



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:44 am BST

PDB ID : 5CO1  
Title : Crystal Structure of Zebrafish Protocadherin-19 EC3-4  
Authors : Cooper, S.R.; Jontes, J.D.; Sotomayor, M.  
Deposited on : 2015-07-19  
Resolution : 2.51 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
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

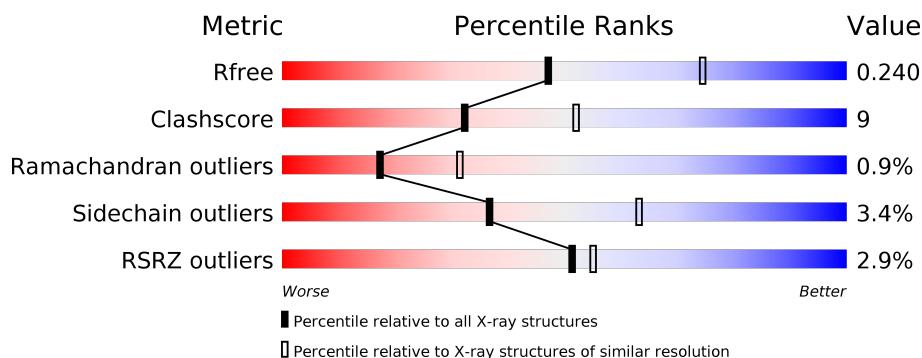
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	219	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div> </div>
1	B	219	<div> <div></div> <div> <div>76%</div> <div>17%</div> <div>• 6%</div> </div> </div>
1	C	219	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>
1	D	219	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6529 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 Protocadherin-19 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1603	1011	267	320	5			
1	B	205	Total	C	N	O	S	0	0	0
			1599	1007	266	321	5			
1	C	210	Total	C	N	O	S	0	0	0
			1631	1024	272	330	5			
1	D	210	Total	C	N	O	S	0	0	0
			1631	1024	272	330	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	MET	-	initiating methionine	UNP C4P340
A	423	LEU	-	expression tag	UNP C4P340
A	424	GLU	-	expression tag	UNP C4P340
A	425	HIS	-	expression tag	UNP C4P340
A	426	HIS	-	expression tag	UNP C4P340
A	427	HIS	-	expression tag	UNP C4P340
A	428	HIS	-	expression tag	UNP C4P340
A	429	HIS	-	expression tag	UNP C4P340
A	430	HIS	-	expression tag	UNP C4P340
B	212	MET	-	initiating methionine	UNP C4P340
B	423	LEU	-	expression tag	UNP C4P340
B	424	GLU	-	expression tag	UNP C4P340
B	425	HIS	-	expression tag	UNP C4P340
B	426	HIS	-	expression tag	UNP C4P340
B	427	HIS	-	expression tag	UNP C4P340
B	428	HIS	-	expression tag	UNP C4P340
B	429	HIS	-	expression tag	UNP C4P340
B	430	HIS	-	expression tag	UNP C4P340
C	212	MET	-	initiating methionine	UNP C4P340
C	423	LEU	-	expression tag	UNP C4P340
C	424	GLU	-	expression tag	UNP C4P340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	expression tag	UNP C4P340
C	426	HIS	-	expression tag	UNP C4P340
C	427	HIS	-	expression tag	UNP C4P340
C	428	HIS	-	expression tag	UNP C4P340
C	429	HIS	-	expression tag	UNP C4P340
C	430	HIS	-	expression tag	UNP C4P340
D	212	MET	-	initiating methionine	UNP C4P340
D	423	LEU	-	expression tag	UNP C4P340
D	424	GLU	-	expression tag	UNP C4P340
D	425	HIS	-	expression tag	UNP C4P340
D	426	HIS	-	expression tag	UNP C4P340
D	427	HIS	-	expression tag	UNP C4P340
D	428	HIS	-	expression tag	UNP C4P340
D	429	HIS	-	expression tag	UNP C4P340
D	430	HIS	-	expression tag	UNP C4P340

