



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:05 pm BST

PDB ID : 2H1N  
Title : 3.0 Å X-ray structure of putative oligoendopeptidase F: crystals grown by vapor diffusion technique  
Authors : Gerdts, C.J.; Tereshko, V.; Dementieva, I.; Collart, F.; Joachimiak, A.; Kossiakoff, A.; Ismagilov, R.F.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2006-05-16  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

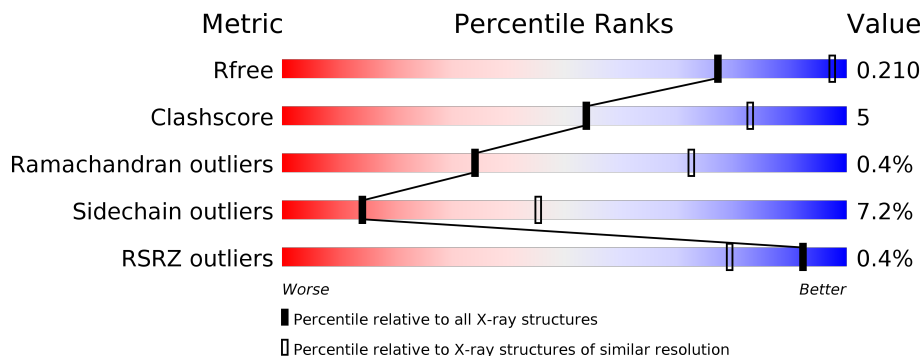
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	567	 83% 14%
1	B	567	 80% 17%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9378 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 Oligoendopeptidase F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	566	4679	2989	799	872	5	14	0	0	0
1	B	566	4679	2989	799	872	5	14	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	C	6	0
			6	6		
3	A	3	Total	C	6	0
			6	6		

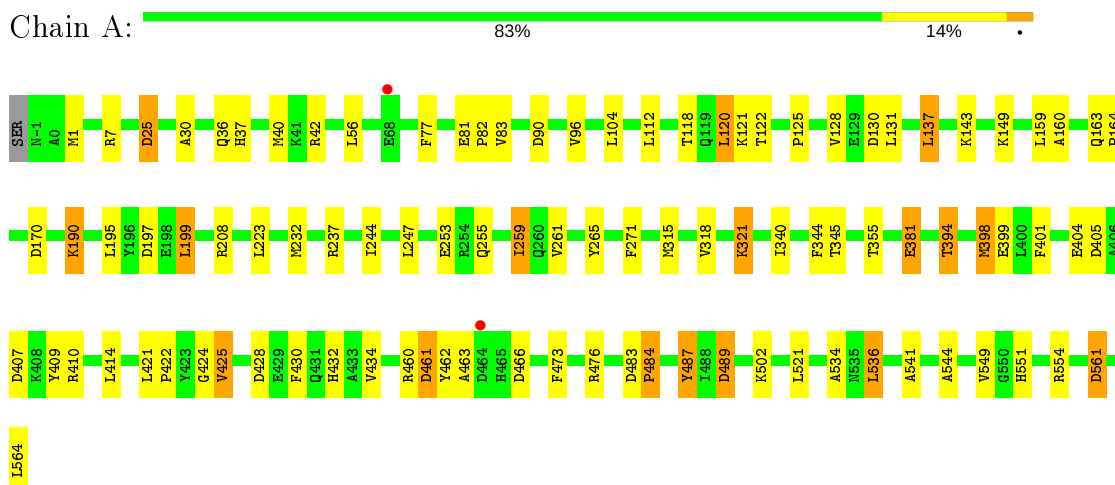
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	3	Total	O	0	0
			3	3		

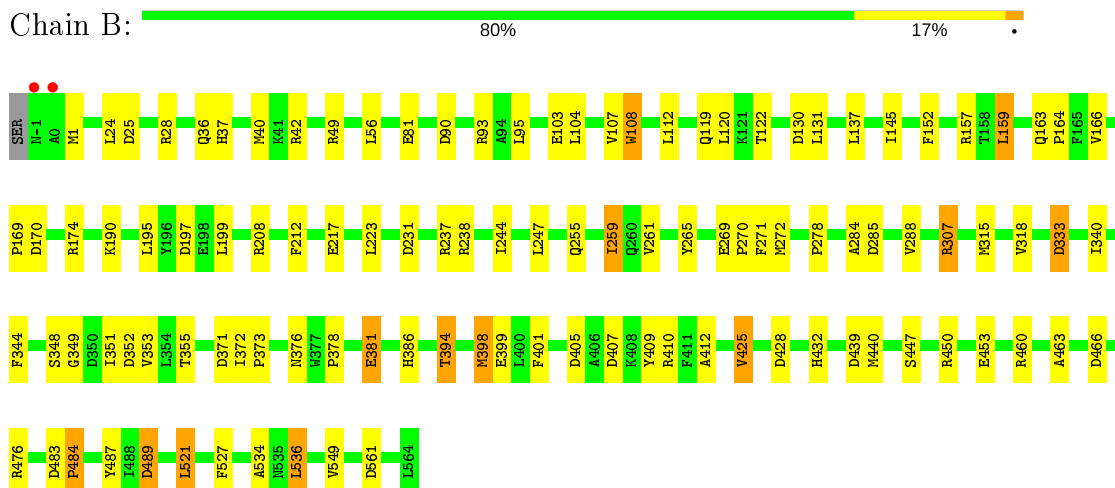
### 3 Residue-property plots [i](#)

