



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 11:08 AM EDT

PDB ID : 2QLB  
Title : Crystal Structure of caspase-7 with inhibitor AC-ESMD-CHO  
Authors : Agniswamy, J.; Fang, B.; Weber, I.  
Deposited on : 2007-07-12  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

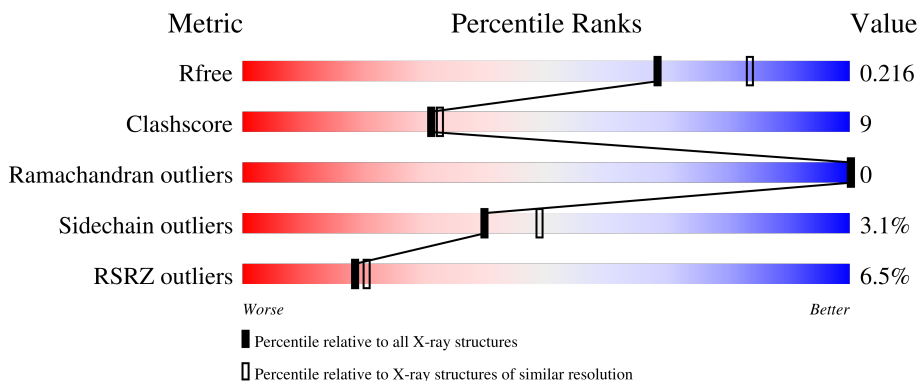
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	173	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 61% 19% • 19%</p>
1	C	173	<div style="display: flex; align-items: center;"> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">62% 17% • 19%</p>
2	B	97	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">11% 82% 12% 5%</p>
2	D	97	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">13% 71% 24% 5%</p>
3	E	5	<div style="display: flex; align-items: center;"> <div style="width: 20%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">20% 60% 20%</p>

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Mol	Chain	Length	Quality of chain
3	F	5	
4	G	5	

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
5	CIT	D	850	-	X	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4049 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 Caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	140	1100	691	188	210	11	0	0	0
1	C	140	1100	691	188	210	11	0	0	0

- Molecule 2 is a protein called Caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	92	758	487	128	139	4	0	0	0
2	D	92	758	487	128	139	4	0	0	0

- Molecule 3 is a protein called Inhibitor AC-ESMD-CHO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	5	34	19	4	10	1	0	0	0
3	F	5	34	19	4	10	1	0	0	0

- Molecule 4 is a protein called Peptide QGHGE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	5	37	20	8	9	0	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 13 6 7	0	0

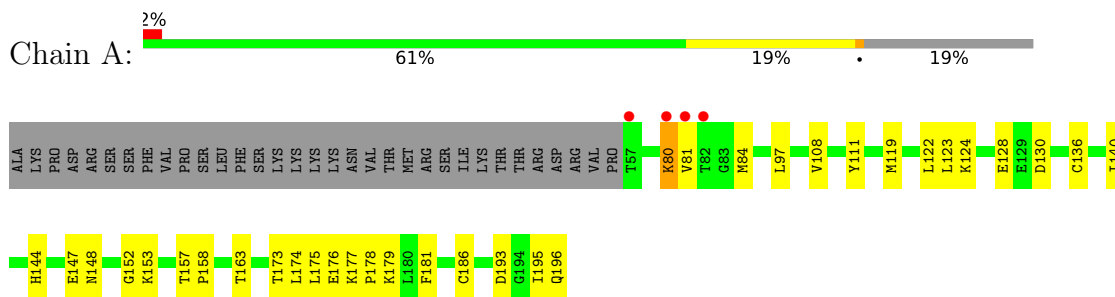
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	28	Total O 28 28	0	0
6	C	91	Total O 91 91	0	0
6	D	32	Total O 32 32	0	0
6	E	1	Total O 1 1	0	0
6	F	2	Total O 2 2	0	0

