wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:10 PM GMT

PDB ID	:	3SKG
Title	:	Crystal structure of beta-site app-cleaving enzyme 1 (BACE-WT) complex with (2S)-2-((3R)-3-acetamido-3-isobutyl-2-oxo-1-pyrrolidinyl)-N-((1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-2-(1,2,3,4-tetrahydro-3-isoquinolinyl)ethyl)-4-phenylbutanamide
Authors	:	Muckelbauer, J.K.
Deposited on	:	2011-06-22
Resolution	:	2.88 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

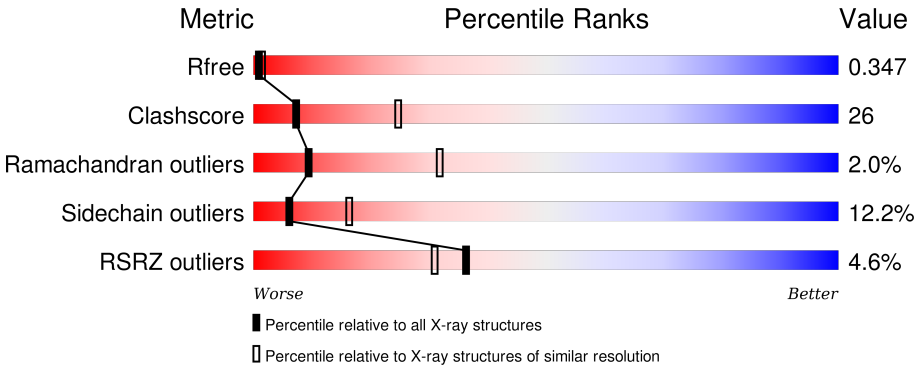
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	455	2% 44% 35% 6% 15%
1	B	455	3% 46% 33% 5% 15%
1	D	455	5% 36% 41% 6% 15%
1	E	455	5% 43% 34% 8% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12434 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	B	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	D	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	E	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-61	MET	-	EXPRESSION TAG	UNP P56817
A	-60	ALA	-	EXPRESSION TAG	UNP P56817
A	-59	SER	-	EXPRESSION TAG	UNP P56817
A	-58	MET	-	EXPRESSION TAG	UNP P56817
A	-57	THR	-	EXPRESSION TAG	UNP P56817
A	-56	GLY	-	EXPRESSION TAG	UNP P56817
A	-55	GLY	-	EXPRESSION TAG	UNP P56817
A	-54	GLN	-	EXPRESSION TAG	UNP P56817
A	-53	GLN	-	EXPRESSION TAG	UNP P56817
A	-52	MET	-	EXPRESSION TAG	UNP P56817
A	-51	GLY	-	EXPRESSION TAG	UNP P56817
A	-50	ARG	-	EXPRESSION TAG	UNP P56817
A	-49	GLY	-	EXPRESSION TAG	UNP P56817
A	-48	SER	-	EXPRESSION TAG	UNP P56817
B	-61	MET	-	EXPRESSION TAG	UNP P56817
B	-60	ALA	-	EXPRESSION TAG	UNP P56817
B	-59	SER	-	EXPRESSION TAG	UNP P56817
B	-58	MET	-	EXPRESSION TAG	UNP P56817
B	-57	THR	-	EXPRESSION TAG	UNP P56817
B	-56	GLY	-	EXPRESSION TAG	UNP P56817
B	-55	GLY	-	EXPRESSION TAG	UNP P56817

