



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:14 PM UTC

PDB ID : 5CO1 / pdb_00005co1
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

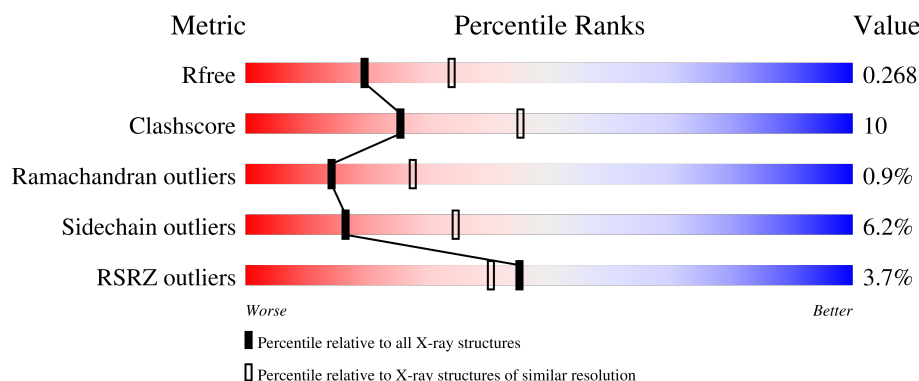
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	6% 69% 21% • 6%
1	B	219	2% 73% 17% • 6%
1	C	219	4% 73% 21% • •
1	D	219	2% 71% 21% • •

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 (CCD ID: CA) (formula: Ca).

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

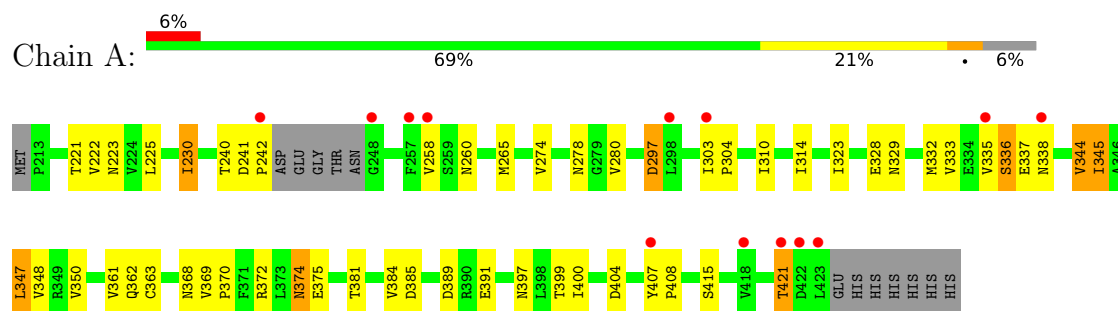
- Molecule 3 is water.

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

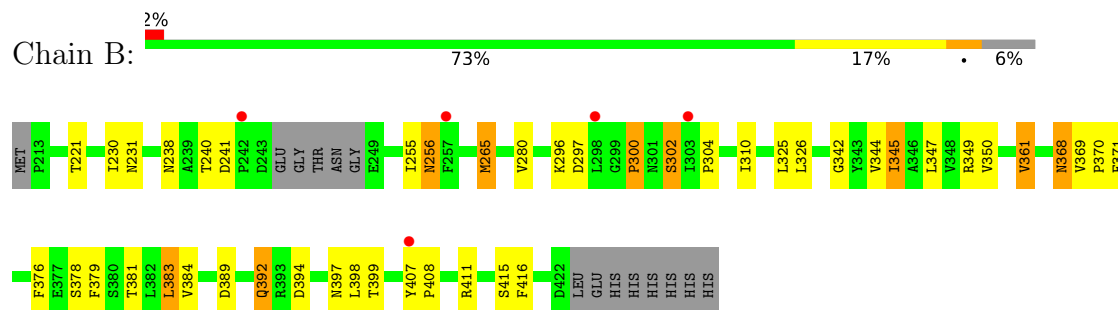
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

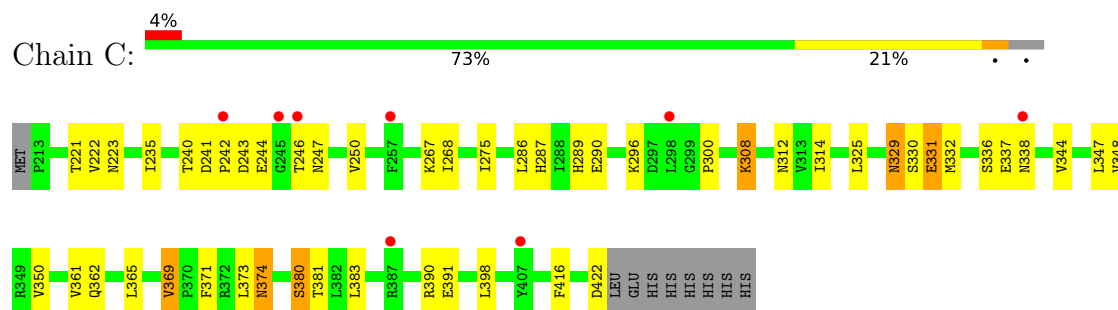
• Molecule 1: Protocadherin-19 isoform 1