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Ca 4 4	0	0
2	A	4	Total Ca 4 4	0	0
2	D	4	Total Ca 4 4	0	0
2	C	4	Total Ca 4 4	0	0

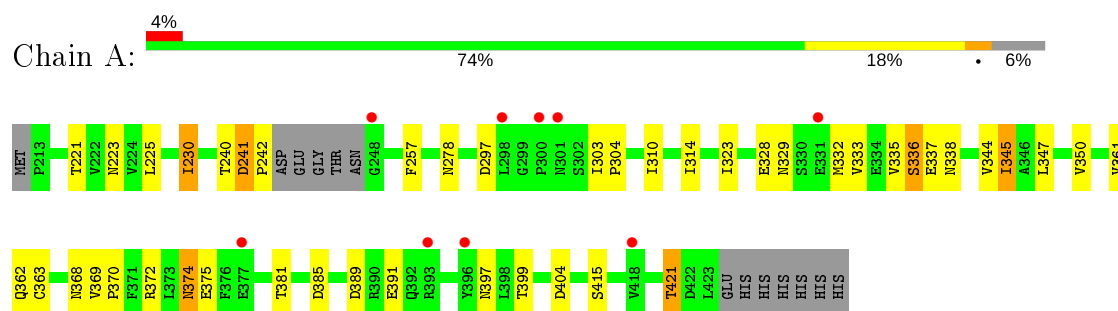
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	14	Total O 14 14	0	0
3	C	13	Total O 13 13	0	0
3	D	12	Total O 12 12	0	0

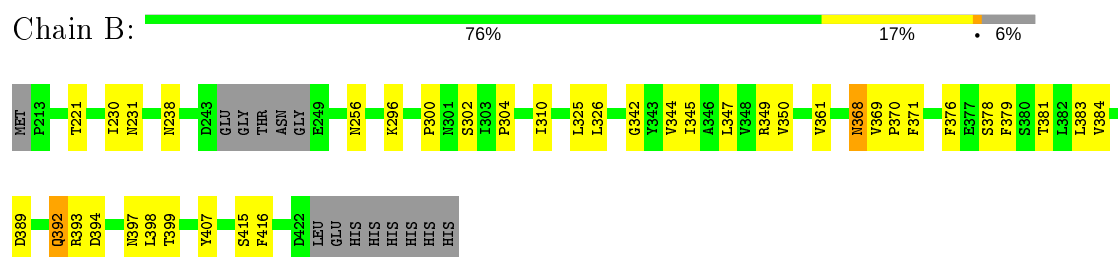
### 3 Residue-property plots

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.

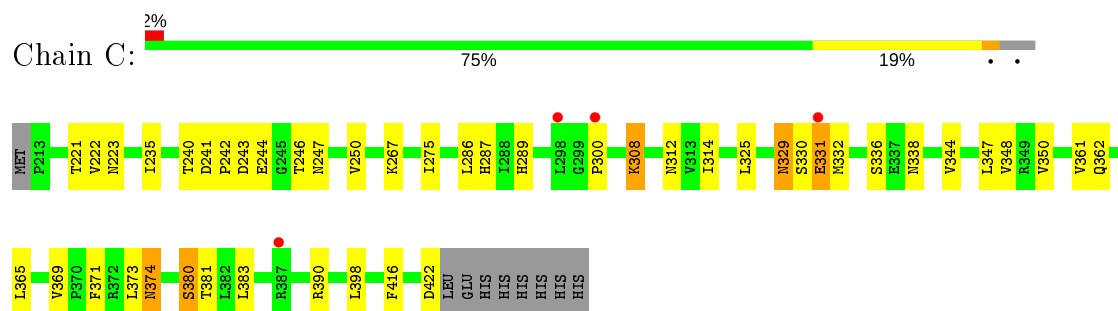
- Molecule 1: Protocadherin-19 isoform 1



