



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:09 AM UTC

PDB ID : 6N2E / pdb_00006n2e
Title : Crystal Structure of Human Protocadherin-15 EC1-3 G16D N369D Q370N
and Mouse Cadherin-23 EC1-2 T15E
Authors : Choudhary, D.; De-la-Torre, P.; Sotomayor, M.
Deposited on : 2018-11-12
Resolution : 2.90 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

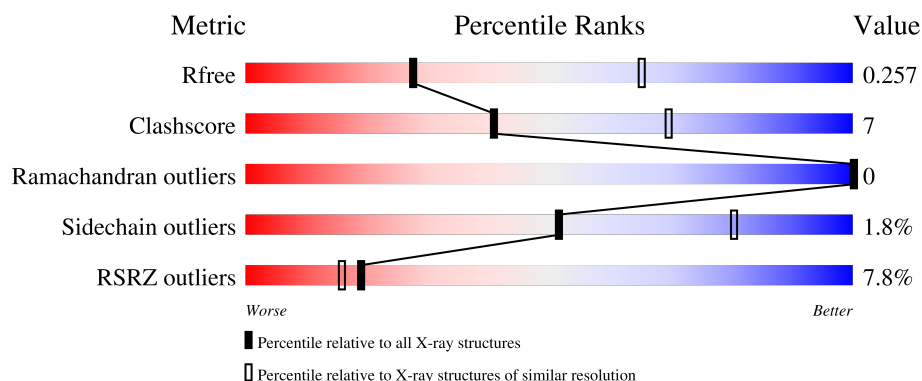
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	379	4% 72% 20% 7%
1	B	379	% 82% 14% %
2	C	214	17% 74% 15% 10%
2	D	214	14% 74% 14% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8779 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-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2805	1769	479	546	11			
1	B	365	Total	C	N	O	S	0	0	0
			2899	1826	495	567	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A087X1T6
A	16	ASP	GLY	engineered mutation	UNP A0A087X1T6
A	369	ASP	ASN	engineered mutation	UNP A0A087X1T6
A	370	ASN	GLN	engineered mutation	UNP A0A087X1T6
A	371	LEU	-	expression tag	UNP A0A087X1T6
A	372	GLU	-	expression tag	UNP A0A087X1T6
A	373	HIS	-	expression tag	UNP A0A087X1T6
A	374	HIS	-	expression tag	UNP A0A087X1T6
A	375	HIS	-	expression tag	UNP A0A087X1T6
A	376	HIS	-	expression tag	UNP A0A087X1T6
A	377	HIS	-	expression tag	UNP A0A087X1T6
A	378	HIS	-	expression tag	UNP A0A087X1T6
B	0	MET	-	initiating methionine	UNP A0A087X1T6
B	16	ASP	GLY	engineered mutation	UNP A0A087X1T6
B	369	ASP	ASN	engineered mutation	UNP A0A087X1T6
B	370	ASN	GLN	engineered mutation	UNP A0A087X1T6
B	371	LEU	-	expression tag	UNP A0A087X1T6
B	372	GLU	-	expression tag	UNP A0A087X1T6
B	373	HIS	-	expression tag	UNP A0A087X1T6
B	374	HIS	-	expression tag	UNP A0A087X1T6
B	375	HIS	-	expression tag	UNP A0A087X1T6
B	376	HIS	-	expression tag	UNP A0A087X1T6
B	377	HIS	-	expression tag	UNP A0A087X1T6
B	378	HIS	-	expression tag	UNP A0A087X1T6

