



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:05 pm GMT

PDB ID : 1M9I  
Title : Crystal Structure Of Phosphorylation-Mimicking Mutant T356D Of Annexin VI  
Authors : Freye-Minks, C.; Kretsinger, R.H.; Creutz, C.E.  
Deposited on : 2002-07-29  
Resolution : 2.65 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

<http://wwpdb.org/validation/2016/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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

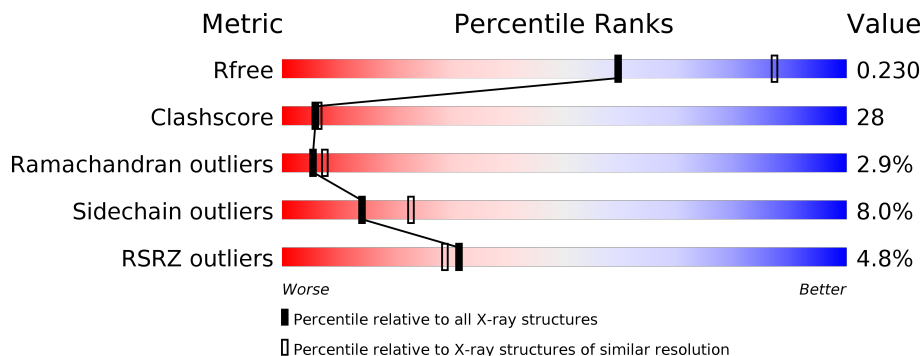
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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. 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	672	<div> <div>5%</div> <div>56%</div> <div>36%</div> <div>6%</div> </div>

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
2	CA	A	701	-	-	-	X
2	CA	A	704	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5417 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 Annexin VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5264	3297	909	1032	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	ASP	THR	ENGINEERED	UNP P08133
A	619	ASP	GLU	SEE REMARK 999	UNP P08133

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		

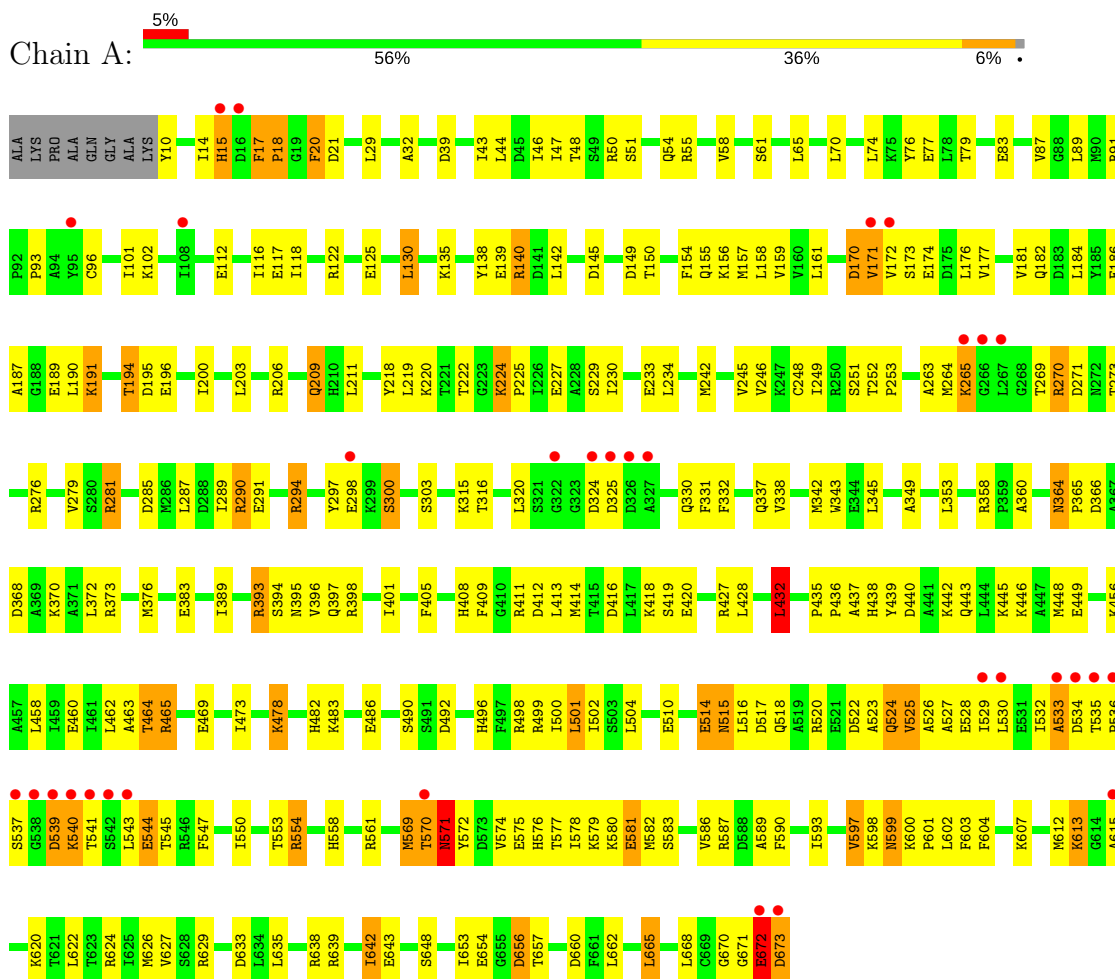
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		