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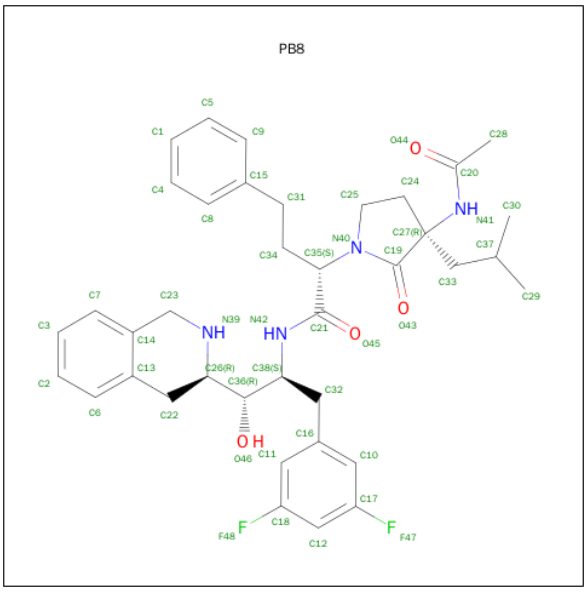
Chain	Residue	Modelled	Actual	Comment	Reference
B	-54	GLN	-	EXPRESSION TAG	UNP P56817
B	-53	GLN	-	EXPRESSION TAG	UNP P56817
B	-52	MET	-	EXPRESSION TAG	UNP P56817
B	-51	GLY	-	EXPRESSION TAG	UNP P56817
B	-50	ARG	-	EXPRESSION TAG	UNP P56817
B	-49	GLY	-	EXPRESSION TAG	UNP P56817
B	-48	SER	-	EXPRESSION TAG	UNP P56817
D	-61	MET	-	EXPRESSION TAG	UNP P56817
D	-60	ALA	-	EXPRESSION TAG	UNP P56817
D	-59	SER	-	EXPRESSION TAG	UNP P56817
D	-58	MET	-	EXPRESSION TAG	UNP P56817
D	-57	THR	-	EXPRESSION TAG	UNP P56817
D	-56	GLY	-	EXPRESSION TAG	UNP P56817
D	-55	GLY	-	EXPRESSION TAG	UNP P56817
D	-54	GLN	-	EXPRESSION TAG	UNP P56817
D	-53	GLN	-	EXPRESSION TAG	UNP P56817
D	-52	MET	-	EXPRESSION TAG	UNP P56817
D	-51	GLY	-	EXPRESSION TAG	UNP P56817
D	-50	ARG	-	EXPRESSION TAG	UNP P56817
D	-49	GLY	-	EXPRESSION TAG	UNP P56817
D	-48	SER	-	EXPRESSION TAG	UNP P56817
E	-61	MET	-	EXPRESSION TAG	UNP P56817
E	-60	ALA	-	EXPRESSION TAG	UNP P56817
E	-59	SER	-	EXPRESSION TAG	UNP P56817
E	-58	MET	-	EXPRESSION TAG	UNP P56817
E	-57	THR	-	EXPRESSION TAG	UNP P56817
E	-56	GLY	-	EXPRESSION TAG	UNP P56817
E	-55	GLY	-	EXPRESSION TAG	UNP P56817
E	-54	GLN	-	EXPRESSION TAG	UNP P56817
E	-53	GLN	-	EXPRESSION TAG	UNP P56817
E	-52	MET	-	EXPRESSION TAG	UNP P56817
E	-51	GLY	-	EXPRESSION TAG	UNP P56817
E	-50	ARG	-	EXPRESSION TAG	UNP P56817
E	-49	GLY	-	EXPRESSION TAG	UNP P56817
E	-48	SER	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is (2S)-2-[(3R)-3-(ACETYLAMINO)-3-(2-METHYLPROPYL)-2-OXOPYR ROLIDIN-1-YL]-N-{(1R,2S)-3-(3,5-DIFLUOROPHENYL)-1-HYDROXY-1-[(3R)-1,2,3 ,4-TETRAHYDROISOQUINOLIN-3-YL]PROPAN-2-YL}-4-PHENYLBUTANAMIDE (three-letter code: PB8) (formula: $C_{38}H_{46}F_2N_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			48	38	2	4	4		
2	B	1	Total	C	F	N	O	0	0
			48	38	2	4	4		
2	D	1	Total	C	F	N	O	0	0
			48	38	2	4	4		
2	E	1	Total	C	F	N	O	0	0
			48	38	2	4	4		

- Molecule 3 is water.