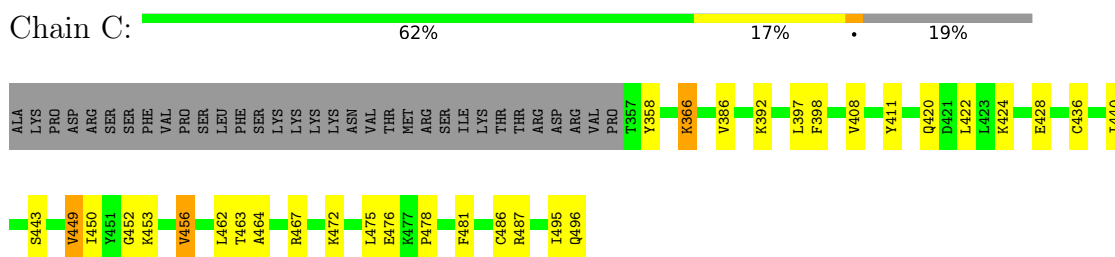
### 3 Residue-property plots [i](#)

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.

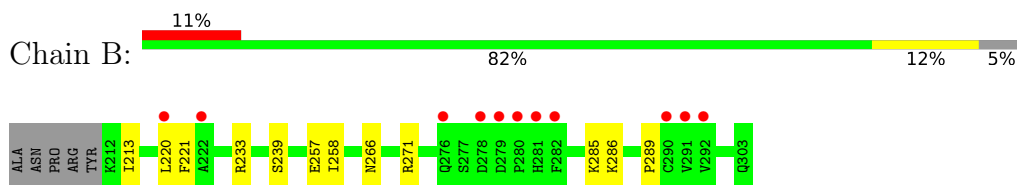
- Molecule 1: Caspase-7



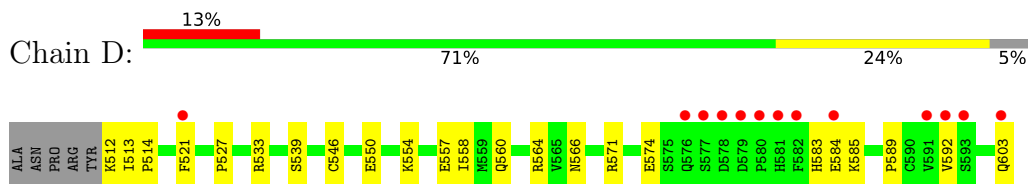
- Molecule 1: Caspase-7



- Molecule 2: Caspase-7

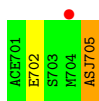


- Molecule 2: Caspase-7



- Molecule 3: Inhibitor AC-ESMD-CHO

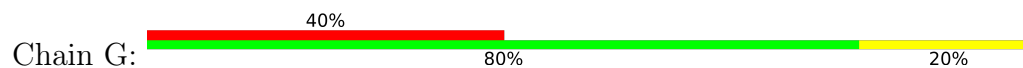




- Molecule 3: Inhibitor AC-ESMD-CHO



- Molecule 4: Peptide QGHGE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.25Å 88.25Å 188.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.25 40.08 – 2.25	Depositor EDS
% Data completeness (in resolution range)	86.0 (50.00-2.25) 86.6 (40.08-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.24Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.187 , 0.223 0.184 , 0.216	Depositor DCC
$R_{free}$ test set	1952 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtrriage
Anisotropy	0.510	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CIT, ACE, ASJ

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	0.34	0/1117	0.57	1/1496 (0.1%)
1	C	0.40	0/1117	0.62	1/1496 (0.1%)
2	B	0.35	0/780	0.59	0/1054
2	D	0.37	0/780	0.63	0/1054
3	E	0.53	0/23	0.92	0/29
3	F	0.81	0/23	1.21	1/29 (3.4%)
4	G	1.51	0/37	2.02	2/46 (4.3%)
All	All	0.40	0/3877	0.64	5/5204 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	452	GLY	N-CA-C	-6.17	97.67	113.10
1	A	152	GLY	N-CA-C	-5.78	98.65	113.10
4	G	813	GLY	C-N-CA	5.41	135.21	121.70
4	G	813	GLY	N-CA-C	-5.40	99.61	113.10
3	F	802	GLU	N-CA-CB	-5.17	101.29	110.60

There are no chirality outliers.

There are no planarity outliers.