### 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 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: Annexin VI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.97 Å 67.97 Å 204.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.21 – 2.65 18.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (18.21-2.65) 97.6 (18.21-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.44 (at 2.49 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.279 0.227 , 0.230	Depositor DCC
$R_{free}$ test set	1325 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.226 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: CA

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	0.38	0/5342	0.60	1/7178 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	432	LEU	CA-CB-CG	5.28	127.45	115.30

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	5264	0	5247	290	0
2	A	5	0	0	1	0
3	A	148	0	0	13	0
All	All	5417	0	5247	291	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 28.

All (291) 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:529:ILE:HD13	1:A:543:LEU:HB3	1.37	1.03
1:A:18:PRO:HD2	1:A:54:GLN:HE22	1.29	0.97
1:A:222:THR:HG22	1:A:224:LYS:H	1.29	0.96
1:A:525:VAL:O	1:A:529:ILE:HG12	1.72	0.88
2:A:705:CA:CA	3:A:706:HOH:O	0.45	0.85
1:A:330:GLN:HB2	1:A:571:ASN:HB3	1.57	0.85
1:A:532:ILE:HG12	1:A:540:LYS:HG3	1.57	0.85
1:A:583:SER:O	1:A:586:VAL:HG12	1.77	0.85
1:A:530:LEU:HG	1:A:577:THR:HB	1.63	0.79
1:A:456:LYS:HZ3	1:A:607:LYS:HE3	1.48	0.78
1:A:530:LEU:HG	1:A:577:THR:CB	2.12	0.78
1:A:14:ILE:HD12	3:A:735:HOH:O	1.85	0.77
1:A:529:ILE:CD1	1:A:543:LEU:HB3	2.12	0.76
1:A:499:ARG:HH12	1:A:545:THR:HG22	1.51	0.76
1:A:672:GLU:O	1:A:673:ASP:HB2	1.87	0.75
1:A:191:LYS:HB3	1:A:191:LYS:NZ	2.01	0.75
1:A:458:LEU:HD23	1:A:501:LEU:HD21	1.71	0.73
1:A:529:ILE:HG13	1:A:547:PHE:CD1	2.23	0.73
1:A:469:GLU:O	1:A:473:ILE:HG12	1.90	0.71
1:A:464:THR:HG22	1:A:465:ARG:HE	1.57	0.70
1:A:44:LEU:HD11	1:A:315:LYS:CB	2.22	0.69
1:A:460:GLU:O	1:A:464:THR:HB	1.92	0.69
1:A:464:THR:HG21	1:A:604:PHE:HZ	1.57	0.69
1:A:18:PRO:HD2	1:A:54:GLN:NE2	2.06	0.69
1:A:48:THR:HG21	1:A:316:THR:HG23	1.74	0.69
1:A:529:ILE:HD13	1:A:543:LEU:CB	2.19	0.69
1:A:580:LYS:HE2	1:A:581:GLU:OE1	1.93	0.69
1:A:500:ILE:HD12	1:A:590:PHE:CE1	2.28	0.68
1:A:440:ASP:HB2	1:A:473:ILE:HD12	1.76	0.68
1:A:118:ILE:O	1:A:122:ARG:HG2	1.93	0.68
1:A:530:LEU:HG	1:A:577:THR:OG1	1.93	0.67
1:A:532:ILE:HD11	1:A:536:PRO:HB2	1.75	0.67
1:A:534:ASP:HB3	1:A:536:PRO:HD2	1.77	0.67
1:A:101:ILE:HD12	1:A:130:LEU:HD11	1.77	0.67
1:A:486:GLU:HG3	1:A:502:ILE:HG23	1.77	0.67
1:A:529:ILE:HB	1:A:530:LEU:HD22	1.76	0.66
1:A:270:ARG:HD2	1:A:270:ARG:N	2.11	0.66
1:A:44:LEU:HD11	1:A:315:LYS:HB3	1.78	0.66
1:A:79:THR:HA	1:A:83:GLU:OE2	1.97	0.64