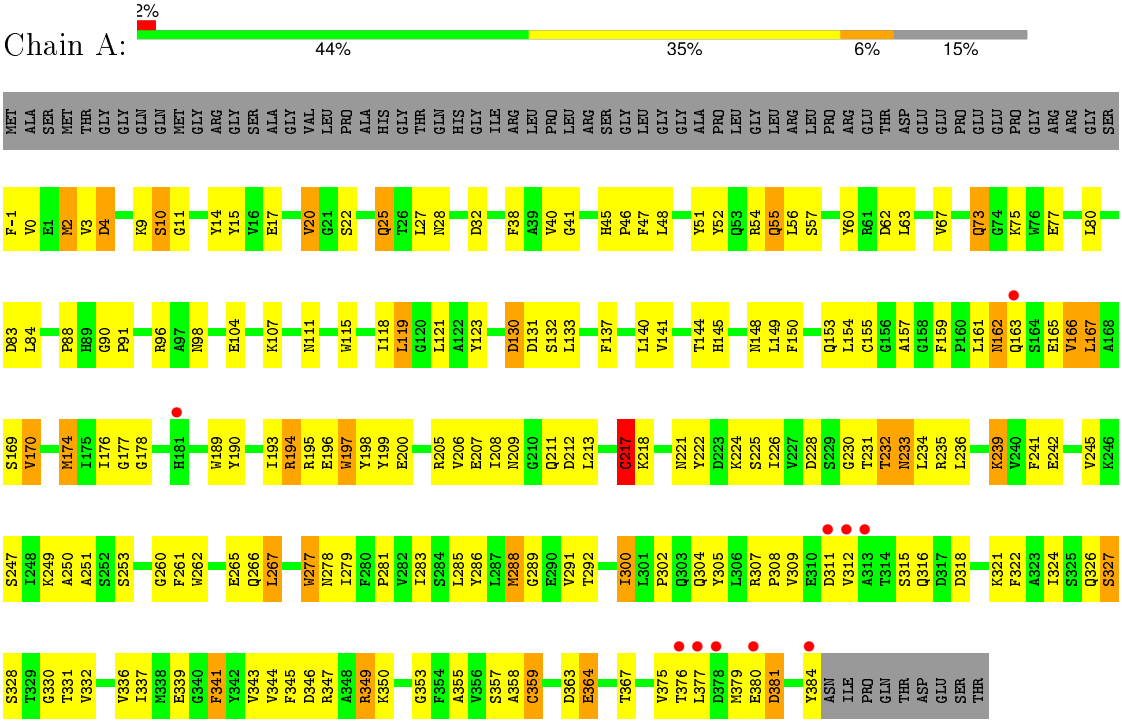
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	38	Total	O	0	0
			38	38		
3	D	20	Total	O	0	0
			20	20		
3	E	24	Total	O	0	0
			24	24		

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.

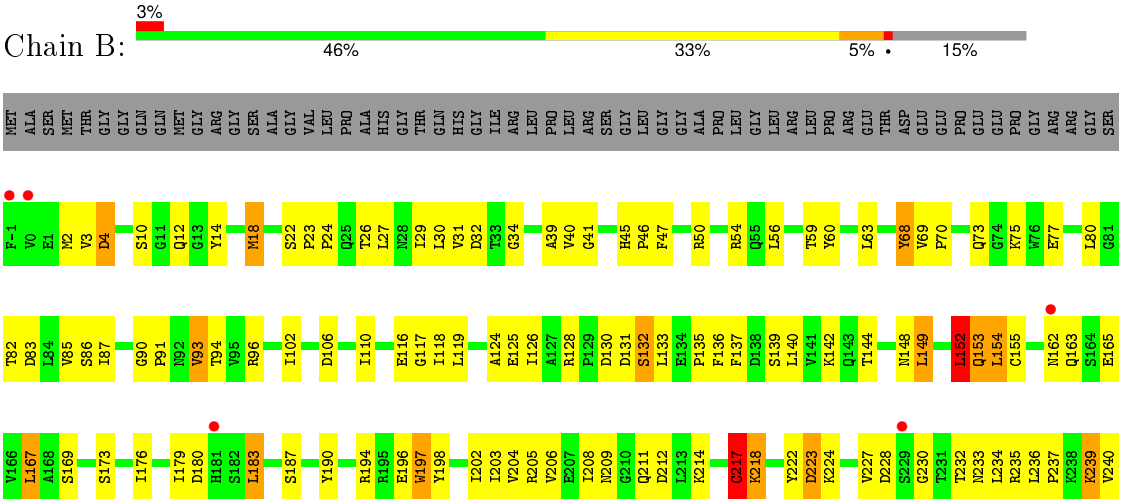
- Molecule 1: Beta-secretase 1

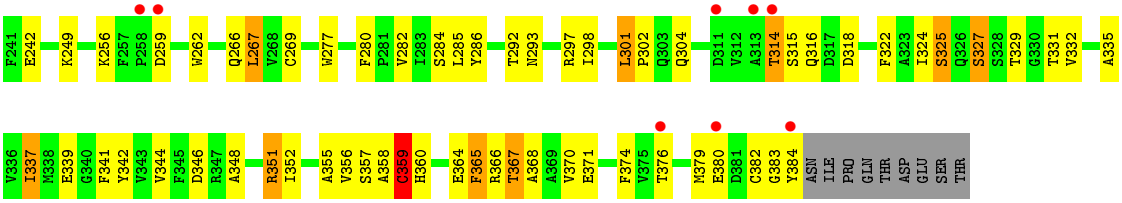
Chain A:



