



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:25 am BST

PDB ID : 1I7W  
Title : BETA-CATENIN/PHOSPHORYLATED E-CADHERIN COMPLEX  
Authors : Huber, A.H.; Weis, W.I.  
Deposited on : 2001-03-10  
Resolution : 2.00 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

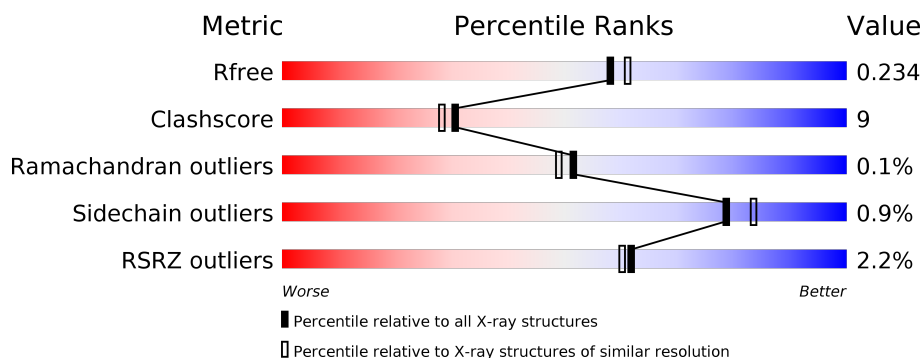
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	538	<div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	C	538	<div> <div>%</div> <div>79%</div> <div>15%</div> <div>5%</div> </div>
2	B	151	<div> <div>12%</div> <div>25%</div> <div>8%</div> <div>66%</div> </div>
2	D	151	<div> <div>2%</div> <div>30%</div> <div>9%</div> <div>60%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9360 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 BETA-CATENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	7	0
			3845	2414	700	704	27			
1	C	509	Total	C	N	O	S	0	12	0
			3963	2490	720	725	28			

- Molecule 2 is a protein called EPITHELIAL-CADHERIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	51	Total	C	N	O	P	S	0	0	0
			393	248	59	84	1	1			
2	D	60	Total	C	N	O	P	S	0	0	0
			480	297	70	109	3	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	684	SEP	SER	MODIFIED RESIDUE	UNP P09803
B	686	SEP	SER	MODIFIED RESIDUE	UNP P09803
B	692	SEP	SER	MODIFIED RESIDUE	UNP P09803
D	684	SEP	SER	MODIFIED RESIDUE	UNP P09803
D	686	SEP	SER	MODIFIED RESIDUE	UNP P09803
D	692	SEP	SER	MODIFIED RESIDUE	UNP P09803

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

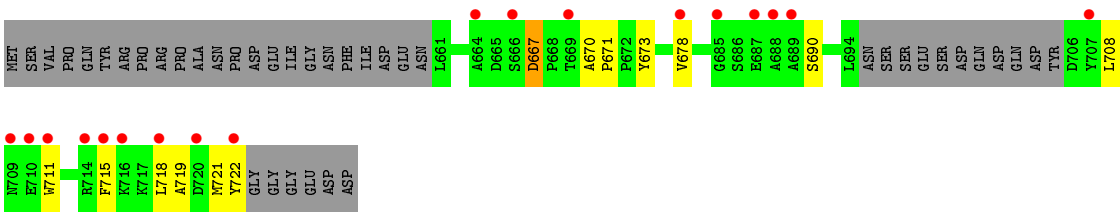
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cl 4 4	0	0
4	C	4	Total Cl 4 4	0	0

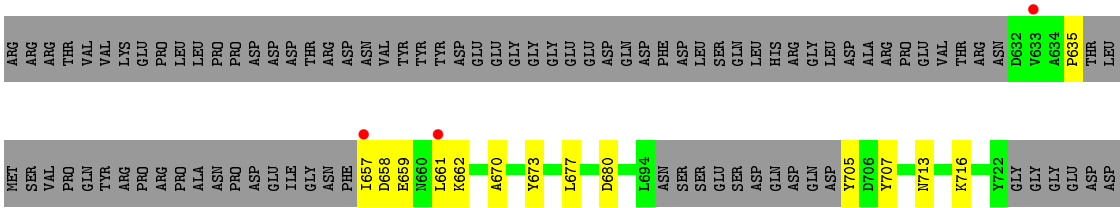
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	291	Total O 291 291	0	0
5	B	7	Total O 7 7	0	0
5	C	344	Total O 344 344	0	2
5	D	27	Total O 27 27	0	0