- Molecule 2 is a protein called Cadherin-23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	193	Total	C	N	O	S	0	0	0
			1507	956	249	301	1			
2	D	189	Total	C	N	O	S	0	0	0
			1488	945	246	296	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q99PF4
C	15	GLU	THR	engineered mutation	UNP Q99PF4
C	206	LEU	-	expression tag	UNP Q99PF4
C	207	GLU	-	expression tag	UNP Q99PF4
C	208	HIS	-	expression tag	UNP Q99PF4
C	209	HIS	-	expression tag	UNP Q99PF4
C	210	HIS	-	expression tag	UNP Q99PF4
C	211	HIS	-	expression tag	UNP Q99PF4
C	212	HIS	-	expression tag	UNP Q99PF4
C	213	HIS	-	expression tag	UNP Q99PF4
D	0	MET	-	initiating methionine	UNP Q99PF4
D	15	GLU	THR	engineered mutation	UNP Q99PF4
D	206	LEU	-	expression tag	UNP Q99PF4
D	207	GLU	-	expression tag	UNP Q99PF4
D	208	HIS	-	expression tag	UNP Q99PF4
D	209	HIS	-	expression tag	UNP Q99PF4
D	210	HIS	-	expression tag	UNP Q99PF4
D	211	HIS	-	expression tag	UNP Q99PF4
D	212	HIS	-	expression tag	UNP Q99PF4
D	213	HIS	-	expression tag	UNP Q99PF4

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Ca	0	0
			5	5		
3	B	5	Total	Ca	0	0
			5	5		
3	C	4	Total	Ca	0	0
			4	4		
3	D	4	Total	Ca	0	0
			4	4		

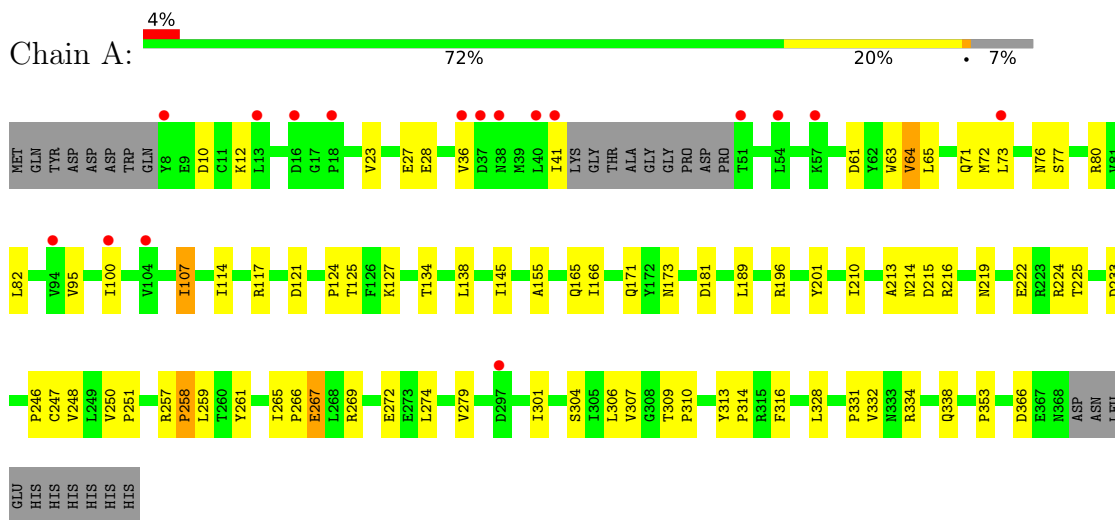
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total 28	O 28	0	0
4	B	32	Total 32	O 32	0	0
4	C	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0

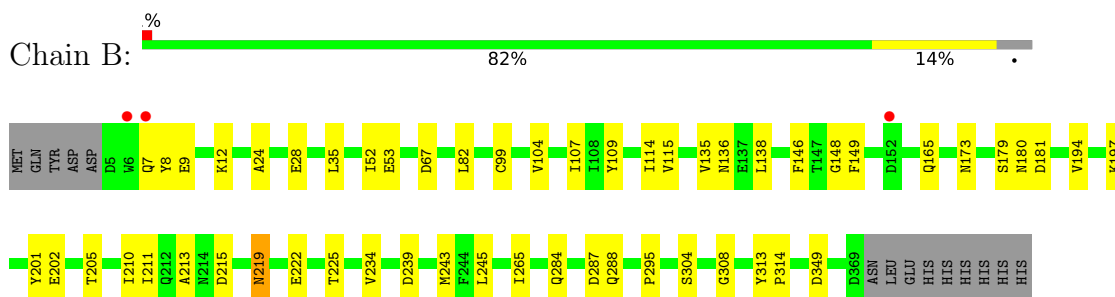
3 Residue-property plots [i](#)

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.