- Molecule 1: Beta-secretase 1

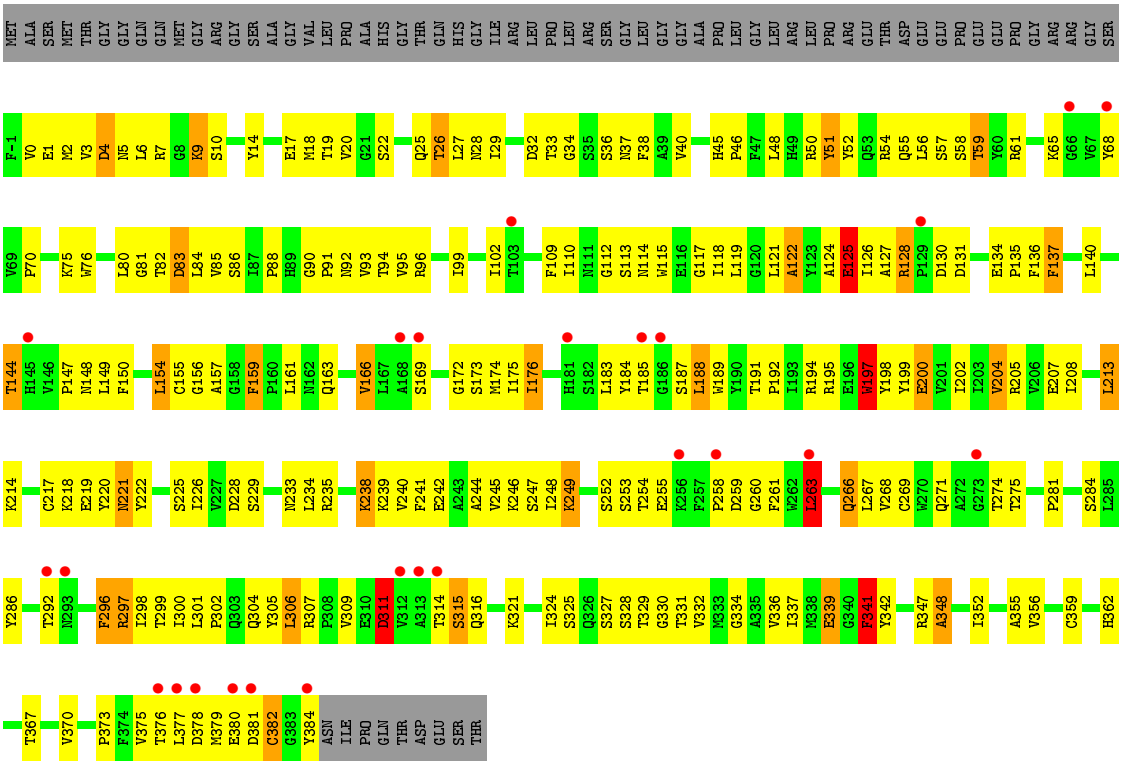
Chain B:





