



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:29 PM GMT

PDB ID : 2A5K  
Title : Crystal structures of SARS coronavirus main peptidase inhibited by an aza-peptide epoxide in space group P212121  
Authors : Lee, T.-W.; Cherney, M.M.; Huitema, C.; Liu, J.; James, K.E.; Powers, J.C.; Eltis, L.D.; James, M.N.  
Deposited on : 2005-06-30  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

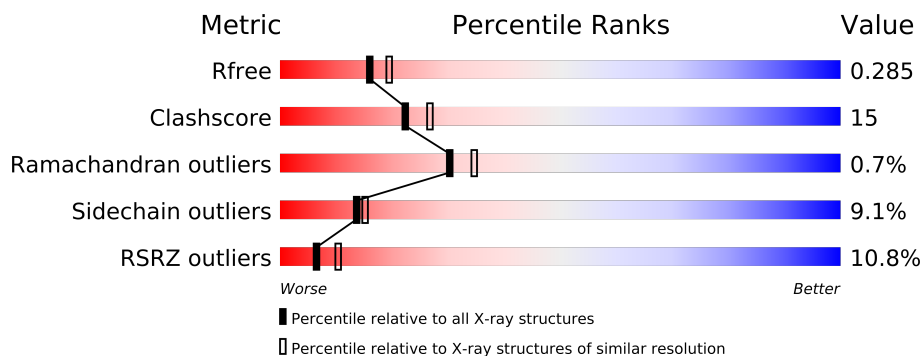
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. 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	307	
1	B	307	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5172 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.

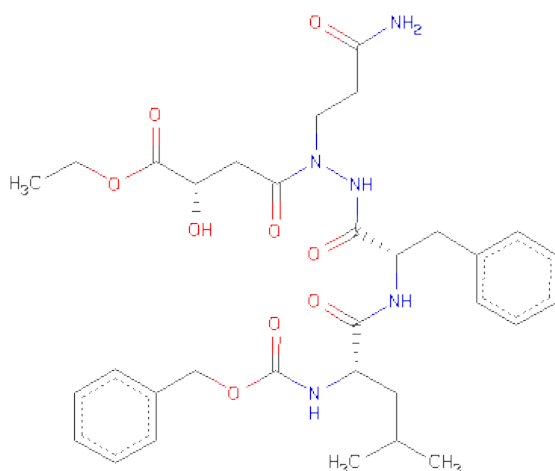
- Molecule 1 is a protein called 3C-like peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	12	0
			2419	1527	418	450	24			
1	B	300	Total	C	N	O	S	0	12	0
			2383	1504	414	442	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	EXPRESSION TAG	UNP P59641
B	0	ALA	-	EXPRESSION TAG	UNP P59641

- Molecule 2 is (5S,8S,14R)-ETHYL 11-(3-AMINO-3-OXOPROPYL)-8-BENZYL-14-HYDROXY-5-ISOBUTYL-3,6,9,12-TETRAOXO-1-PHENYL-2-OXA-4,7,10,11-TETRAAZAPENTADECAN-15-OATE (three-letter code: AZP) (formula: C<sub>32</sub>H<sub>43</sub>N<sub>5</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			46	32	5	9		
2	B	1	Total	C	N	O	0	0
			46	32	5	9		

- Molecule 3 is water.