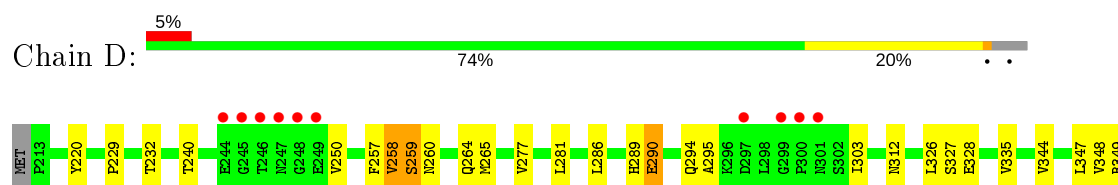
- Molecule 1: Protocadherin-19 isoform 1



- Molecule 1: Protocadherin-19 isoform 1



- Molecule 1: Protocadherin-19 isoform 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.35Å 86.63Å 132.58Å 90.00° 122.13° 90.00°	Depositor
Resolution (Å)	50.00 – 2.51 34.29 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.51) 97.8 (34.29-2.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, $R_{free}$	0.188 , 0.239 0.193 , 0.240	Depositor DCC
$R_{free}$ test set	2360 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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	0.51	0/1630	0.68	0/2219
1	B	0.56	0/1626	0.74	0/2214
1	C	0.59	0/1659	0.72	0/2260
1	D	0.62	0/1659	0.76	0/2260
All	All	0.57	0/6574	0.72	0/8953

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	4
1	D	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	THR	Peptide
1	A	363	CYS	Peptide
1	A	368	ASN	Peptide
1	B	256	ASN	Peptide
1	B	368	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	C	246	THR	Peptide
1	C	247	ASN	Peptide
1	C	308	LYS	Mainchain
1	C	312	ASN	Mainchain
1	D	220	TYR	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1603	0	1587	28	0
1	B	1599	0	1577	22	3
1	C	1631	0	1603	39	1
1	D	1631	0	1603	28	2
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	10	0	0	0	0
3	B	14	0	0	1	0
3	C	13	0	0	0	0
3	D	12	0	0	0	0
All	All	6529	0	6370	113	3