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



- Molecule 1: Oligoendopeptidase F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.99Å 119.99Å 249.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.00) 98.3 (20.00-3.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.98Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.211 0.185 , 0.210	Depositor DCC
$R_{free}$ test set	2088 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.3	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	0/4793	0.87	12/6460 (0.2%)
1	B	0.44	0/4793	0.89	16/6460 (0.2%)
All	All	0.44	0/9586	0.88	28/12920 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ASP	CB-CG-OD2	7.16	124.74	118.30
1	B	352	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	170	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	407	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	285	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	405	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	483	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	90	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	561	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	333	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	231	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	466	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	25	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	439	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	130	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	407	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	405	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	197	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	90	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	489	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	483	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	130	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	25	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	561	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	466	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	489	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	461	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4679	0	4459	47	0
1	B	4679	0	4459	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
All	All	9378	0	8918	97	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 5.

All (97) 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:232:MSE:CE	1:A:232:MSE:SE	2.15	1.45
1:B:440:MSE:SE	1:B:440:MSE:CE	2.20	1.39
1:A:255:GLN:O	1:A:259:ILE:HG22	1.84	0.78
1:B:255:GLN:O	1:B:259:ILE:HG22	1.86	0.74
1:A:259:ILE:HG13	1:A:271:PHE:HD2	1.57	0.70
1:A:398:MSE:CE	1:A:398:MSE:HA	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:HIS:HA	1:A:40:MSE:HE3	1.76	0.68
1:A:355:THR:HG21	1:A:394:THR:HG21	1.76	0.68
1:B:355:THR:HG21	1:B:394:THR:HG21	1.75	0.66
1:B:460:ARG:HH11	1:B:460:ARG:HG3	1.60	0.66
1:B:534:ALA:HB3	1:B:536:LEU:HD22	1.78	0.65
1:B:259:ILE:HG13	1:B:271:PHE:HD2	1.60	0.64
1:A:149:LYS:HE2	1:A:321:LYS:NZ	2.13	0.64
1:A:149:LYS:HE2	1:A:321:LYS:CE	2.28	0.62
1:A:381:GLU:HA	1:A:489:ASP:HB3	1.83	0.61
1:A:561:ASP:HA	1:A:564:LEU:HD12	1.82	0.60
1:B:460:ARG:NH1	1:B:460:ARG:HG3	2.15	0.60
1:B:351:ILE:HG21	1:B:398:MSE:CE	2.33	0.59
1:B:450:ARG:NH1	1:B:453:GLU:OE1	2.34	0.59
1:B:398:MSE:HE3	1:B:401:PHE:CD1	2.37	0.59
1:A:237:ARG:HG2	1:A:425:VAL:HG22	1.85	0.58
1:B:244:ILE:CD1	1:B:549:VAL:HG21	2.34	0.58
1:B:107:VAL:HG12	1:B:107:VAL:O	2.04	0.58