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.10	0.64
1:A:373:ARG:HH22	1:A:411:ARG:NH1	1.96	0.64
1:A:478:LYS:HA	1:A:483:LYS:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:CD1	1:A:130:LEU:HD11	2.28	0.63
1:A:252:THR:OG1	1:A:253:PRO:HD3	1.98	0.63
1:A:360:ALA:H	1:A:397:GLN:HE22	1.47	0.63
1:A:373:ARG:HH12	1:A:411:ARG:NH1	1.95	0.63
1:A:527:ALA:HB1	1:A:570:THR:HG21	1.81	0.63
1:A:613:LYS:NZ	1:A:613:LYS:HB3	2.14	0.63
1:A:518:GLN:CG	1:A:554:ARG:HH21	2.12	0.62
1:A:47:ILE:HG23	1:A:55:ARG:HD3	1.81	0.62
1:A:372:LEU:HD21	1:A:389:ILE:HG21	1.80	0.62
1:A:224:LYS:NZ	1:A:224:LYS:HB3	2.14	0.61
1:A:101:ILE:HG21	1:A:142:LEU:HD11	1.80	0.61
1:A:135:LYS:O	1:A:139:GLU:HA	2.01	0.61
1:A:366:ASP:OD1	1:A:408:HIS:HE1	1.84	0.61
1:A:522:ASP:OD1	1:A:558:HIS:HE1	1.84	0.61
1:A:14:ILE:HD11	1:A:320:LEU:CD2	2.31	0.61
1:A:157:MET:O	1:A:161:LEU:HD13	2.00	0.61
1:A:368:ASP:HB2	1:A:401:ILE:CD1	2.31	0.61
1:A:203:LEU:HD12	1:A:242:MET:HE3	1.83	0.60
1:A:635:LEU:HD23	1:A:635:LEU:C	2.20	0.60
1:A:428:LEU:O	1:A:432:LEU:HD22	2.01	0.60
1:A:577:THR:O	1:A:580:LYS:HB3	2.02	0.60
1:A:61:SER:O	1:A:65:LEU:HD13	2.02	0.60
1:A:456:LYS:HZ3	1:A:607:LYS:CE	2.15	0.60
1:A:138:TYR:O	1:A:139:GLU:HG2	2.02	0.60
1:A:412:ASP:OD2	1:A:414:MET:HB2	2.01	0.60
1:A:394:SER:O	1:A:398:ARG:HG3	2.03	0.59
1:A:600:LYS:HB3	1:A:601:PRO:HD3	1.84	0.59
1:A:654:GLU:HA	1:A:662:LEU:HD21	1.83	0.59
1:A:456:LYS:NZ	1:A:607:LYS:HE3	2.16	0.59
1:A:281:ARG:HG3	1:A:281:ARG:NH1	2.16	0.59
1:A:368:ASP:HB2	1:A:401:ILE:HD12	1.83	0.59
1:A:396:VAL:HG12	3:A:740:HOH:O	2.01	0.59
1:A:586:VAL:HG13	1:A:587:ARG:N	2.18	0.59
1:A:504:LEU:HD11	1:A:593:ILE:HD11	1.84	0.59
1:A:194:THR:HG22	1:A:233:GLU:O	2.03	0.58
1:A:281:ARG:HH11	1:A:281:ARG:HG3	1.67	0.58
1:A:639:ARG:O	1:A:642:ILE:HG22	2.03	0.58
1:A:657:THR:OG1	1:A:662:LEU:HD23	2.01	0.58
1:A:157:MET:SD	1:A:200:ILE:HG23	2.43	0.58
1:A:414:MET:O	1:A:418:LYS:HG3	2.03	0.58
1:A:206:ARG:HD2	3:A:815:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD12	1:A:242:MET:CE	2.34	0.58
1:A:535:THR:N	1:A:536:PRO:HD2	2.19	0.58
1:A:672:GLU:O	1:A:673:ASP:CB	2.53	0.57
1:A:620:LYS:HB3	1:A:620:LYS:NZ	2.20	0.57
1:A:514:GLU:O	1:A:515:ASN:CB	2.52	0.57
1:A:10:TYR:N	3:A:780:HOH:O	2.38	0.57
1:A:499:ARG:NH1	1:A:545:THR:HG22	2.18	0.57
1:A:432:LEU:HD13	1:A:627:VAL:HG22	1.86	0.56
1:A:138:TYR:O	1:A:140:ARG:HG2	2.05	0.56
1:A:456:LYS:NZ	1:A:607:LYS:CE	2.69	0.56
1:A:532:ILE:HG13	1:A:532:ILE:O	2.04	0.56
1:A:219:LEU:O	1:A:222:THR:O	2.23	0.56
1:A:604:PHE:CD2	1:A:629:ARG:HD2	2.41	0.56
1:A:196:GLU:HB2	3:A:842:HOH:O	2.06	0.56
1:A:376:MET:HB3	1:A:420:GLU:HG3	1.86	0.56
1:A:219:LEU:O	1:A:219:LEU:HD12	2.06	0.55
1:A:599:ASN:C	1:A:599:ASN:HD22	2.08	0.55
1:A:478:LYS:HD2	1:A:478:LYS:C	2.27	0.55
1:A:543:LEU:HD23	1:A:543:LEU:C	2.26	0.55