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 (113) 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:C:240:THR:HG21	1:C:250:VAL:HG21	1.61	0.83
1:B:350:VAL:HG11	1:B:361:VAL:HG11	1.62	0.81
1:D:265:MET:HE1	1:D:281:LEU:HA	1.66	0.78
1:B:399:THR:HG22	1:B:415:SER:OG	1.85	0.76
1:D:229:PRO:O	1:D:232:THR:HG22	1.85	0.76
1:D:240:THR:HG21	1:D:250:VAL:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:VAL:HG13	1:B:370:PRO:HD2	1.72	0.70
1:C:325:LEU:HD23	1:C:348:VAL:HG12	1.73	0.69
1:C:350:VAL:CG1	1:C:361:VAL:HG11	2.25	0.65
1:C:369:VAL:HG13	1:C:371:PHE:HD2	1.62	0.65
1:A:399:THR:HG22	1:A:415:SER:OG	1.97	0.65
1:D:350:VAL:CG1	1:D:361:VAL:HG21	2.27	0.65
1:B:350:VAL:CG1	1:B:361:VAL:HG11	2.28	0.63
1:C:361:VAL:HG12	1:C:362:GLN:N	2.12	0.63
1:B:347:LEU:CD2	1:B:381:THR:HG22	2.29	0.61
1:B:230:ILE:O	1:B:231:ASN:HB2	1.98	0.61
1:A:328:GLU:N	1:A:328:GLU:OE1	2.32	0.61
1:C:331:GLU:HA	1:C:416:PHE:HB2	1.83	0.61
1:A:223:ASN:HB3	1:A:314:ILE:CD1	2.31	0.59
1:A:347:LEU:HD22	1:C:347:LEU:HD13	1.84	0.59
1:C:365:LEU:CD2	1:C:373:LEU:HG	2.31	0.59
1:C:221:THR:C	1:C:222:VAL:HG23	2.22	0.58
1:B:369:VAL:HG12	1:B:371:PHE:HD2	1.69	0.56
1:D:348:VAL:HG21	1:D:373:LEU:HD11	1.87	0.56
1:C:381:THR:HG23	1:C:383:LEU:HD23	1.89	0.55
1:A:375:GLU:HG2	1:A:375:GLU:O	2.07	0.54
1:B:342:GLY:HA2	1:B:383:LEU:HD13	1.89	0.54
1:C:350:VAL:HG11	1:C:361:VAL:HG11	1.89	0.54
1:D:229:PRO:O	1:D:232:THR:CG2	2.54	0.53
1:A:338:ASN:OD1	1:D:260:ASN:HB2	2.09	0.53
1:B:238:ASN:HB2	3:B:614:HOH:O	2.07	0.53
1:D:326:LEU:HB2	1:D:347:LEU:HD23	1.90	0.53
1:A:333:VAL:CG1	1:A:345:ILE:HD11	2.39	0.52
1:C:374:ASN:HB2	1:C:381:THR:HG22	1.91	0.52
1:A:404:ASP:OD1	1:A:404:ASP:C	2.47	0.52
1:C:369:VAL:HG11	1:C:398:LEU:HD22	1.91	0.52
1:C:348:VAL:HG23	1:C:380:SER:HB2	1.92	0.52
1:B:221:THR:HG22	1:B:310:ILE:HB	1.91	0.51
1:A:361:VAL:HG12	1:A:362:GLN:N	2.24	0.51
1:D:257:PHE:CE2	1:D:259:SER:HB2	2.45	0.51
1:C:223:ASN:HB3	1:C:314:ILE:HD11	1.92	0.51
1:C:286:LEU:HD23	1:C:289:HIS:CE1	2.46	0.51
1:B:369:VAL:CG1	1:B:370:PRO:HD2	2.40	0.50
1:B:230:ILE:HD12	1:B:231:ASN:ND2	2.27	0.50
1:C:361:VAL:CG1	1:C:362:GLN:N	2.74	0.50
1:A:241:ASP:OD1	1:A:242:PRO:HD2	2.11	0.50
1:D:371:PHE:CZ	1:D:418:VAL:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:HG12	1:C:361:VAL:HG11	1.94	0.50
1:D:350:VAL:HG12	1:D:361:VAL:HG21	1.93	0.50
1:D:376:PHE:N	1:D:376:PHE:CD1	2.81	0.49
1:C:369:VAL:HG13	1:C:371:PHE:CD2	2.47	0.48
1:B:368:ASN:C	1:B:369:VAL:HG23	2.34	0.48
1:C:374:ASN:HB2	1:C:381:THR:CG2	2.43	0.48
1:A:223:ASN:HB3	1:A:314:ILE:HD12	1.94	0.48
1:C:242:PRO:O	1:C:244:GLU:HA	2.14	0.48
1:A:303:ILE:HG13	1:A:304:PRO:HD2	1.97	0.47
1:D:375:GLU:HA	1:D:380:SER:OG	2.14	0.47