1:B:307:ARG:HH11	1:B:307:ARG:HB3	1.68	0.57
1:B:259:ILE:HG13	1:B:271:PHE:CD2	2.39	0.57
1:A:259:ILE:HG13	1:A:271:PHE:CD2	2.40	0.57
1:B:108:TRP:NE1	1:B:372:ILE:HD11	2.19	0.57
1:B:152:PHE:O	1:B:157:ARG:NH1	2.38	0.56
1:A:428:ASP:O	1:A:432:HIS:HD2	1.88	0.56
1:A:534:ALA:HB3	1:A:536:LEU:HD22	1.88	0.56
1:B:349:GLY:O	1:B:353:VAL:HG23	2.05	0.56
1:B:166:VAL:O	1:B:174:ARG:HG2	2.05	0.55
1:B:351:ILE:HG21	1:B:398:MSE:HE2	1.87	0.55
1:A:398:MSE:HE2	1:A:401:PHE:CD1	2.42	0.55
1:A:541:ALA:HB3	1:A:544:ALA:HB2	1.91	0.54
1:A:149:LYS:HE2	1:A:321:LYS:HE2	1.89	0.53
1:B:381:GLU:HA	1:B:489:ASP:HB3	1.90	0.53
1:A:190:LYS:HA	1:A:190:LYS:HE3	1.91	0.52
1:B:398:MSE:HE3	1:B:401:PHE:HD1	1.74	0.52
1:B:95:LEU:HD21	1:B:112:LEU:CD1	2.41	0.51
1:B:265:TYR:CD2	1:B:463:ALA:HB2	2.44	0.51
1:A:81:GLU:HB3	1:A:82:PRO:HD3	1.92	0.51
1:B:237:ARG:HG2	1:B:425:VAL:HG22	1.93	0.51
1:A:460:ARG:HD2	1:A:462:TYR:CZ	2.47	0.50
1:A:253:GLU:OE1	1:A:253:GLU:HA	2.10	0.50
1:A:398:MSE:HE3	1:A:398:MSE:HA	1.93	0.50
1:A:399:GLU:OE2	1:A:410:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HD21	1:B:112:LEU:HD11	1.94	0.49
1:B:381:GLU:HG2	1:B:527:PHE:CD1	2.49	0.48
1:A:125:PRO:O	1:A:128:VAL:HG23	2.14	0.48
1:A:473:PHE:O	1:A:476:ARG:HG2	2.14	0.47
1:B:398:MSE:HG2	1:B:409:TYR:CD2	2.49	0.47
1:A:430:PHE:O	1:A:434:VAL:HG23	2.15	0.47
1:B:284:ALA:O	1:B:288:VAL:HG23	2.15	0.47
1:B:244:ILE:HD11	1:B:549:VAL:HG21	1.96	0.47
1:A:160:ALA:O	1:A:345:THR:HG21	2.14	0.46
1:B:37:HIS:HA	1:B:40:MSE:HE3	1.97	0.46
1:B:378:PRO:HG3	1:B:386:HIS:HE1	1.81	0.46
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.82	0.46
1:A:398:MSE:HG2	1:A:409:TYR:CD2	2.51	0.45
1:B:278:PRO:O	1:B:348:SER:HB3	2.17	0.45
1:A:163:GLN:HB3	1:A:164:PRO:HD3	1.99	0.45
1:A:244:ILE:HD11	1:A:549:VAL:HG21	1.97	0.45
1:A:118:THR:O	1:A:121:LYS:HG2	2.16	0.45
1:B:37:HIS:HD1	1:B:108:TRP:HZ3	1.65	0.45
1:A:398:MSE:HA	1:A:398:MSE:HE2	1.97	0.45
1:A:551:HIS:CD2	1:A:554:ARG:HH12	2.35	0.45
1:A:315:MSE:HE2	1:A:340:ILE:HD12	1.99	0.44
1:A:424:GLY:HA2	1:A:487:TYR:CE2	2.52	0.44
1:B:399:GLU:OE2	1:B:410:ARG:NH2	2.51	0.44
1:B:318:VAL:HA	1:B:344:PHE:HB2	1.99	0.44
1:A:551:HIS:HD2	1:A:554:ARG:HH12	1.66	0.44
1:B:269:GLU:N	1:B:270:PRO:HD2	2.33	0.43
1:B:163:GLN:HB3	1:B:164:PRO:HD3	1.99	0.43
1:B:398:MSE:CE	1:B:401:PHE:CD1	3.01	0.43
1:A:265:TYR:CD2	1:A:463:ALA:HB2	2.53	0.43
1:A:424:GLY:HA2	1:A:487:TYR:HE2	1.84	0.43
1:B:212:PHE:CD2	1:B:217:GLU:HB3	2.53	0.43
1:B:428:ASP:O	1:B:432:HIS:HD2	2.02	0.43
1:A:30:ALA:HB3	1:A:36:GLN:HG3	2.00	0.43
1:B:315:MSE:CE	1:B:340:ILE:HD12	2.49	0.43
1:B:460:ARG:HH11	1:B:460:ARG:CG	2.31	0.42
1:A:421:LEU:HB2	1:A:422:PRO:HD3	2.01	0.42
1:B:145:ILE:HG23	1:B:159:LEU:HD23	2.02	0.42
1:B:169:PRO:HA	1:B:271:PHE:CZ	2.55	0.42
1:A:318:VAL:HA	1:A:344:PHE:HB2	2.01	0.42
1:A:404:GLU:HG2	1:A:404:GLU:H	1.63	0.42
1:B:521:LEU:HA	1:B:521:LEU:HD12	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:O	1:B:108:TRP:HB2	2.21	0.41
1:A:77:PHE:O	1:A:81:GLU:HB2	2.21	0.41
1:B:272:MSE:HE2	1:B:412:ALA:HA	2.02	0.41
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.90	0.41
1:B:36:GLN:HB3	1:B:40:MSE:HE2	2.03	0.41
1:B:315:MSE:HE2	1:B:340:ILE:HD12	2.03	0.41
1:A:137:LEU:HD23	1:A:199:LEU:HD13	2.03	0.41
1:B:373:PRO:HA	1:B:376:ASN:ND2	2.35	0.40
1:A:315:MSE:CE	1:A:340:ILE:HD12	2.50	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	564/567 (100%)	550 (98%)	12 (2%)	2 (0%)	34	72
1	B	564/567 (100%)	553 (98%)	9 (2%)	2 (0%)	34	72
All	All	1128/1134 (100%)	1103 (98%)	21 (2%)	4 (0%)	34	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	PRO
1	B	484	PRO
1	A	487	TYR
1	B	487	TYR