● Molecule 2: EPITHELIAL-CADHERIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.60Å 85.30Å 115.10Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	100.00 – 2.00 76.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (100.00-2.00) 91.4 (76.97-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.206 , 0.245 0.199 , 0.234	Depositor DCC
$R_{free}$ test set	5330 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 63.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9360	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 4.98% 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, CL, SEP

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	0.36	0/3897	0.57	0/5293
1	C	0.37	0/4020	0.57	0/5459
2	B	0.34	0/377	0.54	0/507
2	D	0.31	0/457	0.57	0/615
All	All	0.36	0/8751	0.57	0/11874

There are no bond length outliers.

There are no bond angle outliers.

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	3845	0	3964	70	0
1	C	3963	0	4077	71	0
2	B	393	0	348	11	0
2	D	480	0	421	16	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	1	0
4	C	4	0	0	0	0
5	A	291	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	7	0	0	0	0
5	C	344	0	0	6	0
5	D	27	0	0	3	0
All	All	9360	0	8810	162	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 (162) 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:194:MET:HA	1:A:194:MET:HE3	1.51	0.93
1:A:275:LEU:HD12	5:A:995:HOH:O	1.75	0.87
1:A:160:LEU:HD12	1:A:194:MET:HE1	1.56	0.87
1:A:394:LYS:HE3	1:A:395:GLN:HE21	1.40	0.86
1:A:359:GLU:HG2	1:A:394:LYS:NZ	1.91	0.85
2:D:713:ASN:HA	2:D:716:LYS:HG3	1.62	0.80
1:C:355:PRO:O	1:C:359:GLU:HG2	1.83	0.78
1:C:164:ASP:OD2	1:C:167:VAL:HG23	1.82	0.78
1:A:355:PRO:O	1:A:359:GLU:HG3	1.85	0.76
4:A:704:CL:CL	2:B:690:SER:HB2	2.23	0.76
1:C:648:ASN:O	1:C:651:VAL:HG22	1.85	0.76
1:A:348:SER:O	1:A:354[A]:LYS:HE2	1.85	0.76
1:A:174:MET:HE2	1:A:178:LEU:HD11	1.68	0.74
1:C:163:GLU:CD	1:C:163:GLU:H	1.91	0.73
1:C:354:LYS:HB2	1:C:355:PRO:HD3	1.71	0.72
1:C:586:ASN:O	1:C:590[A]:ILE:HG12	1.88	0.72
1:A:354[B]:LYS:HB3	1:A:355:PRO:HD3	1.69	0.72
1:A:354[A]:LYS:HB2	1:A:355:PRO:HD3	1.73	0.70
1:A:226[B]:GLU:H	1:A:226[B]:GLU:CD	1.95	0.69
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.74	0.68
1:C:625:LYS:HE3	1:C:625:LYS:HA	1.73	0.68
1:C:565:ARG:HG3	1:C:568:GLU:HG3	1.76	0.67
1:A:160:LEU:HD12	1:A:194:MET:CE	2.24	0.66
1:C:617:VAL:O	1:C:621:LEU:HD13	1.95	0.66
1:A:359:GLU:HG2	1:A:394:LYS:HZ3	1.59	0.66
1:C:625:LYS:CE	1:C:625:LYS:HA	2.25	0.66
1:A:359:GLU:HG2	1:A:394:LYS:HZ1	1.60	0.66
1:C:612:ARG:NH2	2:D:670:ALA:HB1	2.12	0.65
1:A:565:ARG:HB3	1:A:567:GLU:OE1	1.97	0.65
1:A:237:ILE:HB	1:A:238:PRO:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:HH11	1:A:627:ALA:HB2	1.60	0.64
1:A:287:ASN:H	1:A:287:ASN:HD22	1.43	0.64
1:A:525:ALA:O	1:A:529:GLU:HG3	1.99	0.62
1:A:156:LEU:HD11	1:A:174:MET:HE1	1.81	0.62
1:A:649:GLU:H	1:A:649:GLU:CD	2.03	0.62