1:A:570:THR:O	1:A:572:TYR:N	2.36	0.55
1:A:550:ILE:O	1:A:554:ARG:HB2	2.06	0.55
1:A:578:ILE:HA	1:A:582:MET:HE3	1.88	0.55
1:A:530:LEU:CG	1:A:577:THR:HB	2.33	0.55
1:A:218:TYR:O	1:A:222:THR:HB	2.07	0.55
1:A:376:MET:CG	1:A:420:GLU:HG3	2.37	0.55
1:A:458:LEU:HD23	1:A:501:LEU:CD2	2.36	0.55
1:A:576:HIS:HD1	1:A:577:THR:N	2.05	0.55
1:A:194:THR:CG2	1:A:234:LEU:HD13	2.36	0.54
1:A:252:THR:N	1:A:253:PRO:CD	2.70	0.54
1:A:445:LYS:NZ	1:A:449:GLU:HB2	2.21	0.54
1:A:44:LEU:HD11	1:A:315:LYS:HB2	1.87	0.54
1:A:125:GLU:H	1:A:125:GLU:CD	2.09	0.54
1:A:117:GLU:OE1	1:A:276:ARG:HD2	2.07	0.54
1:A:365:PRO:HA	1:A:401:ILE:CD1	2.38	0.54
1:A:490:SER:HA	1:A:498:ARG:HD2	1.89	0.54
1:A:225:PRO:HB2	1:A:227:GLU:OE2	2.08	0.54
1:A:269:THR:HG22	1:A:270:ARG:N	2.22	0.54
1:A:290:ARG:HD3	3:A:751:HOH:O	2.06	0.54
1:A:248:CYS:O	1:A:252:THR:HG23	2.07	0.54
1:A:532:ILE:HG12	1:A:540:LYS:CG	2.35	0.54
1:A:440:ASP:OD1	1:A:465:ARG:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:O	1:A:50:ARG:HG2	2.07	0.53
1:A:191:LYS:HZ3	1:A:191:LYS:HB3	1.70	0.53
1:A:187:ALA:HB1	1:A:195:ASP:HB3	1.91	0.53
1:A:294:ARG:HG2	1:A:294:ARG:HH11	1.73	0.53
1:A:300:SER:HB2	1:A:303:SER:H	1.73	0.53
1:A:599:ASN:ND2	1:A:602:LEU:H	2.06	0.53
1:A:642:ILE:O	1:A:642:ILE:HD13	2.09	0.53
1:A:194:THR:HG21	1:A:234:LEU:HD22	1.90	0.53
1:A:530:LEU:HD12	1:A:577:THR:O	2.09	0.53
1:A:514:GLU:OE2	1:A:561:ARG:HD2	2.08	0.53
1:A:273:THR:HG23	1:A:276:ARG:HH12	1.73	0.53
1:A:518:GLN:NE2	1:A:522:ASP:OD2	2.41	0.53
1:A:532:ILE:HG13	1:A:536:PRO:O	2.09	0.53
1:A:20:PHE:CG	1:A:21:ASP:N	2.76	0.52
1:A:445:LYS:HZ2	1:A:449:GLU:HB2	1.74	0.52
1:A:463:ALA:HB1	1:A:593:ILE:HD13	1.91	0.52
1:A:294:ARG:CG	1:A:294:ARG:HH11	2.22	0.52
1:A:540:LYS:C	1:A:540:LYS:HD2	2.30	0.52
1:A:518:GLN:NE2	1:A:554:ARG:NH2	2.58	0.52
1:A:294:ARG:HH12	1:A:331:PHE:HE2	1.58	0.52
1:A:435:PRO:HG2	1:A:438:HIS:HB2	1.91	0.52
1:A:496:HIS:HD2	1:A:499:ARG:HH21	1.57	0.52
1:A:51:SER:O	1:A:55:ARG:HG3	2.09	0.52
1:A:622:LEU:O	1:A:626:MET:HG2	2.09	0.52
1:A:524:GLN:O	1:A:528:GLU:HG3	2.10	0.52
1:A:171:VAL:HG13	1:A:171:VAL:O	2.10	0.51
1:A:211:LEU:HD13	1:A:249:ILE:HD13	1.93	0.51
1:A:653:ILE:HG23	1:A:665:LEU:HD23	1.93	0.51
1:A:269:THR:HG22	1:A:271:ASP:N	2.26	0.51
1:A:629:ARG:HD3	1:A:633:ASP:OD2	2.11	0.51
1:A:170:ASP:OD1	1:A:171:VAL:HG12	2.11	0.51
1:A:373:ARG:HG3	1:A:373:ARG:HH21	1.76	0.51
1:A:413:LEU:O	1:A:413:LEU:HD12	2.11	0.51
1:A:224:LYS:HZ2	1:A:224:LYS:HB3	1.75	0.51
1:A:227:GLU:HG3	1:A:246:VAL:HG11	1.93	0.51
1:A:150:THR:OG1	1:A:155:GLN:HG3	2.11	0.50
1:A:338:VAL:O	1:A:342:MET:HG3	2.12	0.50
1:A:569:MET:O	1:A:570:THR:C	2.49	0.50
1:A:366:ASP:OD1	1:A:408:HIS:CE1	2.65	0.50
1:A:176:LEU:HD11	1:A:206:ARG:HH21	1.77	0.49
1:A:432:LEU:HD11	1:A:668:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:O	1:A:294:ARG:HG2	2.12	0.49