### 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	484/471 (103%)	451 (93%)	33 (7%)	16	48
1	B	484/471 (103%)	447 (92%)	37 (8%)	13	43
All	All	968/942 (103%)	898 (93%)	70 (7%)	14	45

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	7	ARG
1	A	25	ASP
1	A	42	ARG
1	A	56	LEU
1	A	83	VAL
1	A	96	VAL
1	A	104	LEU
1	A	112	LEU
1	A	120	LEU
1	A	122	THR
1	A	131	LEU
1	A	137	LEU
1	A	143	LYS
1	A	159	LEU
1	A	190	LYS
1	A	195	LEU
1	A	199	LEU
1	A	208	ARG
1	A	223	LEU
1	A	247	LEU
1	A	259	ILE
1	A	261	VAL
1	A	321	LYS
1	A	381	GLU
1	A	394	THR
1	A	398	MSE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	425	VAL
1	A	461	ASP
1	A	484	PRO
1	A	502	LYS
1	A	521	LEU
1	A	536	LEU
1	B	1	MSE
1	B	24	LEU
1	B	28	ARG
1	B	42	ARG
1	B	49	ARG
1	B	56	LEU
1	B	81	GLU
1	B	93	ARG
1	B	103	GLU
1	B	108	TRP
1	B	119	GLN
1	B	120	LEU
1	B	122	THR
1	B	131	LEU
1	B	137	LEU
1	B	159	LEU
1	B	190	LYS
1	B	195	LEU
1	B	199	LEU
1	B	208	ARG
1	B	223	LEU
1	B	238	ARG
1	B	247	LEU
1	B	259	ILE
1	B	261	VAL
1	B	307	ARG
1	B	333	ASP
1	B	371	ASP
1	B	381	GLU
1	B	394	THR
1	B	398	MSE
1	B	425	VAL
1	B	447	SER
1	B	476	ARG
1	B	484	PRO
1	B	521	LEU

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Mol	Chain	Res	Type
1	B	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	213	GLN
1	A	376	ASN
1	A	431	GLN
1	A	432	HIS
1	A	451	ASN
1	A	477	GLN
1	A	494	GLN
1	A	551	HIS
1	B	201	HIS
1	B	363	GLN
1	B	376	ASN
1	B	386	HIS
1	B	431	GLN
1	B	432	HIS
1	B	451	ASN
1	B	537	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](#)

Of 8 ligands modelled in this entry, 6 are unknown and 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	552/567 (97%)	-0.54	2 (0%) 92 79	56, 63, 70, 84	55 (9%)
1	B	552/567 (97%)	-0.58	2 (0%) 92 79	57, 63, 70, 89	58 (10%)
All	All	1104/1134 (97%)	-0.56	4 (0%) 92 79	56, 63, 70, 89	113 (10%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	ASN	2.7
1	B	0	ALA	2.3
1	A	68	GLU	2.2
1	A	464	ASP	2.1

### 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. 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	UNL	A	607	2/-	-	-	60,60,60,60	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UNL	B	707	2/-	-	-	60,60,60,60	2
3	UNL	B	705	2/-	-	-	60,60,60,60	2
2	ZN	B	701	1/1	0.99	0.02	66,66,66,66	0
3	UNL	A	605	2/-	-	-	60,60,60,60	2
3	UNL	A	606	2/-	-	-	60,60,60,60	2
2	ZN	A	601	1/1	1.00	0.06	60,60,60,60	0
3	UNL	B	706	2/-	-	-	60,60,60,60	2

## 6.5 Other polymers [i](#)

There are no such residues in this entry.