1:C:257[B]:THR:HG22	1:C:296:ILE:HD13	1.82	0.62
1:A:156:LEU:HD11	1:A:174:MET:CE	2.31	0.61
1:C:185:ARG:HG2	1:C:189[B]:MET:HE3	1.82	0.60
1:A:194:MET:CA	1:A:194:MET:HE3	2.28	0.60
1:C:185:ARG:O	1:C:189[B]:MET:HG2	2.02	0.59
1:A:394:LYS:HE3	1:A:395:GLN:NE2	2.14	0.59
1:C:490:GLY:O	1:C:494:VAL:HG23	2.02	0.59
1:C:153:ILE:HB	1:C:154:PRO:HD3	1.83	0.59
1:C:533:ILE:HB	1:C:534:PRO:HD3	1.84	0.58
1:C:150:THR:HG22	5:C:955:HOH:O	2.03	0.58
1:A:436:MET:CE	1:A:476:GLN:HB2	2.34	0.58
1:C:224[A]:HIS:CD2	1:C:226:GLU:HB2	2.39	0.58
1:A:564:VAL:HA	5:A:939:HOH:O	2.04	0.57
1:A:207:ASP:OD2	1:A:209:GLU:HB3	2.03	0.57
1:C:607:ILE:O	1:C:611:GLN:HG3	2.05	0.57
2:D:658:ASP:O	2:D:662:LYS:HG3	2.04	0.57
1:C:533:ILE:HG23	1:C:590[A]:ILE:HD13	1.85	0.57
1:A:434:ASN:O	1:A:438:VAL:HG23	2.04	0.57
1:A:350:CYS:O	1:A:354[A]:LYS:HG3	2.05	0.56
1:C:523:ASN:C	1:C:526:PRO:HD2	2.26	0.56
1:A:152:ALA:N	2:B:721:MET:HE1	2.20	0.55
1:A:308:ASN:HD22	1:A:311:SER:H	1.54	0.55
1:A:407:GLN:NE2	5:A:959:HOH:O	2.39	0.55
1:A:598:LEU:HD23	1:A:598:LEU:O	2.06	0.55
2:D:705:TYR:HD2	2:D:707:TYR:HH	1.55	0.54
2:D:713:ASN:HA	2:D:716:LYS:CG	2.36	0.54
1:A:287:ASN:N	1:A:287:ASN:HD22	2.00	0.54
2:B:721:MET:HG3	2:B:722:TYR:CD1	2.43	0.53
2:D:657:ILE:O	2:D:661:LEU:HB2	2.08	0.53
1:C:224[A]:HIS:CD2	1:C:226:GLU:H	2.26	0.53
1:C:458:GLU:HG2	1:C:506:LEU:HD22	1.91	0.53
1:C:457:ARG:HH11	1:C:457:ARG:HG3	1.74	0.53
1:A:587:ARG:O	1:A:591:ARG:HG3	2.08	0.53
1:A:350:CYS:SG	5:A:907:HOH:O	2.59	0.52
2:D:713:ASN:HA	2:D:716:LYS:HE2	1.92	0.52
1:C:185:ARG:HD2	1:C:224[B]:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:C	1:A:598:LEU:HD23	2.32	0.51
1:A:620:GLU:O	1:A:623:GLN:HG2	2.11	0.51
2:D:713:ASN:CB	2:D:716:LYS:HE2	2.41	0.51
1:C:533:ILE:CG2	1:C:590[A]:ILE:HD13	2.41	0.50
1:C:184:SER:O	1:C:188:ILE:HG13	2.12	0.50
1:C:161:ASN:OD1	1:C:200:ARG:NH2	2.45	0.50
1:A:458:GLU:HG2	1:A:506:LEU:HD22	1.93	0.50
1:C:287:ASN:HB3	5:C:835:HOH:O	2.11	0.50
2:B:671:PRO:HG3	2:B:673:TYR:CE2	2.47	0.50
2:D:659:GLU:HA	2:D:662:LYS:HE2	1.94	0.49
2:B:721:MET:HG3	2:B:722:TYR:HD1	1.76	0.49
2:D:677:LEU:HG	5:D:751:HOH:O	2.12	0.49
1:C:584:VAL:HG13	1:C:585:HIS:N	2.29	0.48
1:A:174:MET:SD	2:B:718:LEU:HD13	2.53	0.48
1:C:457:ARG:NH1	1:C:457:ARG:HG3	2.27	0.48
1:A:432:TYR:O	1:A:436:MET:HG2	2.13	0.48
1:C:189[A]:MET:HE3	1:C:226:GLU:OE1	2.13	0.48
1:A:198:ILE:HD13	1:A:217:THR:HG21	1.96	0.48
1:C:471:LEU:O	1:C:475:HIS:HE1	1.96	0.48
1:A:330:THR:HG23	1:C:158:LYS:HA	1.95	0.47
1:C:651:VAL:HG23	1:C:652:ALA:N	2.29	0.47
2:B:678:VAL:O	2:B:678:VAL:HG13	2.14	0.47
1:A:338:TRP:CE2	1:A:342:ARG:HD2	2.49	0.47
1:C:507:ILE:O	1:C:511:VAL:HG23	2.14	0.47
1:C:503:HIS:HB2	5:C:1046:HOH:O	2.15	0.47
1:A:287:ASN:ND2	1:A:287:ASN:H	2.11	0.47
1:A:579:ILE:O	1:A:582:ARG:HG3	2.15	0.46
1:C:620:GLU:O	1:C:623:GLN:HG2	2.15	0.46
2:D:713:ASN:O	2:D:716:LYS:HG3	2.16	0.46
1:C:346:VAL:O	1:C:349:VAL:HG22	2.15	0.46
1:A:186:HIS:HA	1:A:189:MET:HG2	1.96	0.46
1:C:625:LYS:HA	1:C:625:LYS:NZ	2.31	0.46
