



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:48 PM GMT

PDB ID : 1F9E
Title : CASPASE-8 SPECIFICITY PROBED AT SUBSITE S4: CRYSTAL STRUCTURE OF THE CASPASE-8-Z-DEVD-CHO
Authors : Blanchard, H.; Donepudi, M.; Tschopp, M.; Kodandapani, L.; Wu, J.C.; Grutter, M.G.
Deposited on : 2000-07-10
Resolution : 2.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

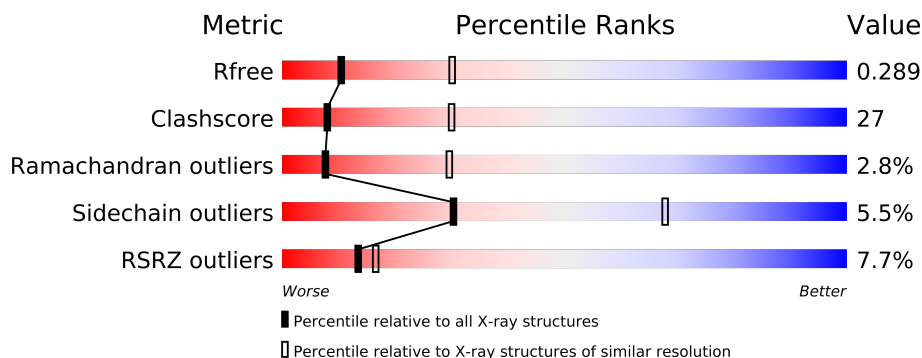
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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.



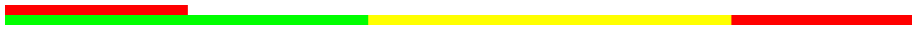
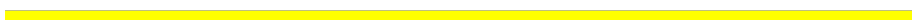
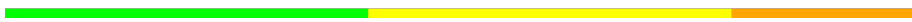


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	153	
1	C	153	
1	E	153	
1	G	153	
1	I	153	
1	K	153	
2	B	89	
2	D	89	
2	F	89	
2	H	89	
2	J	89	
2	L	89	
3	Q	5	
3	R	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	S	5	
3	T	5	
3	U	5	
3	V	5	 

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11926 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CASPASE-8 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	C	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	E	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	G	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	I	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			
1	K	153	Total	C	N	O	S	0	0	0
			1220	774	208	228	10			

- Molecule 2 is a protein called CASPASE-8 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	D	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	F	89	Total	C	N	O	S	0	0	0
			717	450	124	137	6			
2	H	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	J	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			
2	L	89	Total	C	N	O	S	0	0	0
			718	450	124	138	6			

- Molecule 3 is a protein called (PHQ)DEVD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	R	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	S	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	T	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	U	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	V	5	Total	C	N	O	0	0	0
			42	26	4	12			

- Molecule 4 is water.

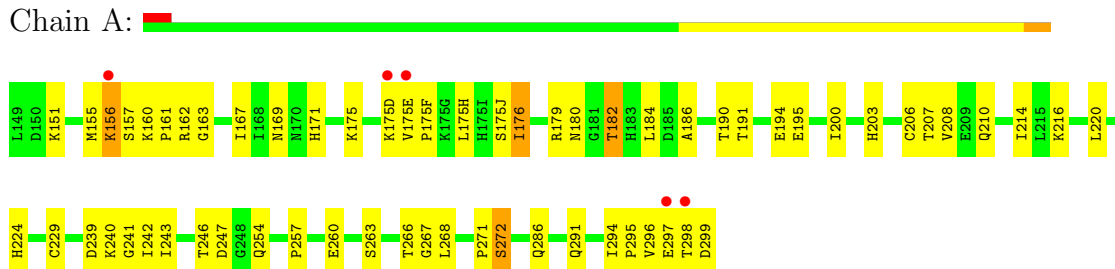
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	7	Total	O	0	0
			7	7		
4	Q	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		
4	D	4	Total	O	0	0
			4	4		
4	E	4	Total	O	0	0
			4	4		
4	F	3	Total	O	0	0
			3	3		
4	G	11	Total	O	0	0
			11	11		
4	H	1	Total	O	0	0
			1	1		
4	I	5	Total	O	0	0
			5	5		
4	K	2	Total	O	0	0
			2	2		
4	L	1	Total	O	0	0
			1	1		