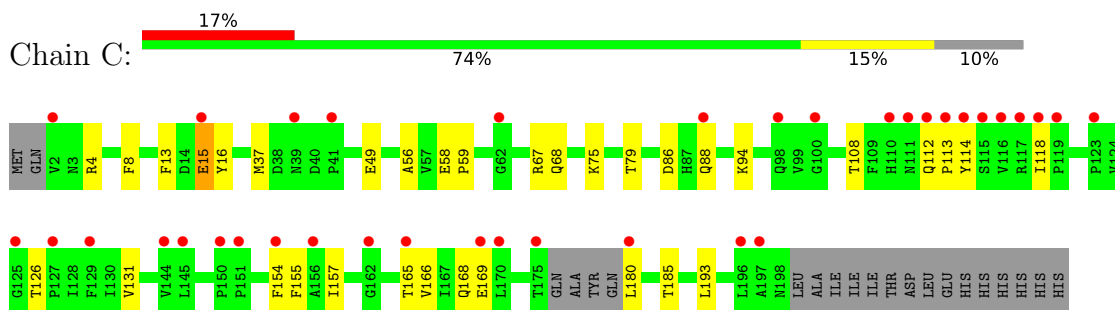
• Molecule 1: Protocadherin-15



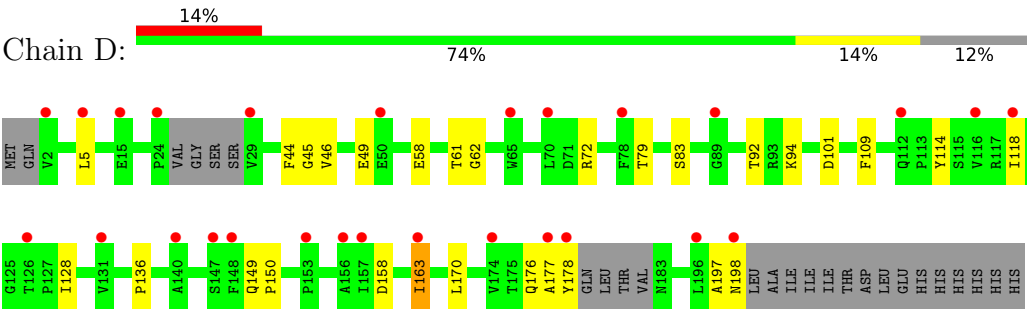
• Molecule 1: Protocadherin-15



• Molecule 2: Cadherin-23



• Molecule 2: Cadherin-23



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.79Å 65.40Å 190.01Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	49.52 – 2.90 49.52 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.52-2.90) 92.9 (49.52-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.225 , 0.253 0.226 , 0.257	Depositor DCC
R_{free} test set	1909 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8779	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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	1.10	6/2866 (0.2%)	1.34	4/3915 (0.1%)
1	B	1.14	6/2965 (0.2%)	1.30	2/4053 (0.0%)
2	C	1.01	1/1543 (0.1%)	1.25	1/2112 (0.0%)
2	D	1.00	1/1524 (0.1%)	1.23	1/2084 (0.0%)
All	All	1.08	14/8898 (0.2%)	1.29	8/12164 (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
2	C	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	PRO	C-O	-8.54	1.13	1.23
1	B	287	ASP	C-O	-7.35	1.15	1.23
1	A	304	SER	C-O	6.93	1.32	1.23
1	A	353	PRO	C-O	-6.26	1.16	1.24
1	B	202	GLU	CD-OE2	6.02	1.36	1.25
1	A	171	GLN	C-O	5.56	1.30	1.23
1	A	248	VAL	C-O	-5.54	1.18	1.24
1	B	295	PRO	C-O	-5.45	1.17	1.24
1	B	304	SER	C-O	5.24	1.30	1.23
1	A	331	PRO	C-O	-5.24	1.17	1.23
1	B	265	ILE	N-CA	5.19	1.49	1.45
2	C	193	LEU	C-O	5.16	1.29	1.24
1	B	52	ILE	C-O	5.07	1.29	1.23
2	D	45	GLY	C-O	5.02	1.28	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLU	CA-C-N	-7.07	112.04	122.86
1	A	267	GLU	C-N-CA	-7.07	112.04	122.86
2	C	88	GLN	CB-CG-CD	-6.05	102.31	112.60
2	D	123	PRO	N-CA-C	5.42	119.54	111.41
1	A	247	CYS	CB-CA-C	-5.29	103.03	111.17
1	A	201	TYR	CA-C-O	-5.26	114.31	120.20
1	B	180	ASN	N-CA-C	-5.17	107.00	113.15
1	B	136	ASN	CA-CB-CG	-5.10	107.50	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	15	GLU	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	2805	0	2753	47	0
1	B	2899	0	2832	32	0
2	C	1507	0	1444	19	0
2	D	1488	0	1416	21	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	28	0	0	0	0
4	B	32	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	8779	0	8445	112	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 7.