1:A:193:GLN:CD	1:A:193:GLN:H	2.19	0.46
1:A:641:THR:O	1:A:644:LEU:HB2	2.15	0.46
1:C:541:VAL:O	1:C:545:GLN:HG3	2.15	0.46
1:C:224[A]:HIS:ND1	5:C:715:HOH:O	2.36	0.46
2:D:713:ASN:HA	2:D:716:LYS:CE	2.45	0.46
1:C:475:HIS:CD2	1:C:477:GLU:H	2.34	0.46
1:C:224[A]:HIS:HD2	1:C:226:GLU:HB2	1.80	0.45
1:A:308:ASN:ND2	1:A:311:SER:H	2.14	0.45
1:C:619:CYS:HA	1:C:658:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:SER:HA	1:C:247[A]:PRO:HD3	1.83	0.45
1:A:449:ARG:O	1:A:453[B]:ARG:HG3	2.16	0.45
1:A:149:ALA:O	1:A:153:ILE:HG12	2.17	0.45
1:C:277:GLY:O	1:C:281:LYS:HG3	2.16	0.45
1:A:543:ALA:O	1:A:547:THR:HG23	2.17	0.45
1:C:182:GLU:HA	1:C:185:ARG:NH1	2.32	0.45
1:A:170:LYS:HB3	2:B:711:TRP:CZ3	2.52	0.44
1:C:200:ARG:HD2	5:C:994:HOH:O	2.17	0.44
1:C:189[A]:MET:SD	1:C:224[A]:HIS:HD2	2.40	0.44
1:A:598:LEU:HD23	1:A:602:LEU:HG	1.99	0.44
1:C:146:ALA:O	1:C:150:THR:HG23	2.18	0.44
1:A:335:LYS:O	1:A:339[A]:THR:HG23	2.18	0.44
1:C:217:THR:O	1:C:221:LEU:HG	2.18	0.43
1:A:393:THR:HG23	1:A:431:ASN:HB2	1.98	0.43
1:A:638:ALA:HB3	1:A:639:PRO:CD	2.48	0.43
2:B:667:ASP:OD1	2:B:670:ALA:N	2.51	0.43
1:C:196:SER:OG	1:C:200:ARG:NH1	2.52	0.43
2:D:713:ASN:CA	2:D:716:LYS:HG3	2.40	0.43
1:A:535:ARG:NH1	1:A:538:GLN:OE1	2.47	0.43
1:C:414:ILE:HG23	1:C:415:ASN:N	2.33	0.43
1:C:458:GLU:HG3	5:C:891:HOH:O	2.17	0.43
1:C:257[B]:THR:HG21	5:D:744:HOH:O	2.18	0.43
1:C:310:GLU:CD	1:C:310:GLU:H	2.22	0.43
1:C:586:ASN:O	1:C:590[B]:ILE:HG13	2.18	0.43
1:A:449:ARG:NE	5:A:911:HOH:O	2.52	0.43
1:C:237:ILE:HB	1:C:238:PRO:HD3	2.01	0.43
1:A:515:ARG:HD3	1:A:515:ARG:C	2.39	0.43
1:A:170:LYS:HB2	2:B:715:PHE:CZ	2.54	0.43
1:C:661:ARG:C	1:C:663:SER:H	2.22	0.43
2:B:708:LEU:HB2	2:B:719:ALA:HB2	2.01	0.43
1:C:651:VAL:CG2	1:C:652:ALA:N	2.82	0.43
1:C:353:ASN:O	1:C:357:ILE:HG13	2.19	0.42
1:C:225:ARG:HG2	1:C:225:ARG:HH11	1.85	0.42
1:C:312:LYS:HE2	1:C:346:VAL:CG1	2.49	0.42
1:A:547:THR:HG22	1:A:567:GLU:OE2	2.20	0.42
1:A:281:LYS:HE3	5:A:748:HOH:O	2.20	0.42
1:C:153:ILE:CD1	1:C:188:ILE:HG12	2.49	0.41
1:A:584:VAL:HG13	1:A:585:HIS:N	2.34	0.41
1:C:575:GLY:O	1:C:578:HIS:HB3	2.21	0.41
2:D:635:PRO:HD3	2:D:673:TYR:CD1	2.56	0.41
1:C:265:HIS:HD2	5:D:745:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG23	1:A:194:MET:HG2	2.03	0.41
2:D:713:ASN:CA	2:D:716:LYS:HE2	2.51	0.41
1:A:437[B]:MET:HA	1:A:437[B]:MET:HE3	2.03	0.41
1:C:312:LYS:HE2	1:C:346:VAL:HG12	2.03	0.41
1:A:393:THR:HG23	1:A:431:ASN:HD22	1.86	0.40
1:A:444:ILE:HG21	1:A:484:ALA:HB3	2.03	0.40
1:C:329[B]:ARG:HG3	1:C:365:ALA:CB	2.51	0.40
2:D:680:ASP:CG	2:D:680:ASP:O	2.59	0.40
1:C:186:HIS:HA	1:C:189[A]:MET:HG2	2.04	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	503/538 (94%)	497 (99%)	6 (1%)	0	100	100
1	C	517/538 (96%)	514 (99%)	3 (1%)	0	100	100
2	B	44/151 (29%)	39 (89%)	4 (9%)	1 (2%)	6	2
2	D	51/151 (34%)	47 (92%)	4 (8%)	0	100	100
All	All	1115/1378 (81%)	1097 (98%)	17 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	667	ASP

