0
1	F	586	PRO	3.0
1	D	-7	LYS	2.9
1	D	445	GLY	2.9
1	B	526	LEU	2.9
1	B	554	PRO	2.9
1	B	450	PHE	2.8
1	A	553	ALA	2.8
1	E	468	PHE	2.8
1	A	518	VAL	2.8
1	F	536	TYR	2.8
1	E	445	GLY	2.8
1	F	554	PRO	2.7
1	E	442	THR	2.7
1	B	510	ASN	2.7
1	C	468	PHE	2.7
1	B	527	VAL	2.6
1	C	510	ASN	2.6
1	F	553	ALA	2.6
1	F	538	ASN	2.6
1	F	487	GLU	2.6
1	B	443	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	570	THR	2.5
1	E	549	GLY	2.5
1	D	444	GLU	2.5
1	D	528	VAL	2.5
1	A	548	ASP	2.5
1	D	554	PRO	2.5
1	E	-7	LYS	2.5
1	F	524	GLU	2.4
1	D	536	TYR	2.4
1	C	443	PRO	2.4
1	E	487	GLU	2.4
1	E	467	THR	2.4
1	A	547	GLN	2.3
1	B	458	THR	2.3
1	D	450	PHE	2.3
1	B	449	GLY	2.3
1	D	510	ASN	2.3
1	A	554	PRO	2.3
1	F	437	LEU	2.3
1	F	518	VAL	2.3
1	B	536	TYR	2.3
1	D	443	PRO	2.3
1	C	549	GLY	2.2
1	F	520	ALA	2.2
1	D	586	PRO	2.2
1	A	565	VAL	2.2
1	C	520	ALA	2.2
1	A	519	MET	2.2
1	E	534	MET	2.2
1	D	555	VAL	2.2
1	D	580	ASP	2.2
1	B	553	ALA	2.2
1	B	538	ASN	2.2
1	F	544	VAL	2.1
1	F	565	VAL	2.1
1	D	585	HIS	2.1
1	B	544	VAL	2.1
1	A	564	ALA	2.1
1	A	450	PHE	2.1
1	A	457	VAL	2.1
1	F	465	ASN	2.0
1	B	543	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	450	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	CL	E	1593	1/1	0.96	0.15	0.75	50,50,50,50	0
3	CL	A	1592	1/1	0.98	0.12	-0.45	19,19,19,19	0
3	CL	C	1591	1/1	0.98	0.10	-0.63	33,33,33,33	0
3	CL	D	1588	1/1	0.95	0.10	-0.75	42,42,42,42	0
3	CL	F	1593	1/1	0.97	0.04	-0.78	37,37,37,37	0
3	CL	D	1587	1/1	0.96	0.12	-0.87	52,52,52,52	0
3	CL	B	1591	1/1	0.98	0.03	-1.06	36,36,36,36	0
3	CL	C	1588	1/1	0.99	0.09	-1.08	34,34,34,34	0
3	CL	E	1591	1/1	0.98	0.04	-1.12	29,29,29,29	0
3	CL	C	1595	1/1	0.95	0.10	-1.19	41,41,41,41	0
3	CL	F	1588	1/1	0.95	0.08	-1.87	40,40,40,40	0
3	CL	C	1593	1/1	0.99	0.07	-2.00	41,41,41,41	0
3	CL	B	1589	1/1	0.99	0.06	-2.30	28,28,28,28	0
3	CL	F	1589	1/1	0.97	0.06	-2.49	32,32,32,32	0
3	CL	D	1590	1/1	0.97	0.07	-2.80	31,31,31,31	0
3	CL	B	1587	1/1	0.95	0.06	-3.45	39,39,39,39	0
3	CL	E	1588	1/1	0.96	0.04	-4.03	32,32,32,32	0
3	CL	A	1588	1/1	0.99	0.03	-5.34	32,32,32,32	0
2	CD	C	1587	1/1	0.99	0.07	-	26,26,26,26	0
2	CD	F	1594	1/1	0.94	0.04	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CD	B	1588	1/1	0.99	0.07	-	26,26,26,26	0
2	CD	C	1589	1/1	0.99	0.05	-	29,29,29,29	0
2	CD	A	1589	1/1	0.99	0.08	-	23,23,23,23	0
2	CD	C	1592	1/1	0.96	0.04	-	68,68,68,68	0
3	CL	A	1594	1/1	0.98	0.03	-	29,29,29,29	0
2	CD	E	1587	1/1	0.99	0.07	-	24,24,24,24	0
2	CD	A	1591	1/1	0.97	0.03	-	58,58,58,58	0
2	CD	E	1590	1/1	0.99	0.06	-	30,30,30,30	0
3	CL	F	1591	1/1	0.97	0.06	-	36,36,36,36	0
2	CD	D	1589	1/1	0.99	0.07	-	23,23,23,23	0
3	CL	D	1592	1/1	0.98	0.10	-	26,26,26,26	0
2	CD	B	1590	1/1	1.00	0.09	-	20,20,20,20	0
3	CL	A	1590	1/1	0.97	0.13	-	26,26,26,26	0
3	CL	C	1590	1/1	0.98	0.09	-	28,28,28,28	0
2	CD	F	1592	1/1	0.99	0.07	-	28,28,28,28	0
2	CD	E	1592	1/1	0.98	0.04	-	55,55,55,55	0
3	CL	F	1587	1/1	0.99	0.06	-	35,35,35,35	0
3	CL	D	1593	1/1	0.98	0.08	-	38,38,38,38	0
2	CD	A	1587	1/1	0.99	0.07	-	27,27,27,27	0
3	CL	E	1589	1/1	0.94	0.06	-	45,45,45,45	0
2	CD	A	1593	1/1	0.98	0.04	-	58,58,58,58	0
2	CD	C	1594	1/1	0.96	0.06	-	55,55,55,55	0
2	CD	F	1590	1/1	0.99	0.07	-	26,26,26,26	0
3	CL	F	1595	1/1	0.97	0.21	-	11,11,11,11	0
2	CD	D	1591	1/1	0.99	0.07	-	24,24,24,24	0
3	CL	B	1592	1/1	0.98	0.19	-	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.