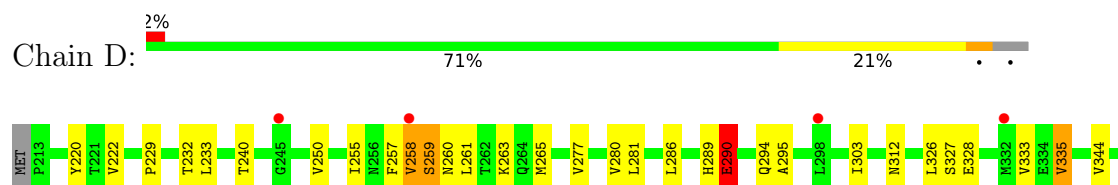
• Molecule 1: Protocadherin-19 isoform 1

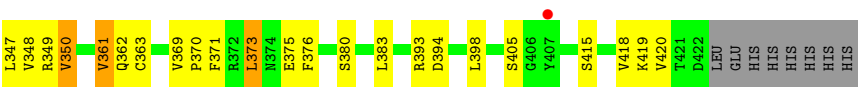


• Molecule 1: Protocadherin-19 isoform 1



• 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, α , β , γ	149.35Å 86.63Å 132.58Å 90.00° 122.13° 90.00°	Depositor
Resolution (Å)	50.00 – 2.51 50.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.51) 97.8 (50.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.188 , 0.239 (Not available) , 0.268	Depositor DCC
R_{free} test set	2360 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.74	0/1630	0.91	0/2219
1	B	0.79	0/1626	1.00	5/2214 (0.2%)
1	C	0.84	1/1659 (0.1%)	0.94	0/2260
1	D	0.85	1/1659 (0.1%)	1.01	3/2260 (0.1%)
All	All	0.81	2/6574 (0.0%)	0.97	8/8953 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	GLU	CA-C	6.87	1.61	1.52
1	D	290	GLU	C-O	-5.90	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ILE	CB-CA-C	-6.51	103.24	112.22
1	B	256	ASN	N-CA-C	6.43	116.94	107.88
1	B	241	ASP	CA-C-N	-5.94	112.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ASP	C-N-CA	-5.94	112.42	119.84
1	D	363	CYS	N-CA-C	5.53	116.37	108.74
1	D	222	VAL	N-CA-C	5.38	116.48	108.46
1	D	255	ILE	CB-CA-C	-5.08	104.23	111.34
1	B	361	VAL	N-CA-C	5.01	115.93	108.46

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
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	30	0
1	B	1599	0	1577	25	3
1	C	1631	0	1603	41	1
1	D	1631	0	1603	31	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6529	0	6370	123	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 10.

All (123) 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: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
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:221:THR:C	1:C:222:VAL:HG23	2.22	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:A:404:ASP:OD1	1:A:404:ASP:C	2.47	0.57
1:B:369:VAL:HG12	1:B:371:PHE:HD2	1.69	0.56
1:A:265:MET:HE1	1:A:280:VAL:O	2.05	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:B:368:ASN:C	1:B:369:VAL:HG23	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:265:MET:HE1	1:D:280:VAL:O	2.11	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
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:CD1	1:D:376:PHE:N	2.81	0.49
1:C:369:VAL:HG13	1:C:371:PHE:CD2	2.47	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:A:407:TYR:HA	1:A:408:PRO:C	2.39	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:C:221:THR:C	1:C:222:VAL:CG2	2.87	0.47
1:A:230:ILE:HD11	1:A:278:ASN:C	2.40	0.46
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:265:MET:CE	1:D:281:LEU:HA	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:OD1	1:A:297:ASP:N	2.48	0.44
1:C:365:LEU:HD23	1:C:373:LEU:HG	1.98	0.44
1:D:261:LEU:HD11	1:D:265:MET:HE2	1.99	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:B:265:MET:HE1	1:B:280:VAL:O	2.19	0.42
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
1:A:221:THR:HG22	1:A:310:ILE:HB	2.02	0.42
1:C:242:PRO:C	1:C:244:GLU:HA	2.45	0.41
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:O	1:D:258:VAL:HG13	2.21	0.41
1:C:308:LYS:HE3	1:D:312:ASN:HD21	1.85	0.41
1:D:286:LEU:HD23	1:D:289:HIS:CE1	2.56	0.41
1:B:300:PRO:C	1:B:302:SER:N	2.79	0.41
1:B:407:TYR:HA	1:B:408:PRO:C	2.45	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:329:ASN:HB3	1:C:332:MET:O	2.20	0.41
1:C:361:VAL:HG12	1:C:362:GLN:H	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:MET:HE1	1:D:281:LEU:HA	2.03	0.41
1:D:294:GLN:HG2	1:D:295:ALA:N	2.35	0.41
1:C:336:SER:C	1:C:337:GLU:O	2.63	0.40
1:C:344:VAL:O	1:C:344:VAL:HG12	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:296:LYS:NZ	1:C:338:ASN:OD1[4_445]	2.16	0.04
1:B:349:ARG:NH2	1:D:344:VAL:O[3_455]	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%)	6	10
1	C	208/219 (95%)	192 (92%)	14 (7%)	2 (1%)	12	24
1	D	208/219 (95%)	192 (92%)	15 (7%)	1 (0%)	24	43
All	All	819/876 (94%)	752 (92%)	60 (7%)	7 (1%)	14	27