1:A:172:VAL:O	1:A:172:VAL:HG13	2.13	0.49
1:A:532:ILE:HG21	1:A:540:LYS:HZ2	1.78	0.49
1:A:439:TYR:O	1:A:443:GLN:HG2	2.12	0.49
1:A:586:VAL:CG1	1:A:587:ARG:N	2.75	0.49
1:A:620:LYS:HB3	1:A:620:LYS:HZ3	1.78	0.49
1:A:540:LYS:O	1:A:540:LYS:HD2	2.12	0.49
1:A:638:ARG:CZ	1:A:670:GLY:HA3	2.42	0.49
1:A:544:GLU:OE2	1:A:544:GLU:HA	2.13	0.49
1:A:194:THR:HG21	1:A:234:LEU:HD13	1.94	0.48
1:A:373:ARG:HD2	1:A:409:PHE:CD2	2.48	0.48
1:A:578:ILE:HG12	1:A:582:MET:HE1	1.95	0.48
1:A:409:PHE:HB2	1:A:411:ARG:HG2	1.95	0.48
1:A:395:ASN:ND2	1:A:436:PRO:HD3	2.29	0.48
1:A:604:PHE:CE2	1:A:629:ARG:HD2	2.48	0.48
1:A:29:LEU:CD2	1:A:43:ILE:HD13	2.44	0.48
1:A:383:GLU:HG2	1:A:660:ASP:OD1	2.14	0.48
1:A:440:ASP:HB2	1:A:473:ILE:CD1	2.42	0.48
1:A:230:ILE:HG23	1:A:234:LEU:HD23	1.94	0.48
1:A:291:GLU:HA	1:A:294:ARG:HD3	1.95	0.48
1:A:437:ALA:HA	1:A:473:ILE:HD13	1.96	0.48
1:A:516:LEU:HD13	3:A:825:HOH:O	2.13	0.48
1:A:523:ALA:O	1:A:526:ALA:HB3	2.14	0.47
1:A:532:ILE:HG21	1:A:540:LYS:NZ	2.29	0.47
1:A:368:ASP:O	1:A:372:LEU:HD23	2.14	0.47
1:A:496:HIS:O	1:A:500:ILE:HG22	2.14	0.47
1:A:500:ILE:HD13	1:A:589:ALA:CB	2.44	0.47
1:A:191:LYS:CB	1:A:191:LYS:NZ	2.75	0.47
1:A:535:THR:N	1:A:536:PRO:CD	2.78	0.47
1:A:589:ALA:O	1:A:593:ILE:HG12	2.15	0.47
1:A:300:SER:HB2	1:A:303:SER:HB2	1.97	0.47
1:A:17:PHE:HD1	1:A:51:SER:HG	1.59	0.47
1:A:191:LYS:HZ2	1:A:191:LYS:HB3	1.79	0.46
1:A:530:LEU:N	1:A:530:LEU:HD22	2.29	0.46
1:A:635:LEU:O	1:A:635:LEU:HD23	2.15	0.46
1:A:285:ASP:O	1:A:289:ILE:HG13	2.15	0.46
1:A:300:SER:CB	1:A:303:SER:H	2.29	0.46
1:A:366:ASP:OD1	1:A:370:LYS:NZ	2.48	0.46
1:A:376:MET:CB	1:A:420:GLU:HG3	2.46	0.46
1:A:269:THR:CG2	1:A:270:ARG:N	2.78	0.46
1:A:514:GLU:HB3	1:A:515:ASN:H	1.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG12	1:A:91:ARG:HH21	1.81	0.46
1:A:298:GLU:OE2	1:A:579:LYS:NZ	2.46	0.46
1:A:373:ARG:NH2	1:A:373:ARG:HG3	2.30	0.46
1:A:393:ARG:HG3	1:A:397:GLN:NE2	2.31	0.46
1:A:416:ASP:O	1:A:419:SER:HB3	2.16	0.46
1:A:154:PHE:CE2	1:A:158:LEU:HD11	2.51	0.46
1:A:535:THR:C	1:A:537:SER:H	2.18	0.46
1:A:365:PRO:HA	1:A:401:ILE:HD13	1.97	0.46
1:A:427:ARG:HH11	1:A:427:ARG:HG2	1.80	0.46
1:A:500:ILE:HD13	1:A:589:ALA:HB1	1.98	0.46
1:A:526:ALA:O	1:A:530:LEU:HD23	2.15	0.46
1:A:534:ASP:CG	1:A:535:THR:H	2.19	0.46
1:A:373:ARG:HH22	1:A:411:ARG:CZ	2.29	0.45
1:A:173:SER:O	1:A:174:GLU:C	2.52	0.45
1:A:157:MET:CE	1:A:161:LEU:HD11	2.46	0.45
1:A:464:THR:HG21	1:A:604:PHE:CZ	2.46	0.45
1:A:593:ILE:O	1:A:597:VAL:HG13	2.16	0.45
1:A:517:ASP:HA	1:A:520:ARG:HH21	1.82	0.45
1:A:518:GLN:HG2	1:A:554:ARG:HH21	1.82	0.45
1:A:54:GLN:O	1:A:58:VAL:HG23	2.16	0.45
1:A:603:PHE:CZ	1:A:607:LYS:HD2	2.52	0.45
1:A:510:GLU:HG3	1:A:553:THR:O	2.16	0.45
1:A:263:ALA:HA	1:A:270:ARG:HD3	1.99	0.45
1:A:393:ARG:HG3	1:A:397:GLN:HE21	1.82	0.44