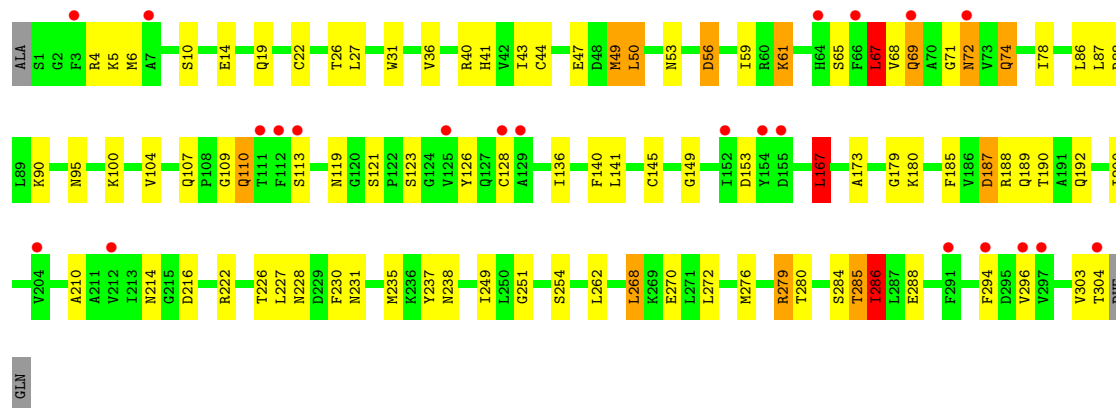
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	96	Total	O	0	0
			96	96		

### 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.

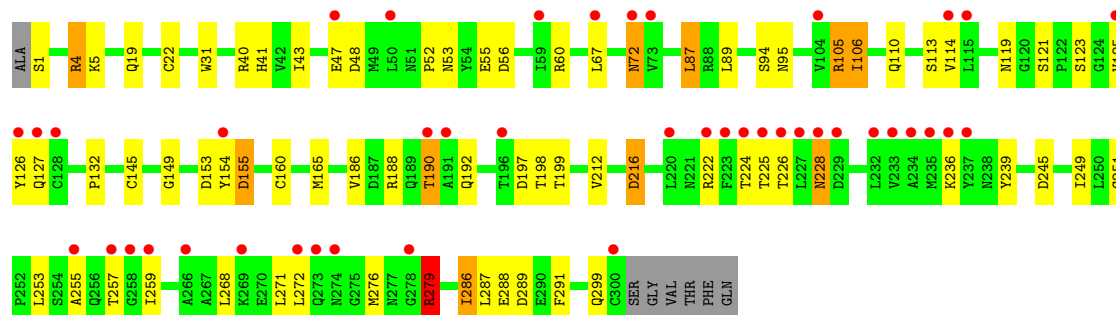
- Molecule 1: 3C-like peptidase

Chain A: 



- Molecule 1: 3C-like peptidase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.35Å 67.48Å 167.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 41.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-2.30) 99.1 (41.83-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.175 , 0.249 0.230 , 0.285	Depositor DCC
$R_{free}$ test set	1685 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.9	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33250 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: AZP

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	1.02	1/2515 (0.0%)	0.99	4/3412 (0.1%)
1	B	0.96	5/2482 (0.2%)	0.94	4/3365 (0.1%)
All	All	0.99	6/4997 (0.1%)	0.97	8/6777 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	THR	C-O	6.21	1.35	1.23
1	B	160	CYS	CB-SG	-6.00	1.72	1.82
1	B	228	ASN	CG-ND2	6.00	1.47	1.32
1	A	44	CYS	CB-SG	-5.74	1.72	1.81
1	B	228	ASN	C-O	5.57	1.33	1.23
1	B	22	CYS	CB-SG	5.21	1.91	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	167	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	67	LEU	CA-CB-CG	6.15	129.45	115.30
1	B	87	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	A	6	MET	CA-CB-CG	5.95	123.41	113.30
1	B	225	THR	O-C-N	5.66	131.75	122.70
1	A	187	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	105	ARG	NE-CZ-NH1	-5.33	117.64	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2419	0	2371	91	0
1	B	2383	0	2335	52	0
2	A	46	0	43	16	0
2	B	46	0	41	3	0
3	A	182	0	0	9	0
3	B	96	0	0	7	0
All	All	5172	0	4790	143	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 15.