1:C:240:THR:CG2	1:C:250:VAL:HG21	2.40	0.47
1:C:287:HIS:ND1	1:D:290:GLU:OE2	2.45	0.47
1:A:361:VAL:CG1	1:A:362:GLN:N	2.78	0.46
1:B:230:ILE:HD12	1:B:231:ASN:HD22	1.80	0.46
1:D:398:LEU:O	1:D:415:SER:HA	2.16	0.46
1:B:369:VAL:HG11	1:B:398:LEU:HD11	1.97	0.46
1:D:361:VAL:HG23	1:D:362:GLN:N	2.30	0.45
1:B:345:ILE:HD11	1:B:384:VAL:HG23	1.98	0.45
1:C:365:LEU:HD21	1:C:373:LEU:HG	1.97	0.45
1:C:374:ASN:CB	1:C:381:THR:HG22	2.47	0.45
1:D:394:ASP:O	1:D:420:VAL:HG12	2.16	0.45
1:D:350:VAL:HG11	1:D:361:VAL:HG21	2.00	0.44
1:A:297:ASP:N	1:A:297:ASP:OD1	2.48	0.44
1:C:365:LEU:HD23	1:C:373:LEU:HG	1.98	0.44
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.68	0.43
1:A:369:VAL:HB	1:A:370:PRO:HD2	2.00	0.43
1:B:376:PHE:HB2	1:B:379:PHE:O	2.18	0.43
1:B:389:ASP:O	1:B:392:GLN:HB3	2.19	0.43
1:A:303:ILE:HG13	1:A:304:PRO:CD	2.49	0.43
1:A:337:GLU:HB2	1:A:389:ASP:HA	2.01	0.43
1:B:326:LEU:HB2	1:B:347:LEU:HB2	2.00	0.43
1:C:390:ARG:NH1	1:C:422:ASP:HB2	2.34	0.43
1:D:344:VAL:O	1:D:344:VAL:HG23	2.18	0.42
1:D:369:VAL:HB	1:D:370:PRO:HD2	2.00	0.42
1:C:361:VAL:CG1	1:C:362:GLN:H	2.32	0.42
1:A:372:ARG:HG2	1:A:385:ASP:HB2	2.01	0.42
1:B:325:LEU:HD11	1:B:416:PHE:CD1	2.54	0.42
1:A:329:ASN:HB2	1:A:332:MET:HB2	2.02	0.42
1:C:374:ASN:OD1	1:C:383:LEU:HD21	2.18	0.42
1:A:374:ASN:HB2	1:A:381:THR:CG2	2.50	0.42
1:A:389:ASP:N	1:A:389:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:THR:HG22	1:A:310:ILE:HB	2.02	0.42
1:C:221:THR:C	1:C:222:VAL:CG2	2.87	0.42
1:A:230:ILE:HD11	1:A:278:ASN:C	2.40	0.42
1:A:337:GLU:N	1:A:421:THR:O	2.48	0.41
1:C:331:GLU:HA	1:C:416:PHE:CB	2.47	0.41
1:A:344:VAL:HB	1:A:381:THR:OG1	2.20	0.41
1:C:373:LEU:HD23	1:C:373:LEU:HA	1.96	0.41
1:D:258:VAL:HG13	1:D:258:VAL:O	2.21	0.41
1:D:286:LEU:HD23	1:D:289:HIS:CE1	2.56	0.41
1:C:308:LYS:HE3	1:D:312:ASN:HD21	1.85	0.41
1:B:369:VAL:CG1	1:B:371:PHE:HD2	2.32	0.41
1:C:329:ASN:ND2	1:C:330:SER:O	2.51	0.41
1:A:323:ILE:HG12	1:A:350:VAL:HG12	2.02	0.41
1:B:399:THR:HG22	1:B:415:SER:HG	1.85	0.41
1:C:235:ILE:CG2	1:C:275:ILE:HD12	2.51	0.41
1:C:361:VAL:HG12	1:C:362:GLN:H	1.81	0.41
1:C:329:ASN:HB3	1:C:332:MET:O	2.20	0.41
1:D:232:THR:HG23	1:D:277:VAL:CG2	2.51	0.41
1:D:327:SER:OG	1:D:328:GLU:N	2.54	0.41
1:D:294:GLN:HG2	1:D:295:ALA:N	2.35	0.41
1:C:344:VAL:HG12	1:C:344:VAL:O	2.21	0.40
1:D:335:VAL:O	1:D:420:VAL:HA	2.21	0.40
1:C:241:ASP:OD2	1:C:243:ASP:HB2	2.20	0.40
1:D:303:ILE:N	1:D:303:ILE:HD13	2.36	0.40
1:A:335:VAL:HG22	1:A:336:SER:N	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:VAL:O	1:D:349:ARG:NH2[3_455]	1.97	0.23
1:B:349:ARG:NH2	1:D:344:VAL:O[3_455]	2.16	0.04
1:B:296:LYS:NZ	1:C:338:ASN:OD1[4_445]	2.16	0.04