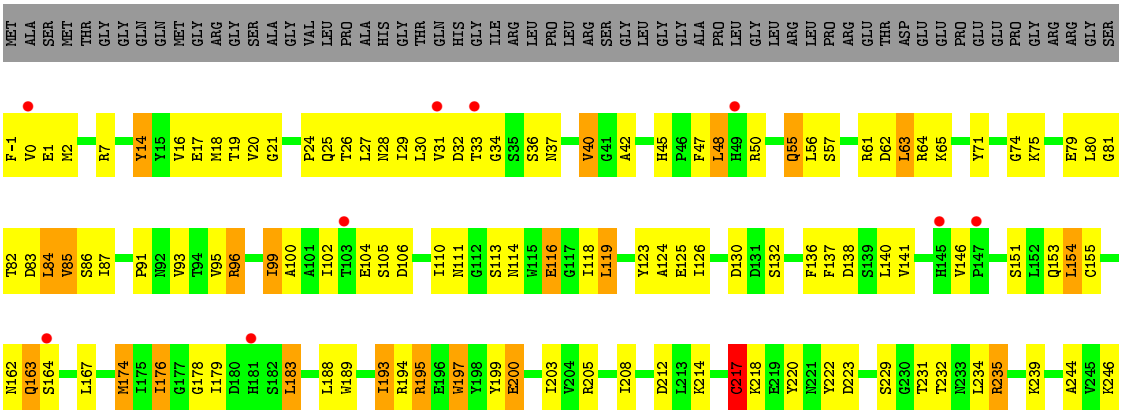
• Molecule 1: Beta-secretase 1

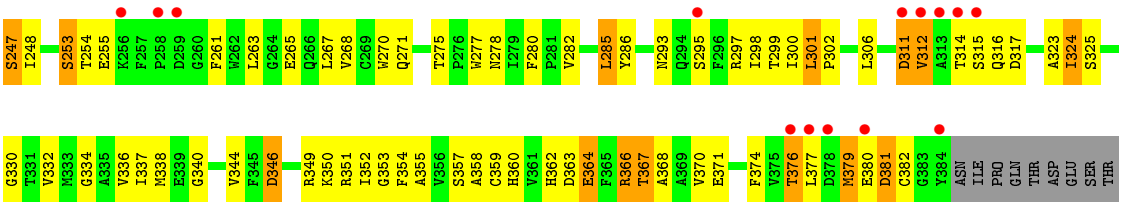
Chain D:



• Molecule 1: Beta-secretase 1

Chain E:




S247 I248 S253 T254 E255 K256 F257 P258 D259 G260 F261 W262 L263 G264 E265 Q266 L267 V268 C269 W270 Q271 T275 P276 W277 N278 I279 F280 P281 V282 L285 Y286 N293 Q294 S295 F296 R297 I298 T299 I300 L301 P302 L306 D311 V312 A313 T314 S315 Q316 D317 A323 I324 S325
G330 T331 V332 M333 G334 A335 V336 I337 M338 E339 G340 V344 F345 D346 R349 K350 R351 I352 G353 F354 A355 V356 S357 A358 C359 H360 V361 H362 D363 E364 F365 R366 T367 A368 A369 V370 E371 F374 V375 T376 L377 D378 M379 E380 D381 C382 G383 Y384 ASN ILE PRO GLN THR ASP GLU SER THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.24Å 130.45Å 86.87Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	30.63 – 2.88 30.63 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.63-2.88) 98.9 (30.63-2.88)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.255 , 0.348 0.256 , 0.347	Depositor DCC
R_{free} test set	2159 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.7	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 42809 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12434	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 22.23 % 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 5.9537e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: PB8

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	1.37	7/3112 (0.2%)	1.21	10/4232 (0.2%)
1	B	1.39	12/3112 (0.4%)	1.24	15/4232 (0.4%)
1	D	1.38	8/3112 (0.3%)	1.22	11/4232 (0.3%)
1	E	1.39	7/3112 (0.2%)	1.26	21/4232 (0.5%)
All	All	1.38	34/12448 (0.3%)	1.23	57/16928 (0.3%)

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	D	0	1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	CYS	CB-SG	-14.77	1.57	1.82
1	E	217	CYS	CB-SG	-11.38	1.62	1.82
1	B	359	CYS	CB-SG	-11.33	1.62	1.82
1	B	364	GLU	CG-CD	9.12	1.65	1.51
1	A	364	GLU	CG-CD	9.08	1.65	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	CYS	CA-CB-SG	-10.02	95.96	114.00
1	E	235	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	B	96	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	E	235	ARG	NE-CZ-NH1	-9.04	115.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	217	CYS	CA-CB-SG	-8.92	97.95	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	197	TRP	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	3034	0	2948	147	0
1	B	3034	0	2948	127	0
1	D	3034	0	2950	188	0
1	E	3034	0	2948	156	0
2	A	48	0	46	9	0
2	B	48	0	46	7	0
2	D	48	0	46	5	0
2	E	48	0	46	10	0
3	A	24	0	0	7	0
3	B	38	0	0	2	0
3	D	20	0	0	2	0
3	E	24	0	0	3	0
All	All	12434	0	11978	629	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 26.