All (112) 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:B:243:MET:HE2	1:B:288:GLN:HG2	1.31	1.08
1:B:243:MET:CE	1:B:288:GLN:HG2	2.16	0.70
1:A:27:GLU:HG2	1:A:117:ARG:O	1.97	0.64
1:A:246:PRO:HD2	1:A:259:LEU:HD21	1.82	0.62
1:B:35:LEU:HD13	1:B:114:ILE:HD13	1.85	0.57
2:C:155:PHE:CE1	2:C:166:VAL:HG22	2.40	0.57
1:A:267:GLU:O	1:A:332:VAL:O	2.22	0.56
1:A:28:GLU:N	1:A:82:LEU:O	2.39	0.56
1:A:28:GLU:HG2	1:A:82:LEU:O	2.05	0.56
1:B:313:TYR:CG	1:B:314:PRO:HD3	2.42	0.54
1:A:334:ARG:O	1:A:338:GLN:NE2	2.40	0.54
2:C:56:ALA:HB2	2:C:67:ARG:HD2	1.89	0.54
1:B:138:LEU:HD21	1:B:239:ASP:HB3	1.90	0.54
2:C:112:GLN:N	2:C:113:PRO:HD2	2.23	0.54
2:C:154:PHE:HA	2:C:168:GLN:HB3	1.91	0.53
1:A:10:ASP:C	1:A:12:LYS:H	2.15	0.53
1:B:313:TYR:N	1:B:314:PRO:CD	2.72	0.52
1:A:165:GLN:O	1:A:216:ARG:HG3	2.09	0.52
1:A:65:LEU:CD1	1:A:76:ASN:HB2	2.40	0.52
1:B:181:ASP:O	1:B:197:LYS:HG3	2.09	0.52
2:D:118:ILE:HD13	2:D:128:ILE:HG21	1.92	0.52
1:A:28:GLU:OE2	1:A:121:ASP:OD2	2.28	0.51
2:D:109:PHE:CD2	2:D:197:ALA:HB2	2.45	0.51
1:A:219:ASN:HB2	1:A:222:GLU:HB2	1.92	0.51
2:D:83:SER:HB3	2:D:92:THR:HG22	1.93	0.51
1:A:165:GLN:O	1:A:215:ASP:HA	2.10	0.51
2:D:72:ARG:HG3	2:D:101:ASP:HB2	1.91	0.51
2:D:176:GLN:HG3	2:D:177:ALA:N	2.26	0.50
1:B:313:TYR:CD2	1:B:314:PRO:HD3	2.46	0.50
1:B:173:ASN:HB2	1:B:210:ILE:CD1	2.42	0.49
2:C:131:VAL:CG2	2:C:157:ILE:HD11	2.42	0.49
1:A:125:THR:O	1:A:155:ALA:HA	2.13	0.49
1:B:146:PHE:CZ	1:B:148:GLY:HA3	2.47	0.49
1:B:165:GLN:O	1:B:215:ASP:HA	2.13	0.49
1:B:181:ASP:O	1:B:181:ASP:OD1	2.31	0.49
1:A:173:ASN:HB2	1:A:210:ILE:HD12	1.95	0.48
1:A:173:ASN:CB	1:A:210:ILE:HD12	2.44	0.48
2:C:49:GLU:HB3	2:D:49:GLU:CB	2.43	0.48
1:A:181:ASP:O	1:A:196:ARG:NH2	2.42	0.48
1:B:219:ASN:OD1	1:B:219:ASN:C	2.55	0.48