All (143) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:145:CYS:SG	2:A:307:AZP:HBM2	1.19	1.71
1:A:50:LEU:HB2	3:A:405:HOH:O	1.58	1.03
1:A:288:GLU:HG3	3:A:341:HOH:O	1.60	1.00
1:A:279[A]:ARG:HH11	1:A:279[A]:ARG:HG2	1.23	1.00
1:A:285[A]:THR:OG1	1:A:286:ILE:N	1.84	0.97
1:A:5:LYS:HE2	3:A:309:HOH:O	1.64	0.95
1:A:49:MET:HB3	2:A:307:AZP:HBI	1.46	0.95
1:A:41:HIS:HD2	2:A:307:AZP:HBS1	1.31	0.95
1:A:72:ASN:H	1:A:72:ASN:ND2	1.65	0.91
1:A:72:ASN:N	1:A:72:ASN:HD22	1.69	0.90
1:B:72:ASN:H	1:B:72:ASN:HD22	1.20	0.88
1:A:72:ASN:H	1:A:72:ASN:HD22	1.18	0.85
1:A:226:THR:HG22	1:A:228:ASN:H	1.47	0.80
1:A:304:THR:HG22	1:B:123:SER:HB2	1.64	0.79
1:A:72:ASN:ND2	1:A:72:ASN:N	2.29	0.78
1:B:72:ASN:H	1:B:72:ASN:ND2	1.80	0.77
1:A:276:MET:HE1	1:A:280:THR:HA	1.67	0.77
1:B:165[A]:MET:SD	2:B:307:AZP:HBF	2.26	0.75
1:B:279[B]:ARG:HH11	1:B:279[B]:ARG:HB3	1.50	0.75
1:A:41:HIS:CD2	2:A:307:AZP:HBS1	2.20	0.75
1:A:192:GLN:HB2	2:A:307:AZP:CAA	2.18	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:19:GLN:NE2	1:A:119:ASN:HB3	2.03	0.73
1:B:279[B]:ARG:NH1	3:B:392:HOH:O	2.22	0.72
1:A:276:MET:HE1	1:A:285[A]:THR:HA	1.72	0.71
2:A:307:AZP:HAF	3:A:397:HOH:O	1.90	0.70
1:B:279[A]:ARG:HA	3:B:353:HOH:O	1.92	0.70
1:B:279[B]:ARG:HH11	1:B:279[B]:ARG:CG	2.04	0.70
1:B:19:GLN:HE21	1:B:119:ASN:HB3	1.57	0.70
1:A:284:SER:OG	1:A:285[A]:THR:O	2.04	0.69
1:A:285[A]:THR:HG23	1:A:286:ILE:HG23	1.75	0.68
1:A:231:ASN:O	1:A:235:MET:HG3	1.94	0.68
1:B:279[B]:ARG:CB	1:B:279[B]:ARG:HH11	2.06	0.68
1:A:226:THR:HG22	1:A:228:ASN:N	2.07	0.68
1:B:132:PRO:HD2	1:B:197:ASP:OD2	1.93	0.67
1:A:49:MET:HB3	2:A:307:AZP:CBI	2.21	0.67
1:A:276:MET:CE	1:A:280:THR:HA	2.25	0.66
1:B:72:ASN:N	1:B:72:ASN:HD22	1.84	0.65
1:B:48:ASP:O	1:B:48:ASP:OD2	2.13	0.65
1:A:279[A]:ARG:NH1	1:A:279[A]:ARG:HG2	2.03	0.65
1:B:5:LYS:HE2	1:B:288:GLU:OE1	1.98	0.63
1:A:69:GLN:NE2	1:A:72:ASN:HA	2.14	0.63
1:A:285[A]:THR:O	1:A:286:ILE:O	2.17	0.63
1:A:126:TYR:HE1	1:A:128[B]:CYS:SG	2.22	0.63
1:A:67:LEU:HD11	3:A:471:HOH:O	1.99	0.63