### 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	413/447 (92%)	409 (99%)	4 (1%)	76	81
1	C	428/447 (96%)	424 (99%)	4 (1%)	78	83
2	B	37/128 (29%)	37 (100%)	0	100	100
2	D	47/128 (37%)	47 (100%)	0	100	100
All	All	925/1150 (80%)	917 (99%)	8 (1%)	78	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	MET
1	A	287	ASN
1	A	396	GLU
1	A	480	MET
1	C	163	GLU
1	C	287	ASN
1	C	546	ASP
1	C	625	LYS

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	165	GLN
1	A	206	ASN
1	A	287	ASN
1	A	308	ASN
1	A	415	ASN
1	A	578	HIS
1	C	177	GLN
1	C	302	GLN
1	C	309	GLN
1	C	375	GLN
1	C	407	GLN
1	C	430	ASN
1	C	475	HIS
1	C	538	GLN
1	C	578	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SEP	D	686	2	8,9,10	0.68	0	8,12,14	2.05	3 (37%)
2	SEP	D	684	2	8,9,10	0.65	0	8,12,14	1.90	5 (62%)
2	SEP	B	684	2	4,5,10	0.59	0	0,5,14	0.00	-
2	SEP	D	692	2	8,9,10	0.75	0	8,12,14	1.84	2 (25%)
2	SEP	B	692	2	8,9,10	0.74	0	8,12,14	1.82	2 (25%)
2	SEP	B	686	2	4,5,10	0.57	0	0,5,14	0.00	-