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%)	170 (91%)	17 (9%)	9	19
1	B	187/199 (94%)	178 (95%)	9 (5%)	23	46
1	C	190/199 (96%)	182 (96%)	8 (4%)	26	52
1	D	190/199 (96%)	177 (93%)	13 (7%)	14	31
All	All	754/796 (95%)	707 (94%)	47 (6%)	16	34

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	VAL
1	A	230	ILE
1	A	258	VAL
1	A	260	ASN
1	A	274	VAL
1	A	297	ASP
1	A	336	SER
1	A	344	VAL
1	A	345	ILE
1	A	347	LEU
1	A	348	VAL
1	A	374	ASN
1	A	384	VAL
1	A	391	GLU
1	A	397	ASN

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Mol	Chain	Res	Type
1	A	400	ILE
1	A	421	THR
1	B	240	THR
1	B	255	ILE
1	B	265	MET
1	B	297	ASP
1	B	378	SER
1	B	383	LEU
1	B	394	ASP
1	B	397	ASN
1	B	411	ARG
1	C	267	LYS
1	C	268	ILE
1	C	296	LYS
1	C	329	ASN
1	C	369	VAL
1	C	374	ASN
1	C	380	SER
1	C	391	GLU
1	D	233	LEU
1	D	259	SER
1	D	263	LYS
1	D	290	GLU
1	D	333	VAL
1	D	335	VAL
1	D	350	VAL
1	D	361	VAL
1	D	373	LEU
1	D	383	LEU
1	D	393	ARG
1	D	405	SER
1	D	419	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	368	ASN
1	A	374	ASN
1	B	231	ASN
1	B	312	ASN
1	C	231	ASN

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Mol	Chain	Res	Type
1	C	238	ASN
1	C	366	GLN
1	C	368	ASN
1	D	231	ASN
1	D	312	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
1	A	206/219 (94%)	0.29	13 (6%) 26 23	40, 78, 141, 168	0
1	B	205/219 (93%)	-0.07	5 (2%) 59 55	38, 64, 127, 156	0
1	C	210/219 (95%)	0.07	8 (3%) 44 39	27, 65, 141, 171	0
1	D	210/219 (95%)	0.09	5 (2%) 59 55	29, 66, 142, 183	0
All	All	831/876 (94%)	0.10	31 (3%) 45 40	27, 68, 140, 183	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	7.0
1	A	242	PRO	6.9
1	B	303	ILE	4.8
1	A	257	PHE	4.2
1	C	245	GLY	4.1
1	A	407	TYR	3.4
1	A	298	LEU	3.2
1	B	242	PRO	3.2
1	A	303	ILE	3.0
1	D	258	VAL	3.0
1	A	418	VAL	2.9
1	B	407	TYR	2.9
1	D	407	TYR	2.9
1	C	246	THR	2.9
1	C	338	ASN	2.8
1	A	248	GLY	2.8
1	A	421	THR	2.8
1	A	422	ASP	2.6
1	A	338	ASN	2.6
1	C	242	PRO	2.4
1	B	257	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	2.4
1	A	335	VAL	2.4
1	D	245	GLY	2.4
1	C	407	TYR	2.3
1	D	298	LEU	2.2
1	C	298	LEU	2.2
1	A	258	VAL	2.2
1	C	387	ARG	2.1
1	C	257	PHE	2.1
1	D	332	MET	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 oligosaccharides 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, 95th 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	D	504	1/1	0.98	0.04	69,69,69,69	0
2	CA	B	504	1/1	0.99	0.03	55,55,55,55	0
2	CA	D	501	1/1	0.99	0.02	65,65,65,65	0
2	CA	A	1004	1/1	0.99	0.02	69,69,69,69	0
2	CA	B	501	1/1	1.00	0.02	62,62,62,62	0
2	CA	B	502	1/1	1.00	0.01	45,45,45,45	0
2	CA	B	503	1/1	1.00	0.01	45,45,45,45	0
2	CA	A	1002	1/1	1.00	0.01	47,47,47,47	0
2	CA	C	501	1/1	1.00	0.04	65,65,65,65	0
2	CA	C	502	1/1	1.00	0.01	44,44,44,44	0
2	CA	C	503	1/1	1.00	0.02	45,45,45,45	0
2	CA	C	504	1/1	1.00	0.02	63,63,63,63	0
2	CA	A	1003	1/1	1.00	0.02	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	502	1/1	1.00	0.03	41,41,41,41	0
2	CA	D	503	1/1	1.00	0.01	45,45,45,45	0
2	CA	A	1001	1/1	1.00	0.02	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.