1:A:514:GLU:O	1:A:515:ASN:HB2	2.17	0.44
1:A:112:GLU:O	1:A:116:ILE:HG13	2.16	0.44
1:A:373:ARG:HH12	1:A:411:ARG:HH11	1.65	0.44
1:A:373:ARG:NH1	1:A:411:ARG:NH1	2.64	0.44
1:A:612:MET:HB3	1:A:656:ASP:CG	2.38	0.44
1:A:177:VAL:O	1:A:181:VAL:HG23	2.18	0.44
1:A:486:GLU:HG3	1:A:502:ILE:CG2	2.47	0.44
1:A:648:SER:HB2	1:A:673:ASP:HB2	2.00	0.44
1:A:539:ASP:C	1:A:541:THR:H	2.20	0.44
1:A:93:PRO:O	1:A:96:CYS:HB3	2.18	0.44
1:A:155:GLN:O	1:A:159:VAL:HG23	2.18	0.43
1:A:209:GLN:HE21	1:A:209:GLN:HB3	1.66	0.43
1:A:613:LYS:HB3	1:A:613:LYS:HZ2	1.82	0.43
1:A:300:SER:HB2	1:A:303:SER:CB	2.49	0.43
1:A:435:PRO:HA	1:A:436:PRO:HD3	1.89	0.43
1:A:76:TYR:HD2	1:A:77:GLU:HG2	1.83	0.43
1:A:281:ARG:NH2	3:A:731:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:MET:O	1:A:265:LYS:C	2.57	0.43
1:A:70:LEU:O	1:A:74:LEU:HG	2.19	0.43
1:A:189:GLU:HG2	1:A:229:SER:OG	2.19	0.43
1:A:543:LEU:O	1:A:543:LEU:HD23	2.19	0.43
1:A:156:LYS:HD2	3:A:767:HOH:O	2.18	0.43
1:A:222:THR:HG22	1:A:224:LYS:N	2.13	0.43
1:A:194:THR:HG21	1:A:234:LEU:CD2	2.48	0.43
1:A:561:ARG:HD3	3:A:825:HOH:O	2.19	0.43
1:A:102:LYS:HE3	3:A:827:HOH:O	2.19	0.42
1:A:448:MET:HA	1:A:492:ASP:OD2	2.18	0.42
1:A:285:ASP:OD2	1:A:285:ASP:N	2.50	0.42
1:A:182:GLN:HE21	1:A:186:GLU:CD	2.22	0.42
1:A:343:TRP:CH2	1:A:598:LYS:HB2	2.54	0.42
1:A:220:LYS:HE2	3:A:790:HOH:O	2.19	0.42
1:A:222:THR:CG2	1:A:224:LYS:HG2	2.49	0.42
1:A:364:ASN:HD21	1:A:366:ASP:HB3	1.85	0.42
1:A:427:ARG:NH1	1:A:427:ARG:HG2	2.34	0.42
1:A:533:ALA:O	1:A:536:PRO:HG2	2.20	0.42
1:A:140:ARG:NH2	1:A:145:ASP:OD2	2.52	0.42
1:A:29:LEU:HD22	1:A:43:ILE:HD13	2.02	0.42
1:A:574:VAL:HG13	1:A:575:GLU:N	2.34	0.42
1:A:140:ARG:NH2	1:A:140:ARG:HB2	2.35	0.42
1:A:297:TYR:O	1:A:298:GLU:C	2.57	0.42
1:A:315:LYS:HE3	1:A:315:LYS:HB3	1.88	0.42
1:A:224:LYS:HB2	1:A:225:PRO:HD2	2.02	0.41
1:A:442:LYS:HZ1	1:A:446:LYS:HZ1	1.68	0.41
1:A:345:LEU:HD12	1:A:349:ALA:HB2	2.03	0.41
1:A:482:HIS:O	1:A:483:LYS:HB2	2.21	0.41
1:A:170:ASP:OD1	1:A:171:VAL:N	2.54	0.41
1:A:428:LEU:HD22	1:A:665:LEU:HD13	2.02	0.41
1:A:500:ILE:CD1	1:A:589:ALA:HB1	2.50	0.41
1:A:364:ASN:HD22	1:A:364:ASN:C	2.24	0.41
1:A:20:PHE:CD2	1:A:20:PHE:C	2.93	0.41
1:A:373:ARG:HB2	1:A:405:PHE:CE2	2.55	0.41
1:A:376:MET:HG2	1:A:420:GLU:HG3	2.03	0.41
1:A:182:GLN:O	1:A:186:GLU:HG3	2.20	0.41
1:A:490:SER:HA	1:A:498:ARG:CD	2.51	0.41
1:A:32:ALA:HB1	1:A:39:ASP:HB3	2.02	0.40
1:A:445:LYS:O	1:A:449:GLU:HB3	2.20	0.40
1:A:532:ILE:HD13	1:A:540:LYS:HE3	2.03	0.40
1:A:460:GLU:OE1	1:A:624:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD23	1:A:279:VAL:HG13	2.03	0.40
1:A:671:GLY:O	1:A:672:GLU:C	2.59	0.40
1:A:194:THR:HG21	1:A:234:LEU:CD1	2.51	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	662/672 (98%)	591 (89%)	52 (8%)	19 (3%)	<a href="#">5</a> <a href="#">7</a>