1:A:270:GLU:HG3	3:A:350:HOH:O	1.99	0.62
1:B:31:TRP:CD2	1:B:95:ASN:HB2	2.35	0.62
1:A:188[A]:ARG:HG3	1:A:190:THR:HG22	1.81	0.61
1:A:49:MET:CB	2:A:307:AZP:HBI	2.25	0.61
1:A:145:CYS:SG	2:A:307:AZP:HBM1	2.34	0.60
1:B:19:GLN:NE2	1:B:119:ASN:HB3	2.17	0.60
1:B:145:CYS:SG	2:B:307:AZP:CBK	2.89	0.60
1:A:110:GLN:HB3	3:A:473:HOH:O	2.00	0.59
1:A:10:SER:O	1:A:14:GLU:HG3	2.02	0.58
1:B:31:TRP:CE2	1:B:95:ASN:HB2	2.39	0.58
1:A:4:ARG:HD2	1:B:126:TYR:CD1	2.38	0.57
1:B:279[B]:ARG:HA	3:B:353:HOH:O	2.03	0.57
1:B:52:PRO:O	1:B:188[B]:ARG:NH1	2.36	0.57
1:B:212:VAL:HA	1:B:216:ASP:O	2.04	0.56
1:B:279[B]:ARG:HG2	1:B:279[B]:ARG:HH11	1.70	0.56
1:A:167:LEU:HD21	1:A:173:ALA:HB2	1.89	0.55
1:A:276:MET:CE	1:A:285[A]:THR:HA	2.35	0.55
1:A:126:TYR:CE1	1:A:128[B]:CYS:SG	3.00	0.55
1:B:41:HIS:HD2	2:B:307:AZP:HBS1	1.72	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:279[B]:ARG:HG2	1:B:279[B]:ARG:NH1	2.23	0.54
1:A:88[A]:ARG:NH1	3:A:407:HOH:O	2.32	0.53
1:A:279[A]:ARG:CG	1:A:279[A]:ARG:HH11	2.09	0.53
1:A:107:GLN:O	1:A:110:GLN:HG3	2.09	0.53
1:A:187:ASP:HB2	2:A:307:AZP:HGB	1.91	0.53
1:B:257:THR:OG1	1:B:259:ILE:HD12	2.10	0.52
1:A:69:GLN:OE1	1:A:74:GLN:NE2	2.42	0.52
1:A:285[B]:THR:O	1:A:286:ILE:CG1	2.57	0.52
1:A:19:GLN:HE21	1:A:26:THR:HG21	1.75	0.52
1:A:192:GLN:HB2	2:A:307:AZP:CAB	2.39	0.52
1:B:253:LEU:O	1:B:257:THR:HG23	2.11	0.51
1:A:140:PHE:O	1:A:141:LEU:HD23	2.11	0.51
1:A:145:CYS:SG	2:A:307:AZP:CBK	2.93	0.51
1:A:41:HIS:HD2	2:A:307:AZP:CBS	2.11	0.51
1:B:87:LEU:HD13	1:B:89:LEU:HD21	1.93	0.51
1:A:113:SER:O	1:A:149:GLY:HA2	2.11	0.50
1:B:186:VAL:HG21	1:B:188[A]:ARG:HE	1.77	0.50
1:B:114:VAL:O	1:B:125:VAL:HA	2.12	0.50
1:A:188[A]:ARG:HG3	1:A:190:THR:CG2	2.42	0.49
1:A:251:GLY:O	1:A:254:SER:HB3	2.12	0.49
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.95	0.48
1:A:285[B]:THR:O	1:A:286:ILE:HG23	2.14	0.48
1:A:268:LEU:HD22	1:A:272:LEU:HG	1.94	0.48
1:B:251:GLY:O	1:B:255:ALA:N	2.42	0.48
1:A:180:LYS:HE2	3:A:391:HOH:O	2.13	0.48