1:A:313:TYR:N	1:A:314:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HG23	1:A:114:ILE:HG23	1.95	0.47
1:A:41:ILE:HB	1:A:71:GLN:NE2	2.29	0.47
1:B:308:GLY:HA3	1:B:313:TYR:CE2	2.49	0.47
1:A:266:PRO:HB2	1:A:269:ARG:HG2	1.96	0.47
2:C:126:THR:O	2:C:165:THR:HA	2.15	0.47
1:A:124:PRO:HB3	1:A:166:ILE:HD12	1.97	0.47
1:B:245:LEU:HB2	1:B:284:GLN:HG3	1.97	0.47
2:C:8:PHE:HB3	2:C:13:PHE:CE2	2.50	0.47
2:C:49:GLU:HB3	2:D:49:GLU:HB3	1.97	0.47
1:A:269:ARG:HB2	1:A:274:LEU:HD11	1.96	0.46
2:D:114:TYR:HB2	2:D:198:ASN:O	2.14	0.46
1:A:306:LEU:HG	1:A:307:VAL:HG13	1.98	0.46
1:A:213:ALA:O	1:A:225:THR:HA	2.16	0.45
1:A:77:SER:O	1:A:80:ARG:O	2.35	0.45
2:C:79:THR:CG2	2:C:94:LYS:HD2	2.46	0.45
1:A:309:THR:HA	1:A:310:PRO:C	2.42	0.45
1:A:100:ILE:HG12	1:A:107:ILE:HG12	1.99	0.45
2:D:79:THR:HG22	2:D:94:LYS:HD2	1.99	0.45
2:D:58:GLU:HG2	2:D:61:THR:OG1	2.17	0.45
1:A:261:TYR:HB3	1:A:279:VAL:CG1	2.47	0.45
1:A:366:ASP:OD1	1:A:366:ASP:C	2.60	0.44
1:B:9:GLU:O	1:B:12:LYS:HB2	2.17	0.44
2:D:44:PHE:CD2	2:D:62:GLY:CA	3.00	0.44
1:B:24:ALA:HA	1:B:115:VAL:O	2.17	0.44
1:A:61:ASP:HB2	1:A:63:TRP:CD1	2.52	0.44
1:B:213:ALA:O	1:B:225:THR:HA	2.18	0.43
1:A:36:VAL:HB	1:A:73:LEU:HB2	2.00	0.43
2:D:72:ARG:NH1	2:D:136:PRO:O	2.51	0.43
1:B:149:PHE:HE2	1:B:211:ILE:HG21	1.83	0.43
1:A:246:PRO:O	1:A:259:LEU:HD22	2.19	0.43
1:A:138:LEU:HD22	1:B:138:LEU:HD22	1.99	0.43
1:A:214:ASN:HA	1:A:224:ARG:O	2.19	0.43
1:B:53:GLU:O	1:B:99:CYS:HA	2.19	0.43
1:B:67:ASP:OD1	1:B:67:ASP:C	2.61	0.43
1:B:107:ILE:CG2	1:B:109:TYR:CE1	3.02	0.43
1:A:72:MET:C	1:A:73:LEU:HD12	2.44	0.43
1:A:189:LEU:CD1	2:D:5:LEU:HD11	2.49	0.43
2:D:79:THR:CG2	2:D:94:LYS:HD2	2.49	0.43
2:C:112:GLN:O	2:C:114:TYR:N	2.52	0.42
1:B:349:ASP:OD1	1:B:349:ASP:C	2.62	0.42
2:C:86:ASP:OD1	2:C:86:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:GLU:HG2	2:D:49:GLU:HB3	2.01	0.42