### 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	1100	0	1085	24	0
1	C	1100	0	1085	26	0
2	B	758	0	731	9	0
2	D	758	0	731	18	0
3	E	34	0	28	2	0
3	F	34	0	28	3	0
4	G	37	0	26	0	0
5	D	13	0	5	4	0
6	A	61	0	0	1	0
6	B	28	0	0	0	0
6	C	91	0	0	3	0
6	D	32	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
All	All	4049	0	3719	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (69) 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:186:CYS:H	3:E:705:ASJ:H	1.53	0.72
1:C:486:CYS:H	3:F:805:ASJ:H	1.57	0.68
2:D:592:VAL:HG11	5:D:850:CIT:H21	1.78	0.65
1:A:186:CYS:N	3:E:705:ASJ:H	2.13	0.64
1:A:177:LYS:O	1:A:179:LYS:HE2	1.98	0.63
1:C:464:ALA:O	1:C:467:ARG:HG3	1.98	0.63
2:B:233:ARG:HA	2:B:239:SER:HA	1.81	0.61
2:D:533:ARG:HA	2:D:539:SER:HA	1.84	0.59
1:C:366:LYS:NZ	1:C:366:LYS:HB3	2.17	0.59
1:C:392:LYS:NZ	1:C:392:LYS:HB2	2.18	0.58
1:A:195:ILE:O	1:A:196:GLN:HG3	2.04	0.57
2:D:527:PRO:HG3	5:D:850:CIT:O3	2.04	0.57
1:C:424:LYS:O	1:C:428:GLU:HG3	2.04	0.57
1:C:436:CYS:HB3	1:C:478:PRO:HG2	1.87	0.57
1:C:486:CYS:N	3:F:805:ASJ:H	2.20	0.56
1:A:130:ASP:OD1	1:A:173:THR:HG21	2.05	0.55
1:A:196:GLN:HG2	1:C:475:LEU:HD21	1.90	0.54
1:A:163:THR:HG21	2:B:221:PHE:HE1	1.74	0.53
1:A:195:ILE:HG13	1:A:196:GLN:N	2.23	0.53
1:A:163:THR:HG22	1:A:181:PHE:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:SER:HB3	1:C:450:ILE:HD11	1.90	0.52
2:D:546:CYS:O	2:D:550:GLU:HG3	2.10	0.52
2:D:566:ASN:OD1	2:D:589:PRO:HB2	2.10	0.52
1:C:472:LYS:HD3	6:C:70:HOH:O	2.09	0.52
2:D:560:GLN:O	2:D:564:ARG:HG3	2.11	0.51
1:A:136:CYS:HB3	1:A:178:PRO:HG2	1.92	0.51
2:B:257:GLU:OE2	2:B:258:ILE:HG22	2.11	0.51
1:A:124:LYS:O	1:A:128:GLU:HG3	2.11	0.50
1:C:463:THR:HG21	2:D:521:PHE:HE2	1.77	0.50
2:D:583:HIS:CD2	2:D:584:GLU:HG3	2.48	0.49
1:C:436:CYS:CB	1:C:478:PRO:HG2	2.43	0.49
1:C:495:ILE:HG13	1:C:496:GLN:N	2.28	0.49
1:C:397:LEU:HD13	1:C:440:ILE:HG21	1.95	0.49
2:D:557:GLU:OE2	2:D:558:ILE:HG22	2.13	0.48
1:A:81:VAL:HG13	6:A:255:HOH:O	2.13	0.48
2:B:220:LEU:C	2:B:220:LEU:HD23	2.34	0.48
2:B:266:ASN:OD1	2:B:289:PRO:HB2	2.12	0.48
1:A:84:MET:HB3	1:A:144:HIS:CD2	2.49	0.47