The worst 5 of 629 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:A:73:GLN:HG2	3:A:414:HOH:O	1.43	1.18
1:D:376:THR:HA	3:D:412:HOH:O	1.53	1.07
1:E:63:LEU:HD12	1:E:80:LEU:HB3	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:394:PB8:H28A	2:E:394:PB8:H31A	1.30	1.07
2:E:394:PB8:H28A	2:E:394:PB8:C31	1.88	1.01

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	384/455 (84%)	338 (88%)	39 (10%)	7 (2%)	11 35
1	B	384/455 (84%)	338 (88%)	42 (11%)	4 (1%)	19 52
1	D	384/455 (84%)	336 (88%)	37 (10%)	11 (3%)	6 21
1	E	384/455 (84%)	337 (88%)	38 (10%)	9 (2%)	8 28
All	All	1536/1820 (84%)	1349 (88%)	156 (10%)	31 (2%)	9 32

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	107	LYS
1	D	55	GLN
1	D	92	ASN
1	D	380	GLU

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	329/381 (86%)	294 (89%)	35 (11%)	8 23
1	B	329/381 (86%)	290 (88%)	39 (12%)	6 17
1	D	329/381 (86%)	282 (86%)	47 (14%)	4 11
1	E	329/381 (86%)	289 (88%)	40 (12%)	6 16
All	All	1316/1524 (86%)	1155 (88%)	161 (12%)	6 16

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	359	CYS
1	D	185	THR
1	E	301	LEU
1	D	9	LYS
1	D	94	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	B	153	GLN
1	B	360	HIS
1	A	271	GLN
1	B	211	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
2	PB8	A	394	-	50,52,52	2.30	12 (24%)	58,74,74	2.69	23 (39%)
2	PB8	B	394	-	50,52,52	1.98	11 (22%)	58,74,74	3.12	24 (41%)
2	PB8	D	394	-	50,52,52	2.24	12 (24%)	58,74,74	3.07	28 (48%)
2	PB8	E	394	-	50,52,52	1.98	15 (30%)	58,74,74	3.03	27 (46%)

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
2	PB8	A	394	-	-	2/39/64/64	0/5/5/5
2	PB8	B	394	-	-	2/39/64/64	0/5/5/5
2	PB8	D	394	-	-	2/39/64/64	0/5/5/5
2	PB8	E	394	-	-	2/39/64/64	0/5/5/5

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	394	PB8	C14-C13	-5.82	1.29	1.40
2	A	394	PB8	C14-C13	-5.62	1.29	1.40
2	B	394	PB8	C14-C13	-5.61	1.29	1.40
2	E	394	PB8	C27-C19	-5.54	1.47	1.52
2	D	394	PB8	C27-C19	-5.27	1.47	1.52

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	394	PB8	C25-N40-C19	-9.79	107.14	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	394	PB8	O43-C19-C27	-8.59	118.06	126.42
2	E	394	PB8	O43-C19-C27	-7.32	119.30	126.42
2	D	394	PB8	C32-C38-N42	-7.19	102.28	110.14
2	B	394	PB8	C25-C24-C27	-6.68	96.41	104.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	394	PB8	C28-C20-N41-C27
2	B	394	PB8	O44-C20-N41-C27
2	E	394	PB8	C28-C20-N41-C27
2	E	394	PB8	O44-C20-N41-C27
2	D	394	PB8	O44-C20-N41-C27

There are no ring outliers.

4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	394	PB8	9	0
2	B	394	PB8	7	0
2	D	394	PB8	5	0
2	E	394	PB8	10	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, 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	386/455 (84%)	0.17	10 (2%)	59	55	4, 18, 36, 59	0
1	B	386/455 (84%)	0.12	13 (3%)	49	42	3, 16, 35, 47	0
1	D	386/455 (84%)	0.47	25 (6%)	22	16	10, 24, 39, 59	0
1	E	386/455 (84%)	0.42	23 (5%)	25	19	10, 23, 41, 57	0
All	All	1544/1820 (84%)	0.30	71 (4%)	36	31	3, 20, 38, 59	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	THR	5.7
1	E	378	ASP	4.9
1	B	313	ALA	4.4
1	E	311	ASP	4.3
1	E	376	THR	4.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	PB8	E	394	48/48	0.91	0.21	-0.29	6,15,20,22	0
2	PB8	B	394	48/48	0.93	0.19	-0.50	3,10,15,20	0
2	PB8	A	394	48/48	0.93	0.19	-0.81	2,11,21,24	0
2	PB8	D	394	48/48	0.93	0.18	-1.28	3,15,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.