2:C:58:GLU:CD	2:C:58:GLU:C	2.88	0.42
1:B:179:SER:C	1:B:181:ASP:H	2.27	0.42
1:B:308:GLY:HA3	1:B:313:TYR:CD2	2.55	0.42
2:D:170:LEU:HG	2:D:178:TYR:OH	2.20	0.42
1:B:173:ASN:HB2	1:B:210:ILE:HD13	2.02	0.41
1:A:189:LEU:HD21	2:D:5:LEU:CD1	2.50	0.41
2:D:158:ASP:HB2	2:D:163:ILE:CD1	2.51	0.41
2:C:15:GLU:O	2:C:16:TYR:HB3	2.21	0.41
1:A:134:THR:HA	1:A:233:ASP:O	2.21	0.41
1:B:201:TYR:CD1	1:B:205:THR:HG22	2.55	0.41
1:B:28:GLU:N	1:B:82:LEU:O	2.50	0.41
1:A:266:PRO:HB2	1:A:269:ARG:CG	2.51	0.41
1:A:189:LEU:HD11	2:D:5:LEU:CD1	2.51	0.41
1:A:65:LEU:HD11	1:A:76:ASN:HB2	2.03	0.41
2:C:4:ARG:HD2	2:C:37:MET:HB2	2.03	0.41
2:D:149:GLN:HA	2:D:150:PRO:HA	1.93	0.41
1:A:10:ASP:C	1:A:12:LYS:N	2.79	0.41
1:A:196:ARG:HH21	1:A:196:ARG:HG2	1.85	0.41
2:C:180:LEU:HD23	2:C:180:LEU:HA	1.88	0.41
1:A:250:VAL:O	1:A:251:PRO:C	2.64	0.41
1:A:316:PHE:O	1:A:328:LEU:HA	2.22	0.41
2:C:131:VAL:HG21	2:C:157:ILE:HD11	2.02	0.41
1:A:257:ARG:HA	1:A:258:PRO:HD3	1.88	0.40
1:B:219:ASN:ND2	1:B:222:GLU:HG3	2.37	0.40
2:C:58:GLU:HA	2:C:59:PRO:HD3	1.80	0.40
1:B:8:TYR:CD1	1:B:104:VAL:HG21	2.56	0.40
2:D:44:PHE:CD2	2:D:62:GLY:HA3	2.56	0.40
1:A:64:VAL:CG2	1:A:95:VAL:HG11	2.52	0.40
1:B:135:VAL:O	1:B:234:VAL:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/379 (92%)	338 (97%)	10 (3%)	0	100	100
1	B	363/379 (96%)	354 (98%)	9 (2%)	0	100	100
2	C	189/214 (88%)	178 (94%)	11 (6%)	0	100	100
2	D	183/214 (86%)	178 (97%)	5 (3%)	0	100	100
All	All	1083/1186 (91%)	1048 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	321/344 (93%)	314 (98%)	7 (2%)	45	77
1	B	330/344 (96%)	327 (99%)	3 (1%)	70	90
2	C	172/191 (90%)	166 (96%)	6 (4%)	32	66
2	D	168/191 (88%)	166 (99%)	2 (1%)	63	86
All	All	991/1070 (93%)	973 (98%)	18 (2%)	51	80