1:C:392:LYS:HB2	1:C:392:LYS:HZ3	1.79	0.47
1:A:193:ASP:OD2	2:B:285:LYS:NZ	2.49	0.45
1:A:119:MET:O	1:A:123:LEU:HD23	2.16	0.45
1:A:97:LEU:HD13	1:A:140:ILE:HG21	1.99	0.44
2:D:512:LYS:C	2:D:513:ILE:HD12	2.38	0.44
2:D:533:ARG:HE	3:F:805:ASJ:CG	2.30	0.44
1:A:111:TYR:CG	1:A:122:LEU:HD21	2.53	0.44
1:C:463:THR:HG21	2:D:521:PHE:CE2	2.52	0.44
1:C:487:ARG:HH22	5:D:850:CIT:C5	2.30	0.44
1:A:176:GLU:CG	2:B:213:ILE:HD13	2.48	0.44
2:D:571:ARG:HG2	2:D:571:ARG:HH11	1.83	0.44
1:A:147:GLU:O	1:A:148:ASN:HB2	2.18	0.44
1:A:136:CYS:CB	1:A:178:PRO:HG2	2.47	0.43
1:A:174:LEU:HA	1:A:177:LYS:HD2	1.99	0.43
1:C:358:TYR:HB3	6:C:42:HOH:O	2.18	0.43
2:D:527:PRO:CG	5:D:850:CIT:O3	2.66	0.43
1:C:386:VAL:HG23	6:C:1029:HOH:O	2.18	0.43
1:A:175:LEU:O	1:A:176:GLU:HB2	2.17	0.43
2:D:513:ILE:HD12	2:D:513:ILE:N	2.34	0.42
1:C:463:THR:HG22	1:C:481:PHE:CE2	2.54	0.42
1:C:411:TYR:CG	1:C:422:LEU:HD11	2.55	0.42
1:C:420:GLN:NE2	1:C:462:LEU:HD23	2.34	0.42
2:D:574:GLU:HG2	2:D:584:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:LYS:HE3	1:C:453:LYS:HB2	1.79	0.42
1:C:449:VAL:CG1	1:C:456:VAL:HG13	2.50	0.41
2:D:585:LYS:HA	2:D:585:LYS:HD3	1.85	0.41
1:A:157:THR:HA	1:A:158:PRO:HD3	1.92	0.41
1:A:80:LYS:HD2	1:A:80:LYS:N	2.36	0.41
2:B:271:ARG:NH2	1:C:476:GLU:OE2	2.54	0.41
2:B:286:LYS:HB3	2:D:514:PRO:HG3	2.04	0.40
1:C:449:VAL:HG13	1:C:456:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/173 (80%)	133 (96%)	5 (4%)	0	100	100
1	C	138/173 (80%)	134 (97%)	4 (3%)	0	100	100
2	B	90/97 (93%)	89 (99%)	1 (1%)	0	100	100
2	D	90/97 (93%)	89 (99%)	1 (1%)	0	100	100
3	E	3/5 (60%)	3 (100%)	0	0	100	100
3	F	3/5 (60%)	3 (100%)	0	0	100	100
4	G	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
All	All	465/555 (84%)	452 (97%)	13 (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	120/152 (79%)	117 (98%)	3 (2%)	47	56
1	C	120/152 (79%)	115 (96%)	5 (4%)	30	34
2	B	84/88 (96%)	84 (100%)	0	100	100
2	D	84/88 (96%)	82 (98%)	2 (2%)	49	58
3	E	3/3 (100%)	2 (67%)	1 (33%)	0	0
3	F	3/3 (100%)	1 (33%)	2 (67%)	0	0
4	G	3/3 (100%)	3 (100%)	0	100	100
All	All	417/489 (85%)	404 (97%)	13 (3%)	40	49