## 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	202/219 (92%)	184 (91%)	18 (9%)	0	100	100
1	B	201/219 (92%)	184 (92%)	13 (6%)	4 (2%)	7	12
1	C	208/219 (95%)	192 (92%)	14 (7%)	2 (1%)	15	28
1	D	208/219 (95%)	192 (92%)	15 (7%)	1 (0%)	29	48
All	All	819/876 (94%)	752 (92%)	60 (7%)	7 (1%)	17	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	300	PRO
1	B	392	GLN
1	C	331	GLU
1	D	258	VAL
1	B	302	SER
1	B	300	PRO
1	B	304	PRO

### 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	187/199 (94%)	178 (95%)	9 (5%)	25	48
1	B	187/199 (94%)	182 (97%)	5 (3%)	44	71
1	C	190/199 (96%)	185 (97%)	5 (3%)	46	72
1	D	190/199 (96%)	183 (96%)	7 (4%)	34	60
All	All	754/796 (95%)	728 (97%)	26 (3%)	37	63

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	ILE
1	A	241	ASP
1	A	257	PHE
1	A	336	SER
1	A	345	ILE
1	A	374	ASN
1	A	391	GLU
1	A	397	ASN
1	A	421	THR
1	B	378	SER
1	B	393	ARG
1	B	394	ASP
1	B	397	ASN
1	B	407	TYR
1	C	267	LYS
1	C	329	ASN
1	C	336	SER
1	C	374	ASN
1	C	380	SER
1	D	259	SER
1	D	264	GLN
1	D	290	GLU
1	D	374	ASN
1	D	405	SER
1	D	414	LYS
1	D	419	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	231	ASN
1	B	312	ASN
1	C	368	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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	206/219 (94%)	-0.09	9 (4%) 34 37	41, 78, 141, 168	0
1	B	205/219 (93%)	-0.30	0 100 100	38, 64, 127, 156	0
1	C	210/219 (95%)	-0.24	4 (1%) 66 69	27, 65, 141, 171	0
1	D	210/219 (95%)	-0.14	11 (5%) 27 29	29, 66, 142, 183	0
All	All	831/876 (94%)	-0.19	24 (2%) 51 55	27, 68, 140, 183	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	THR	7.7
1	D	247	ASN	6.0
1	A	300	PRO	5.5
1	D	245	GLY	5.5
1	D	244	GLU	4.1
1	C	298	LEU	3.5
1	A	301	ASN	3.2
1	D	391	GLU	3.2
1	A	331	GLU	3.2
1	A	298	LEU	2.9
1	D	301	ASN	2.6
1	A	393	ARG	2.6
1	C	300	PRO	2.4
1	A	418	VAL	2.4
1	D	297	ASP	2.2
1	C	331	GLU	2.2
1	A	248	GLY	2.2
1	D	299	GLY	2.2
1	D	248	GLY	2.1
1	A	396	TYR	2.1
1	D	249	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	377	GLU	2.0
1	C	387	ARG	2.0
1	D	300	PRO	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1004	1/1	0.98	0.11	69,69,69,69	0
2	CA	A	1003	1/1	0.99	0.08	53,53,53,53	0
2	CA	D	504	1/1	0.99	0.11	69,69,69,69	0
2	CA	C	502	1/1	0.99	0.11	44,44,44,44	0
2	CA	C	503	1/1	0.99	0.07	45,45,45,45	0
2	CA	A	1002	1/1	0.99	0.09	47,47,47,47	0
2	CA	B	502	1/1	0.99	0.08	45,45,45,45	0
2	CA	D	501	1/1	0.99	0.06	65,65,65,65	0
2	CA	C	504	1/1	0.99	0.13	63,63,63,63	0
2	CA	A	1001	1/1	0.99	0.06	63,63,63,63	0
2	CA	D	502	1/1	0.99	0.08	41,41,41,41	0
2	CA	B	501	1/1	0.99	0.06	62,62,62,62	0
2	CA	D	503	1/1	1.00	0.09	45,45,45,45	0
2	CA	B	503	1/1	1.00	0.09	45,45,45,45	0
2	CA	C	501	1/1	1.00	0.04	65,65,65,65	0
2	CA	B	504	1/1	1.00	0.14	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.