1:A:276:MET:HE1	1:A:285[B]:THR:HA	1.95	0.48
1:A:285[A]:THR:HG21	3:B:359:HOH:O	2.14	0.47
1:A:237:TYR:O	1:A:238:ASN:CB	2.63	0.47
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.50	0.47
1:A:276:MET:CE	1:A:285[B]:THR:HA	2.45	0.47
1:A:19:GLN:NE2	1:A:26:THR:HG21	2.29	0.47
1:A:210:ALA:HB2	1:A:296:VAL:HG13	1.96	0.47
1:A:185:PHE:CE1	2:A:307:AZP:HAB	2.50	0.46
1:A:53:ASN:OD1	1:A:56:ASP:HB2	2.15	0.46
1:A:189:GLN:HG3	2:A:307:AZP:OAL	2.14	0.46
1:A:185:PHE:CD1	2:A:307:AZP:HAB	2.51	0.46
1:A:69:GLN:NE2	1:A:71:GLY:O	2.46	0.45
1:B:276:MET:O	1:B:279[A]:ARG:HD2	2.16	0.45
1:A:210:ALA:O	1:A:214:ASN:ND2	2.49	0.45
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.74	0.45
1:B:113:SER:O	1:B:149:GLY:HA2	2.17	0.45
1:A:100:LYS:HB3	1:A:100:LYS:HE2	1.82	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:226:THR:HG22	1:B:228:ASN:N	2.32	0.45
1:A:285[B]:THR:O	1:A:286:ILE:CB	2.66	0.44
1:B:40:ARG:O	1:B:43:ILE:HG12	2.17	0.44
1:A:285[B]:THR:O	1:A:286:ILE:HG12	2.17	0.44
1:B:279[A]:ARG:HG3	1:B:279[A]:ARG:H	1.56	0.44
1:B:190:THR:O	1:B:192:GLN:HG2	2.18	0.44
1:A:78:ILE:HG13	1:A:90:LYS:HD3	2.00	0.43
1:A:43:ILE:HB	1:A:61:LYS:HE2	2.00	0.43
1:B:4:ARG:HD3	1:B:4:ARG:HH11	1.61	0.43
1:A:40:ARG:HA	1:A:87:LEU:HG	2.01	0.43
1:A:78:ILE:HD11	1:A:90:LYS:HD3	2.01	0.43
1:A:136:ILE:HG21	1:A:136:ILE:HD13	1.82	0.43
1:B:245:ASP:O	1:B:249:ILE:HG13	2.19	0.42
1:B:291:PHE:HB2	3:B:327:HOH:O	2.18	0.42
1:B:186:VAL:HG23	1:B:188[A]:ARG:HG3	2.02	0.42
1:B:48:ASP:HA	3:B:396:HOH:O	2.19	0.42
1:B:288:GLU:HG2	1:B:291:PHE:CD1	2.55	0.42
1:B:5:LYS:HD2	1:B:127[B]:GLN:OE1	2.19	0.42
1:B:106:ILE:HG13	1:B:110:GLN:HB2	2.01	0.41
1:A:78:ILE:CG1	1:A:90:LYS:HD3	2.50	0.41
1:A:19:GLN:HE21	1:A:119:ASN:HB3	1.83	0.41
1:B:272:LEU:HA	1:B:272:LEU:HD23	1.80	0.41
1:A:86:LEU:HG	1:A:179:GLY:HA2	2.03	0.41
1:A:230:PHE:HZ	1:A:268:LEU:HD13	1.85	0.41
1:B:199:THR:HG21	1:B:239:TYR:CZ	2.56	0.41
1:A:36:VAL:HG21	1:A:68:VAL:HG11	2.02	0.40
1:B:53:ASN:CG	1:B:56:ASP:OD1	2.59	0.40
1:B:271:LEU:HD13	1:B:287:LEU:HD21	2.02	0.40