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

Mol	Chain	Res	Type
1	A	80	LYS
1	A	108	VAL
1	A	153	LYS
1	C	366	LYS
1	C	398	PHE
1	C	408	VAL
1	C	449	VAL
1	C	456	VAL
2	D	554	LYS
2	D	603	GLN
3	E	702	GLU
3	F	802	GLU
3	F	803	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	C	420	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](#)

2 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	ASJ	E	705	1,3	7,7,7	0.73	0	5,8,8	1.54	1 (20%)
3	ASJ	F	805	1,3	7,7,7	1.19	0	5,8,8	2.10	1 (20%)

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	ASJ	E	705	1,3	-	4/6/6/6	-
3	ASJ	F	805	1,3	-	4/6/6/6	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	805	ASJ	CB-CA-C	-4.16	104.68	112.21
3	E	705	ASJ	CB-CA-C	-2.89	106.98	112.21

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	705	ASJ	O-C-CA-N
3	E	705	ASJ	O-C-CA-CB
3	E	705	ASJ	N-CA-CB-CG
3	F	805	ASJ	O-C-CA-N
3	F	805	ASJ	O-C-CA-CB
3	F	805	ASJ	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	F	805	ASJ	N-CA-CB-CG
3	E	705	ASJ	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	705	ASJ	2	0
3	F	805	ASJ	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CIT	D	850	-	12,12,12	1.75	2 (16%)	17,17,17	2.11	6 (35%)

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
5	CIT	D	850	-	-	12/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	850	CIT	C4-C3	3.95	1.58	1.53
5	D	850	CIT	C2-C3	2.70	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	850	CIT	O6-C6-C3	4.78	121.34	113.05
5	D	850	CIT	O4-C5-O3	-3.73	114.01	123.30
5	D	850	CIT	C3-C4-C5	2.63	120.18	113.81
5	D	850	CIT	C4-C3-C6	-2.62	104.47	110.11
5	D	850	CIT	O3-C5-C4	-2.37	116.01	122.94
5	D	850	CIT	O6-C6-O5	-2.06	117.28	123.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	850	CIT	C1-C2-C3-C4
5	D	850	CIT	C1-C2-C3-C6
5	D	850	CIT	C2-C3-C4-C5
5	D	850	CIT	C6-C3-C4-C5
5	D	850	CIT	C2-C3-C6-O5
5	D	850	CIT	C2-C3-C6-O6
5	D	850	CIT	O7-C3-C6-O5
5	D	850	CIT	O7-C3-C6-O6
5	D	850	CIT	C1-C2-C3-O7
5	D	850	CIT	O7-C3-C4-C5
5	D	850	CIT	C4-C3-C6-O5
5	D	850	CIT	C3-C4-C5-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	850	CIT	4	0

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	140/173 (80%)	-0.12	4 (2%) 51 55	34, 51, 66, 76	0
1	C	140/173 (80%)	-0.24	0 100 100	30, 41, 58, 78	0
2	B	92/97 (94%)	0.46	11 (11%) 4 3	32, 45, 85, 95	0
2	D	92/97 (94%)	0.42	13 (14%) 2 2	31, 43, 84, 90	0
3	E	3/5 (60%)	0.69	1 (33%) 0 0	73, 73, 74, 78	0
3	F	3/5 (60%)	0.68	0 100 100	63, 63, 65, 74	0
4	G	5/5 (100%)	2.42	2 (40%) 0 0	107, 108, 112, 112	0
All	All	475/555 (85%)	0.10	31 (6%) 18 20	30, 46, 76, 112	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	278	ASP	5.8
4	G	811	GLY	4.4
2	D	578	ASP	4.0
2	B	280	PRO	3.8
2	B	276	GLN	3.7
2	D	580	PRO	3.6
2	B	291	VAL	3.4
2	D	592	VAL	3.2
2	D	582	PHE	3.2
2	D	521	PHE	2.9
2	B	290	CYS	2.8
4	G	813	GLY	2.7
2	B	292	VAL	2.7
2	B	282	PHE	2.6
1	A	80	LYS	2.6
2	D	576	GLN	2.5
2	B	279	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	281	HIS	2.4
2	D	591	VAL	2.4
1	A	57	THR	2.3
1	A	81	VAL	2.3
2	D	593	SER	2.3
2	D	603	GLN	2.2
2	D	579	ASP	2.2
3	E	704	MET	2.2
1	A	82	THR	2.2
2	B	222	ALA	2.1
2	D	581	HIS	2.1
2	D	584	GLU	2.1
2	B	220	LEU	2.1
2	D	577	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	ASJ	E	705	8/8	0.90	0.13	50,57,59,63	0
3	ASJ	F	805	8/8	0.95	0.10	47,51,51,54	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
5	CIT	D	850	13/13	0.68	0.48	118,119,120,120	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.