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	SEP	D	686	2	-	1/5/8/10	-
2	SEP	D	684	2	-	0/5/8/10	-
2	SEP	B	684	2	-	0/2/4/10	-
2	SEP	D	692	2	-	0/5/8/10	-
2	SEP	B	692	2	-	0/5/8/10	-
2	SEP	B	686	2	-	1/2/4/10	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	686	SEP	OG-CB-CA	3.35	111.41	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	692	SEP	O3P-P-OG	-3.01	98.71	106.73
2	B	692	SEP	O3P-P-OG	-2.92	98.96	106.73
2	D	692	SEP	O3P-P-O2P	2.41	116.84	107.64
2	B	692	SEP	O3P-P-O2P	2.38	116.74	107.64
2	D	686	SEP	O2P-P-OG	-2.33	100.52	106.73
2	D	684	SEP	O3P-P-O2P	2.32	116.50	107.64
2	D	686	SEP	O3P-P-O2P	2.24	116.21	107.64
2	D	684	SEP	O3P-P-OG	-2.23	100.79	106.73
2	D	684	SEP	OG-CB-CA	2.16	110.25	108.14
2	D	684	SEP	O2P-P-OG	-2.12	101.09	106.73
2	D	684	SEP	OG-P-O1P	-2.06	100.71	106.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	686	SEP	CA-CB-OG-P
2	B	686	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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

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	500/538 (92%)	-0.13	1 (0%) 95 94	27, 41, 71, 95	0
1	C	509/538 (94%)	-0.20	3 (0%) 89 88	22, 39, 66, 97	0
2	B	48/151 (31%)	1.53	18 (37%) 0 0	39, 84, 112, 113	0
2	D	57/151 (37%)	0.76	3 (5%) 26 25	37, 76, 105, 111	0
All	All	1114/1378 (80%)	-0.04	25 (2%) 62 60	22, 42, 84, 113	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	715	PHE	6.7
2	D	661	LEU	5.9
2	B	689	ALA	5.4
2	B	718	LEU	5.4
2	B	716	LYS	4.2
2	B	722	TYR	4.1
2	B	664	ALA	4.1
2	B	707	TYR	4.0
2	B	688	ALA	3.2
2	B	666	SER	3.0
2	B	711	TRP	2.7
2	B	687	GLU	2.7
2	B	678	VAL	2.7
2	D	657	ILE	2.7
1	C	549	ARG	2.7
1	A	647	ARG	2.5
2	B	685	GLY	2.5
2	D	633	VAL	2.4
1	C	551	THR	2.4
2	B	669	THR	2.4
2	B	709	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	714	ARG	2.1
1	C	647	ARG	2.1
2	B	710	GLU	2.0
2	B	720	ASP	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
2	SEP	B	686	6/11	0.54	0.30	91,91,91,91	0
2	SEP	B	684	6/11	0.76	0.21	72,77,80,80	0
2	SEP	D	684	10/11	0.90	0.13	59,70,87,88	0
2	SEP	D	686	10/11	0.91	0.12	59,64,75,76	0
2	SEP	B	692	10/11	0.97	0.09	49,53,55,56	0
2	SEP	D	692	10/11	0.99	0.09	38,41,43,47	0

## 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	ZN	A	1	1/1	0.82	0.08	61,61,61,61	1
3	ZN	C	2	1/1	0.91	0.08	61,61,61,61	1
4	CL	C	708	1/1	0.95	0.06	49,49,49,49	0
4	CL	A	707	1/1	0.97	0.07	42,42,42,42	0
4	CL	C	706	1/1	0.98	0.07	41,41,41,41	0
4	CL	C	701	1/1	0.98	0.11	40,40,40,40	0
4	CL	A	704	1/1	0.99	0.09	52,52,52,52	0
4	CL	C	702	1/1	0.99	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	A	705	1/1	0.99	0.13	38,38,38,38	0
4	CL	A	703	1/1	0.99	0.12	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.