3 Residue-property plots

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

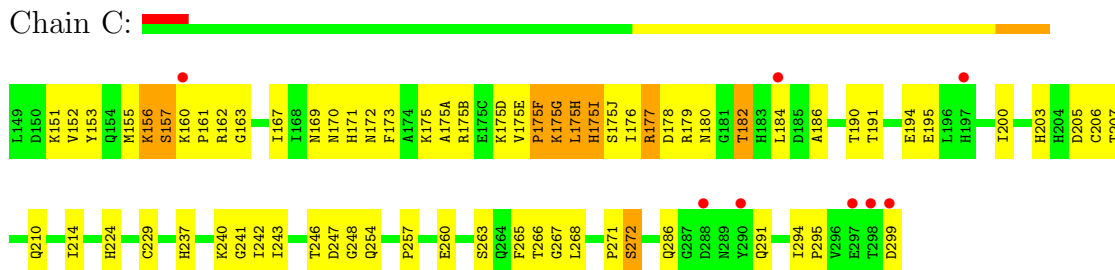
• Molecule 1: CASPASE-8 ALPHA CHAIN

Chain A:



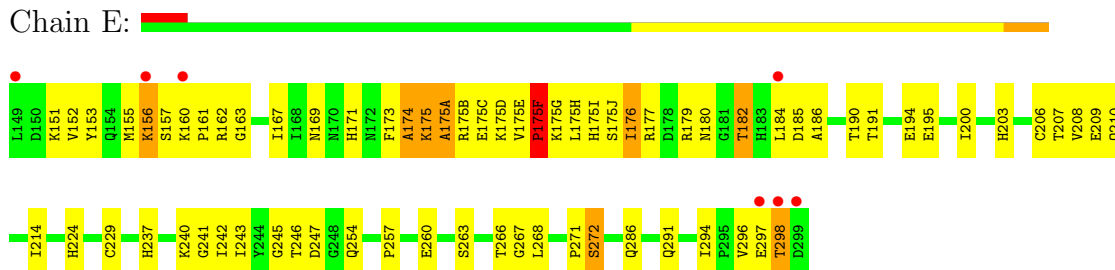
• Molecule 1: CASPASE-8 ALPHA CHAIN

Chain C:



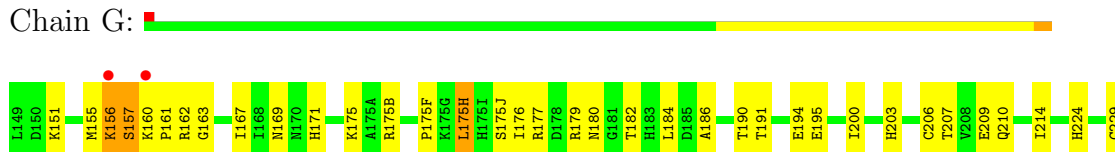
• Molecule 1: CASPASE-8 ALPHA CHAIN

Chain E:



• Molecule 1: CASPASE-8 ALPHA CHAIN

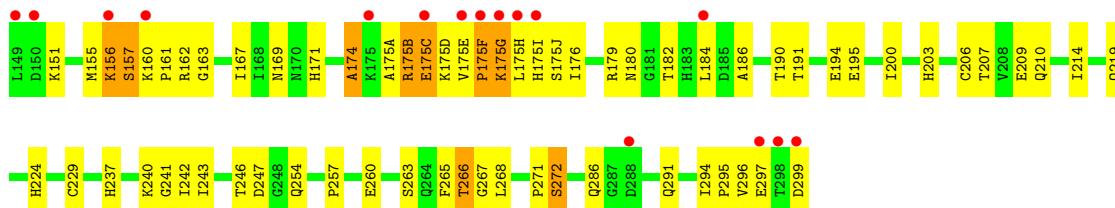
Chain G:





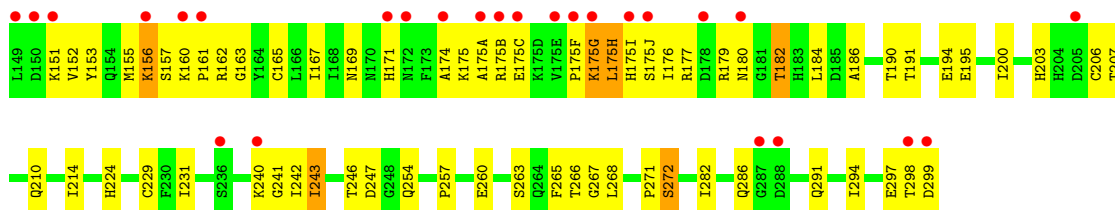
• Molecule 1: CASPASE-8 ALPHA CHAIN

Chain I:



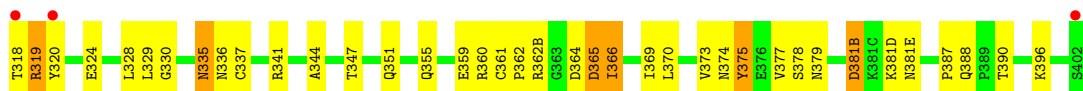
• Molecule 1: CASPASE-8 ALPHA CHAIN

Chain K:



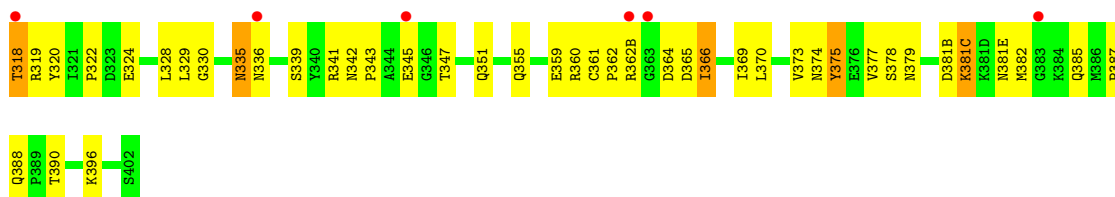
• Molecule 2: CASPASE-8 BETA CHAIN

Chain B:



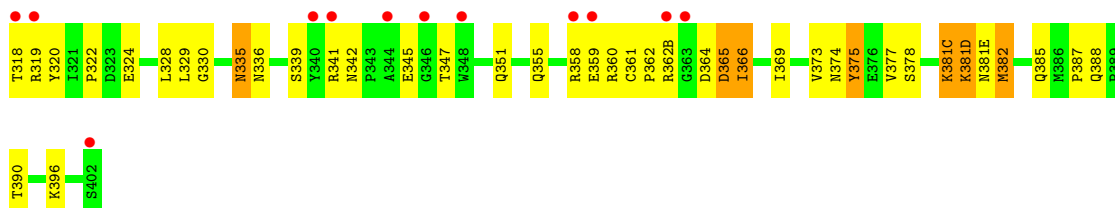
• Molecule 2: CASPASE-8 BETA CHAIN

Chain D:



• Molecule 2: CASPASE-8 BETA CHAIN

Chain F:



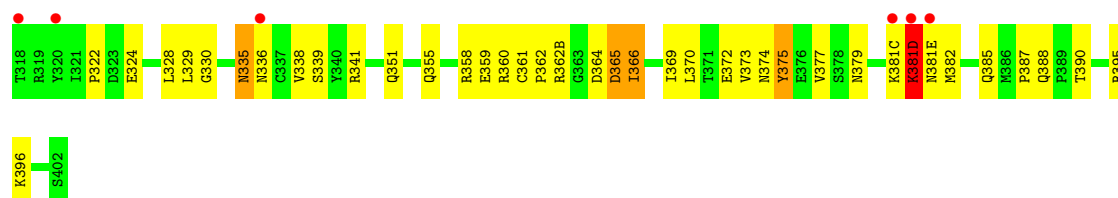
• Molecule 2: CASPASE-8 BETA CHAIN

Chain H: 