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ASP
1	A	265	LYS
1	A	300	SER
1	A	324	ASP
1	A	514	GLU
1	A	515	ASN
1	A	571	ASN
1	A	672	GLU
1	A	325	ASP
1	A	539	ASP
1	A	570	THR
1	A	18	PRO
1	A	171	VAL
1	A	251	SER
1	A	544	GLU
1	A	15	HIS
1	A	569	MET
1	A	533	ALA

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Mol	Chain	Res	Type
1	A	615	ALA

### 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	565/569 (99%)	520 (92%)	45 (8%)	14	23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	17	PHE
1	A	20	PHE
1	A	130	LEU
1	A	140	ARG
1	A	149	ASP
1	A	184	LEU
1	A	190	LEU
1	A	191	LYS
1	A	194	THR
1	A	209	GLN
1	A	224	LYS
1	A	245	VAL
1	A	270	ARG
1	A	281	ARG
1	A	287	LEU
1	A	290	ARG
1	A	294	ARG
1	A	332	PHE
1	A	337	GLN
1	A	353	LEU
1	A	358	ARG
1	A	364	ASN
1	A	393	ARG
1	A	432	LEU

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Mol	Chain	Res	Type
1	A	462	LEU
1	A	464	THR
1	A	465	ARG
1	A	478	LYS
1	A	501	LEU
1	A	524	GLN
1	A	525	VAL
1	A	540	LYS
1	A	554	ARG
1	A	571	ASN
1	A	581	GLU
1	A	597	VAL
1	A	599	ASN
1	A	613	LYS
1	A	642	ILE
1	A	643	GLU
1	A	656	ASP
1	A	665	LEU
1	A	672	GLU
1	A	673	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	179	GLN
1	A	182	GLN
1	A	272	ASN
1	A	307	ASN
1	A	337	GLN
1	A	364	ASN
1	A	397	GLN
1	A	403	GLN
1	A	408	HIS
1	A	443	GLN
1	A	496	HIS
1	A	518	GLN
1	A	558	HIS
1	A	599	ASN