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	314/307 (102%)	303 (96%)	10 (3%)	1 (0%)	50 60

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	309/307 (101%)	285 (92%)	20 (6%)	4 (1%)	18	17
All	All	623/614 (102%)	588 (94%)	30 (5%)	5 (1%)	30	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	286	ILE
1	A	286	ILE
1	B	154[C]	TYR
1	B	279[A]	ARG
1	B	279[B]	ARG

### 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	273/263 (104%)	244 (89%)	29 (11%)	10	10
1	B	269/263 (102%)	246 (91%)	23 (9%)	15	17
All	All	542/526 (103%)	490 (90%)	52 (10%)	14	13

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	27	LEU
1	A	47	GLU
1	A	49	MET
1	A	50	LEU
1	A	56	ASP
1	A	59	ILE
1	A	61	LYS
1	A	65	SER
1	A	67	LEU
1	A	69	GLN
1	A	72	ASN
1	A	74	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	104	VAL
1	A	110	GLN
1	A	121	SER
1	A	123	SER
1	A	153	ASP
1	A	167	LEU
1	A	216	ASP
1	A	222	ARG
1	A	227	LEU
1	A	268	LEU
1	A	279[A]	ARG
1	A	279[B]	ARG
1	A	285[A]	THR
1	A	285[B]	THR
1	A	286	ILE
1	A	303	VAL
1	B	1	SER
1	B	47	GLU
1	B	55	GLU
1	B	60	ARG
1	B	67	LEU
1	B	72	ASN
1	B	94	SER
1	B	105	ARG
1	B	106	ILE
1	B	121	SER
1	B	153[A]	ASP
1	B	153[B]	ASP
1	B	155[A]	ASP
1	B	155[B]	ASP
1	B	190	THR
1	B	198	THR
1	B	216	ASP
1	B	222	ARG
1	B	268	LEU
1	B	279[A]	ARG
1	B	279[B]	ARG
1	B	286	ILE
1	B	289	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	72	ASN
1	A	228	ASN
1	A	277	ASN
1	B	19	GLN
1	B	69	GLN
1	B	72	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	AZP	A	307	1	47,47,47	1.64	4 (8%)	61,61,61	1.93	11 (18%)
2	AZP	B	307	1	47,47,47	1.67	4 (8%)	61,61,61	1.69	11 (18%)