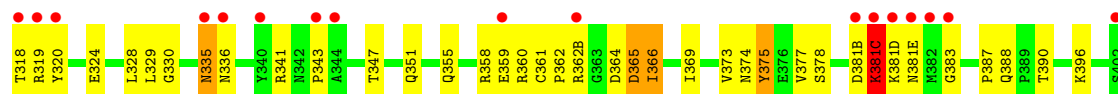
- Molecule 2: CASPASE-8 BETA CHAIN

Chain J: 



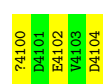
- Molecule 2: CASPASE-8 BETA CHAIN

Chain L: 



- Molecule 3: (PHQ)DEVD

Chain Q: 



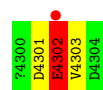
- Molecule 3: (PHQ)DEVD

Chain R: 



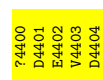
- Molecule 3: (PHQ)DEVD

Chain S: 



- Molecule 3: (PHQ)DEVD

Chain T: 



- Molecule 3: (PHQ)DEVD

Chain U: 

24500
D4501
E4502
V4503
D4504

- Molecule 3: (PHQ)DEVD

Chain V: 

24600
D4601
E4602
V4603
D4604

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.03Å 188.75Å 209.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.90 19.93 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-2.90) 99.5 (19.93-2.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.93Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.289 0.241 , 0.289	Depositor DCC
R_{free} test set	4318 reflections (10.07%)	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 42872 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11926	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	0/1248	0.69	0/1682
1	C	0.52	0/1248	0.71	0/1682
1	E	0.50	0/1248	0.72	0/1682
1	G	0.55	0/1248	0.71	0/1682
1	I	0.49	0/1248	0.71	0/1682
1	K	0.48	0/1248	0.70	0/1682
2	B	0.51	0/732	0.74	0/989
2	D	0.48	0/732	0.71	0/989
2	F	0.54	0/731	0.74	0/989
2	H	0.53	0/732	0.71	0/989
2	J	0.46	0/732	0.69	0/989
2	L	0.49	0/732	0.71	0/989
3	Q	2.09	1/23 (4.3%)	1.84	0/30
3	R	2.35	0/23	1.96	0/30
3	S	2.16	1/23 (4.3%)	1.71	0/30
3	T	2.21	1/23 (4.3%)	2.06	1/30 (3.3%)
3	U	2.18	1/23 (4.3%)	1.68	0/30
3	V	2.16	0/23	1.89	0/30
All	All	0.56	4/12017 (0.0%)	0.73	1/16206 (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
3	Q	1	0
3	R	1	1
3	S	1	1
3	T	1	1
3	U	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	V	0	1
All	All	5	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	4102	GLU	CD-OE2	5.31	1.31	1.25
3	U	4502	GLU	CD-OE1	5.24	1.31	1.25
3	S	4302	GLU	CD-OE2	5.21	1.31	1.25
3	T	4402	GLU	CD-OE1	5.13	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	4401	ASP	N-CA-C	-5.57	95.95	111.00

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	Q	4101	ASP	CA
3	R	4201	ASP	CA
3	S	4301	ASP	CA
3	T	4401	ASP	CA
3	U	4501	ASP	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	R	4203	VAL	Mainchain
3	S	4303	VAL	Mainchain
3	T	4403	VAL	Mainchain
3	U	4503	VAL	Mainchain
3	V	4603	VAL	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1220	0	1198	72	0
1	C	1220	0	1198	84	0
1	E	1220	0	1198	87	0
1	G	1220	0	1198	60	0
1	I	1220	0	1198	80	0
1	K	1220	0	1198	85	0
2	B	718	0	712	53	0
2	D	718	0	712	53	0
2	F	717	0	712	49	0
2	H	718	0	712	39	0
2	J	718	0	712	47	0
2	L	718	0	712	54	0
3	Q	42	0	28	2	0
3	R	42	0	28	2	0
3	S	42	0	28	3	0
3	T	42	0	28	2	0
3	U	42	0	28	2	0
3	V	42	0	28	3	0
4	A	6	0	0	2	0
4	B	7	0	0	2	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	3	0	0	0	0
4	G	11	0	0	4	0
4	H	1	0	0	0	0
4	I	5	0	0	1	0
4	K	2	0	0	0	0
4	L	1	0	0	0	0
4	Q	1	0	0	0	0
All	All	11926	0	11628	630	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