### 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 5 ligands modelled in this entry, 5 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 ⓘ

### 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	664/672 (98%)	0.04	32 (4%) 31 29	14, 37, 85, 179	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	SER	18.0
1	A	534	ASP	7.9
1	A	535	THR	6.4
1	A	672	GLU	6.2
1	A	541	THR	5.9
1	A	172	VAL	5.8
1	A	538	GLY	5.5
1	A	540	LYS	5.4
1	A	326	ASP	5.2
1	A	324	ASP	5.0
1	A	265	LYS	4.6
1	A	543	LEU	4.5
1	A	267	LEU	4.3
1	A	325	ASP	4.2
1	A	537	SER	4.2
1	A	533	ALA	3.7
1	A	536	PRO	3.6
1	A	16	ASP	3.5
1	A	327	ALA	3.0
1	A	108	ILE	2.7
1	A	95	TYR	2.6
1	A	298	GLU	2.6
1	A	673	ASP	2.5
1	A	530	LEU	2.5
1	A	15	HIS	2.5
1	A	171	VAL	2.5
1	A	322	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	615	ALA	2.3
1	A	539	ASP	2.3
1	A	529	ILE	2.2
1	A	570	THR	2.2
1	A	266	GLY	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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	701	1/1	0.54	0.32	2.27	160,160,160,160	1
2	CA	A	704	1/1	0.84	0.23	2.23	161,161,161,161	1
2	CA	A	705	1/1	0.64	0.24	1.57	176,176,176,176	1
2	CA	A	702	1/1	0.80	0.22	-0.39	142,142,142,142	1
2	CA	A	703	1/1	0.91	0.07	-1.81	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.