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	AZP	A	307	1	-	0/51/53/53	0/2/2/2
2	AZP	B	307	1	-	0/51/53/53	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	307	AZP	OBR-CBP	6.65	1.47	1.33
2	B	307	AZP	OBR-CBP	6.51	1.47	1.33
2	B	307	AZP	OAH-CAI	5.95	1.47	1.35
2	B	307	AZP	NAX-NAZ	5.61	1.47	1.39
2	A	307	AZP	NAX-NAZ	5.53	1.46	1.39
2	A	307	AZP	OAH-CAI	4.67	1.45	1.35
2	A	307	AZP	CBA-CBB	-2.15	1.49	1.52
2	B	307	AZP	CA-N	2.05	1.50	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	307	AZP	OBR-CBP-CBO	6.78	120.36	111.44
2	B	307	AZP	OBR-CBP-CBO	6.65	120.17	111.44
2	A	307	AZP	CAU-NAX-NAZ	6.09	126.75	120.01
2	A	307	AZP	CBB-CBA-NAZ	-4.89	106.77	111.87
2	A	307	AZP	CBA-CBB-CBC	-4.53	104.34	112.63
2	A	307	AZP	CAG-OAH-CAI	-4.35	104.90	115.98
2	B	307	AZP	CAT-CAU-NAX	3.83	120.36	114.19
2	B	307	AZP	CBB-CBA-NAZ	3.44	115.46	111.87
2	A	307	AZP	CBM-CBK-NAZ	3.01	121.75	117.69
2	B	307	AZP	CAG-OAH-CAI	-2.81	108.82	115.98
2	B	307	AZP	CBS-OBR-CBP	-2.73	109.75	116.64
2	B	307	AZP	CB-CA-N	-2.73	103.74	110.52
2	A	307	AZP	CAU-CAT-NAS	-2.72	103.63	111.28
2	B	307	AZP	OAH-CAI-N	2.71	117.06	110.57
2	B	307	AZP	O-C-NAS	-2.36	118.39	122.93
2	A	307	AZP	OAH-CAI-OAL	-2.27	119.22	124.19
2	B	307	AZP	CBO-CBM-CBK	2.23	117.56	113.19
2	A	307	AZP	CB-CA-C	-2.23	104.69	110.57
2	B	307	AZP	OAL-CAI-N	-2.22	120.95	124.90
2	A	307	AZP	OBL-CBK-CBM	-2.20	118.00	122.25
2	A	307	AZP	OAH-CAI-N	2.18	115.79	110.57
2	B	307	AZP	CA-N-CAI	2.01	126.12	120.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	304/307 (99%)	0.47	22 (7%) 15 22	30, 45, 61, 80	6 (1%)
1	B	300/307 (97%)	0.86	43 (14%) 3 5	27, 46, 59, 68	9 (3%)
All	All	604/614 (98%)	0.66	65 (10%) 6 10	27, 45, 60, 80	15 (2%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	CYS	8.2
1	B	125	VAL	7.0
1	A	125	VAL	6.6
1	B	232	LEU	6.2
1	B	222	ARG	6.2
1	B	223	PHE	6.0
1	B	50	LEU	5.8
1	B	226	THR	5.4
1	B	227	LEU	5.0
1	B	154[C]	TYR	4.8
1	A	294[A]	PHE	4.5
1	B	59	ILE	4.4
1	B	255	ALA	4.3
1	B	266	ALA	3.5
1	B	274	ASN	3.5
1	A	128[A]	CYS	3.4
1	B	191	ALA	3.4
1	B	72	ASN	3.4
1	B	233	VAL	3.3
1	B	258	GLY	3.3
1	B	257	THR	3.2
1	B	236[A]	LYS	3.2
1	B	127[A]	GLN	3.2
1	B	224	THR	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	273	GLN	3.2
1	B	234	ALA	3.2
1	A	3	PHE	3.2
1	B	237	TYR	3.0
1	A	212	VAL	2.9
1	A	112	PHE	2.8
1	A	155[A]	ASP	2.8
1	A	7	ALA	2.7
1	B	73	VAL	2.7
1	A	64[A]	HIS	2.7
1	B	229	ASP	2.6
1	B	47	GLU	2.6
1	A	129	ALA	2.6
1	A	111	THR	2.6
1	B	220	LEU	2.6
1	B	235	MET	2.6
1	A	66	PHE	2.6
1	B	269	LYS	2.5
1	A	154	TYR	2.5
1	B	126	TYR	2.5
1	B	196	THR	2.4
1	A	297	VAL	2.4
1	B	104	VAL	2.4
1	B	115	LEU	2.4
1	A	72	ASN	2.3
1	B	225	THR	2.3
1	A	204	VAL	2.3
1	B	228	ASN	2.2
1	A	113	SER	2.2
1	A	296	VAL	2.2
1	B	67	LEU	2.2
1	B	278	GLY	2.1
1	A	291	PHE	2.1
1	B	190	THR	2.1
1	B	300	CYS	2.1
1	A	69	GLN	2.1
1	B	272	LEU	2.1
1	B	114	VAL	2.0
1	A	152	ILE	2.0
1	B	259	ILE	2.0
1	A	304	THR	2.0

## 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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	AZP	A	307	46/46	0.18	1.63	53,58,63,64	0
2	AZP	B	307	46/46	0.23	1.24	61,70,81,81	0

## 6.5 Other polymers

There are no such residues in this entry.