The worst 5 of 630 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:298:THR:HG23	2:H:319:ARG:HH21	1.15	1.10
2:B:319:ARG:HH22	1:C:299:ASP:HB2	1.13	1.09
1:A:160:LYS:HB2	1:A:161:PRO:HD3	1.35	1.08
1:K:160:LYS:HB2	1:K:161:PRO:HD3	1.38	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:160:LYS:HB2	1:C:161:PRO:HD3	1.38	1.05

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/153 (99%)	134 (89%)	15 (10%)	2 (1%)	18	54
1	C	151/153 (99%)	125 (83%)	19 (13%)	7 (5%)	4	14
1	E	151/153 (99%)	128 (85%)	13 (9%)	10 (7%)	2	5
1	G	151/153 (99%)	132 (87%)	17 (11%)	2 (1%)	18	54
1	I	151/153 (99%)	126 (83%)	16 (11%)	9 (6%)	2	7
1	K	151/153 (99%)	131 (87%)	15 (10%)	5 (3%)	6	24
2	B	87/89 (98%)	78 (90%)	7 (8%)	2 (2%)	10	36
2	D	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
2	F	87/89 (98%)	78 (90%)	8 (9%)	1 (1%)	21	60
2	H	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
2	J	87/89 (98%)	80 (92%)	5 (6%)	2 (2%)	10	36
2	L	87/89 (98%)	79 (91%)	7 (8%)	1 (1%)	21	60
3	Q	2/5 (40%)	2 (100%)	0	0	100	100
3	R	2/5 (40%)	2 (100%)	0	0	100	100
3	S	2/5 (40%)	2 (100%)	0	0	100	100
3	T	2/5 (40%)	2 (100%)	0	0	100	100
3	U	2/5 (40%)	2 (100%)	0	0	100	100
3	V	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1440/1482 (97%)	1264 (88%)	135 (9%)	41 (3%)	8	29

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	319	ARG
1	C	175(F)	PRO
1	C	175(G)	LYS
1	C	175(H)	LEU
1	C	175(J)	SER

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	135/135 (100%)	129 (96%)	6 (4%)	39	77
1	C	135/135 (100%)	129 (96%)	6 (4%)	39	77
1	E	135/135 (100%)	128 (95%)	7 (5%)	32	71
1	G	135/135 (100%)	127 (94%)	8 (6%)	28	64
1	I	135/135 (100%)	131 (97%)	4 (3%)	53	89
1	K	135/135 (100%)	129 (96%)	6 (4%)	39	77
2	B	82/82 (100%)	77 (94%)	5 (6%)	26	62
2	D	82/82 (100%)	76 (93%)	6 (7%)	20	51
2	F	82/82 (100%)	75 (92%)	7 (8%)	15	42
2	H	82/82 (100%)	77 (94%)	5 (6%)	26	62
2	J	82/82 (100%)	77 (94%)	5 (6%)	26	62
2	L	82/82 (100%)	76 (93%)	6 (7%)	20	51
3	Q	3/3 (100%)	3 (100%)	0	100	100
3	R	3/3 (100%)	2 (67%)	1 (33%)	0	1
3	S	3/3 (100%)	2 (67%)	1 (33%)	0	1
3	T	3/3 (100%)	3 (100%)	0	100	100
3	U	3/3 (100%)	3 (100%)	0	100	100
3	V	3/3 (100%)	3 (100%)	0	100	100
All	All	1320/1320 (100%)	1247 (94%)	73 (6%)	30	68