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	107	ILE
1	A	127	LYS
1	A	145	ILE
1	A	265	ILE
1	A	272	GLU
1	A	301	ILE
1	B	7	GLN
1	B	194	VAL
1	B	219	ASN

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Mol	Chain	Res	Type
2	C	68	GLN
2	C	75	LYS
2	C	108	THR
2	C	118	ILE
2	C	169	GLU
2	C	185	THR
2	D	46	VAL
2	D	163	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	128	HIS
1	A	288	GLN
1	B	122	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 18 ligands modelled in this entry, 18 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	352/379 (92%)	0.10	17 (4%) 35 28	39, 62, 129, 147	0
1	B	365/379 (96%)	-0.16	3 (0%) 82 77	38, 58, 89, 127	0
2	C	193/214 (90%)	1.22	36 (18%) 3 3	82, 106, 145, 173	0
2	D	189/214 (88%)	1.14	30 (15%) 5 4	91, 113, 136, 143	0
All	All	1099/1186 (92%)	0.39	86 (7%) 19 16	38, 80, 132, 173	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	2	VAL	5.2
2	C	175	THR	5.1
2	D	24	PRO	3.8
2	D	198	ASN	3.5
2	D	131	VAL	3.4
2	C	150	PRO	3.4
2	D	163	ILE	3.3
2	C	116	VAL	3.3
2	D	178	TYR	3.3
2	C	196	LEU	3.2
2	C	170	LEU	3.2
2	D	123	PRO	3.2
1	A	94	VAL	3.1
1	B	6	TRP	3.1
2	D	147	SER	3.0
2	D	29	VAL	2.9
1	B	7	GLN	2.9
2	C	180	LEU	2.9
2	C	154	PHE	2.9
2	D	177	ALA	2.8
2	D	2	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	112	GLN	2.7
2	C	151	PRO	2.6
2	D	140	ALA	2.6
1	A	8	TYR	2.6
1	A	51	THR	2.6
1	B	152	ASP	2.6
2	D	174	VAL	2.6
2	D	156	ALA	2.6
2	C	115	SER	2.6
2	C	165	THR	2.6
2	D	5	LEU	2.5
2	C	110	HIS	2.5
2	C	88	GLN	2.5
2	D	118	ILE	2.5
1	A	297	ASP	2.5
1	A	104	VAL	2.4
2	C	62	GLY	2.4
2	D	65	TRP	2.4
2	C	145	LEU	2.4
1	A	73	LEU	2.4
2	C	127	PRO	2.4
2	C	100	GLY	2.3
2	D	78	PHE	2.3
1	A	57	LYS	2.3
1	A	37	ASP	2.3
1	A	41	ILE	2.3
2	C	41	PRO	2.3
2	C	156	ALA	2.3
2	D	50	GLU	2.3
2	C	144	VAL	2.3
2	D	124	VAL	2.3
2	C	111	ASN	2.2
2	C	118	ILE	2.2
2	D	157	ILE	2.2
2	C	39	ASN	2.2
2	D	112	GLN	2.2
1	A	36	VAL	2.2
2	C	129	PHE	2.2
1	A	40	LEU	2.2
2	C	197	ALA	2.2
2	D	70	LEU	2.2
2	D	196	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	54	LEU	2.2
2	C	15	GLU	2.2
2	D	15	GLU	2.2
2	C	98	GLN	2.2
1	A	16	ASP	2.2
2	C	113	PRO	2.2
2	D	116	VAL	2.2
2	D	89	GLY	2.2
2	C	162	GLY	2.1
2	D	126	THR	2.1
1	A	13	LEU	2.1
1	A	100	ILE	2.1
1	A	18	PRO	2.1
2	D	148	PHE	2.1
2	C	119	PRO	2.1
2	C	117	ARG	2.1
2	C	114	TYR	2.1
2	C	123	PRO	2.0
1	A	38	ASN	2.0
2	C	125	GLY	2.0
2	C	169	GLU	2.0
2	D	120	GLU	2.0
2	D	153	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 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	401	1/1	0.96	0.09	106,106,106,106	0
3	CA	C	302	1/1	0.96	0.04	102,102,102,102	0
3	CA	C	304	1/1	0.97	0.04	100,100,100,100	0
3	CA	D	301	1/1	0.97	0.05	139,139,139,139	0
3	CA	C	303	1/1	0.98	0.04	92,92,92,92	0
3	CA	D	302	1/1	0.98	0.03	106,106,106,106	0
3	CA	D	303	1/1	0.98	0.05	120,120,120,120	0
3	CA	B	401	1/1	0.99	0.04	64,64,64,64	0
3	CA	C	301	1/1	0.99	0.07	97,97,97,97	0
3	CA	A	403	1/1	0.99	0.03	76,76,76,76	0
3	CA	A	405	1/1	0.99	0.03	39,39,39,39	0
3	CA	D	304	1/1	0.99	0.05	87,87,87,87	0
3	CA	B	402	1/1	1.00	0.03	58,58,58,58	0
3	CA	B	403	1/1	1.00	0.02	60,60,60,60	0
3	CA	B	404	1/1	1.00	0.03	42,42,42,42	0
3	CA	B	405	1/1	1.00	0.02	44,44,44,44	0
3	CA	A	402	1/1	1.00	0.03	89,89,89,89	0
3	CA	A	404	1/1	1.00	0.03	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.