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	365	ASP
1	G	175	LYS
2	L	335	ASN
2	F	382	MET
1	G	175(J)	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	286	GLN
1	G	210	GLN
1	K	286	GLN
1	E	291	GLN
2	F	336	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ASA	Q	4104	1,3	7,7,7	2.15	2 (28%)	8,8,8	1.20	0
3	ASA	R	4204	1,3	7,7,7	1.59	2 (28%)	8,8,8	2.33	1 (12%)
3	ASA	S	4304	1,3	7,7,7	2.15	2 (28%)	8,8,8	0.89	0
3	ASA	T	4404	1,3	7,7,7	1.93	2 (28%)	8,8,8	0.76	0
3	ASA	U	4504	1,3	7,7,7	1.69	2 (28%)	8,8,8	0.80	0
3	ASA	V	4604	1	7,7,7	2.02	2 (28%)	8,8,8	1.06	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
3	ASA	Q	4104	1,3	-	0/5/6/6	0/0/0/0
3	ASA	R	4204	1,3	-	0/5/6/6	0/0/0/0
3	ASA	S	4304	1,3	-	0/5/6/6	0/0/0/0
3	ASA	T	4404	1,3	-	0/5/6/6	0/0/0/0
3	ASA	U	4504	1,3	-	0/5/6/6	0/0/0/0
3	ASA	V	4604	1	-	0/5/6/6	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	4304	ASA	CA-C	4.71	1.55	1.50
3	Q	4104	ASA	CA-C	4.60	1.54	1.50
3	V	4604	ASA	CA-C	4.37	1.54	1.50
3	T	4404	ASA	CA-C	4.29	1.54	1.50
3	U	4504	ASA	CA-C	3.37	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	4204	ASA	O-C-CA	-6.30	111.01	125.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	153/153 (100%)	0.05	5 (3%) 44 53	26, 51, 79, 97	0
1	C	153/153 (100%)	0.21	8 (5%) 26 32	30, 60, 85, 100	0
1	E	153/153 (100%)	0.40	7 (4%) 31 38	34, 65, 94, 99	0
1	G	153/153 (100%)	-0.01	2 (1%) 74 82	23, 49, 81, 96	0
1	I	153/153 (100%)	0.43	16 (10%) 7 9	42, 64, 96, 100	0
1	K	153/153 (100%)	0.76	26 (16%) 2 3	45, 72, 99, 100	0
2	B	89/89 (100%)	-0.02	3 (3%) 43 51	26, 48, 84, 95	0
2	D	89/89 (100%)	0.22	6 (6%) 17 21	27, 57, 91, 98	0
2	F	89/89 (100%)	0.67	12 (13%) 4 5	28, 66, 97, 99	0
2	H	89/89 (100%)	-0.10	3 (3%) 43 51	31, 49, 85, 96	0
2	J	89/89 (100%)	0.45	6 (6%) 17 21	37, 66, 97, 100	0
2	L	89/89 (100%)	0.92	17 (19%) 2 2	39, 70, 97, 100	0
3	Q	5/5 (100%)	-0.52	0 100 100	30, 39, 44, 66	0
3	R	5/5 (100%)	0.32	0 100 100	69, 70, 87, 100	0
3	S	5/5 (100%)	1.34	1 (20%) 2 2	72, 86, 93, 100	0
3	T	5/5 (100%)	-0.73	0 100 100	31, 33, 40, 48	0
3	U	5/5 (100%)	1.12	0 100 100	78, 92, 99, 100	0
3	V	5/5 (100%)	1.58	2 (40%) 1 0	98, 100, 100, 100	0
All	All	1482/1482 (100%)	0.33	114 (7%) 13 16	23, 60, 95, 100	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	402	SER	5.7
2	L	318	THR	4.7
1	K	160	LYS	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	298	THR	4.7
2	F	359	GLU	4.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ASA	U	4504	8/8	0.29	-	65,76,82,89	0
3	ASA	S	4304	8/8	0.33	-	68,89,96,100	0
3	ASA	Q	4104	8/8	0.18	-	41,42,45,48	0
3	ASA	V	4604	8/8	0.50	-	89,99,100,100	0
3	ASA	R	4204	8/8	0.17	-	60,65,72,80	0
3	ASA	T	4404	8/8	0.18	-	19,30,35,35	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.