



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2020 – 12:12 PM EDT

PDB ID : 6N2E
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 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	:	2.14.6
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)	:	2.14.6

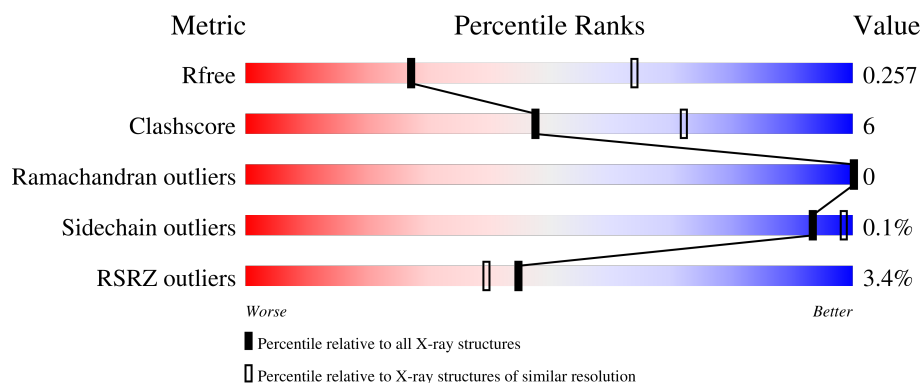
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 on 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	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
1	B	379	<div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	C	214	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
2	D	214	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>12%</div> </div> </div>

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 (three-letter code: CA) (formula: Ca).

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

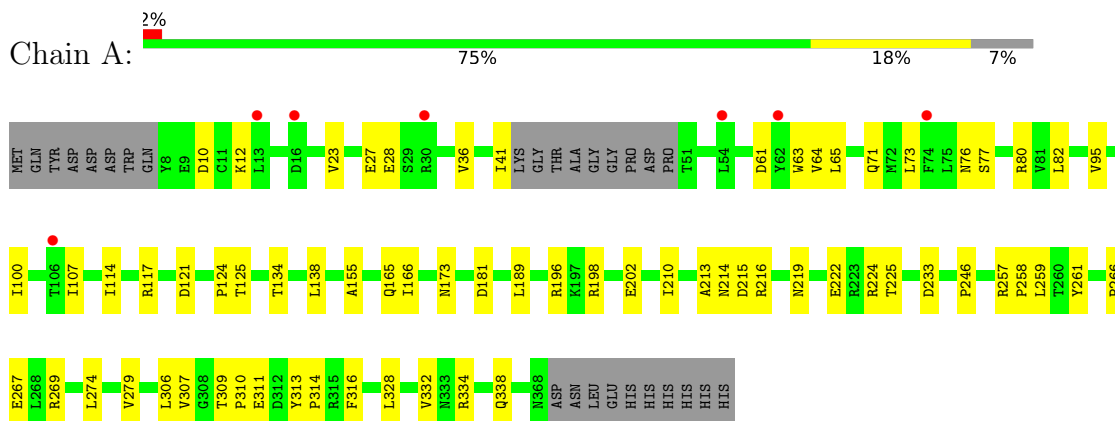
- Molecule 4 is water.

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

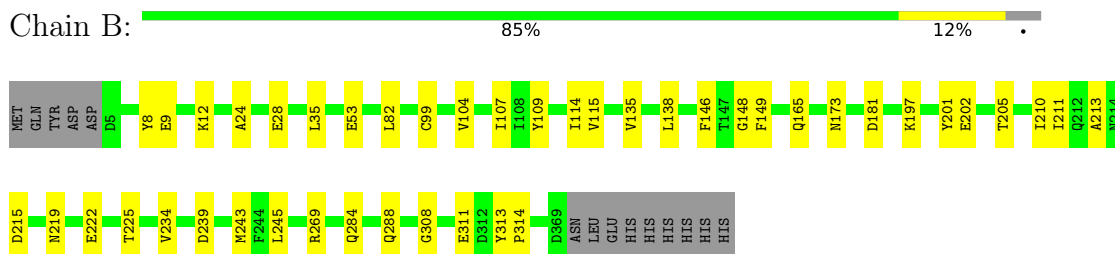
3 Residue-property plots [i](#)

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.

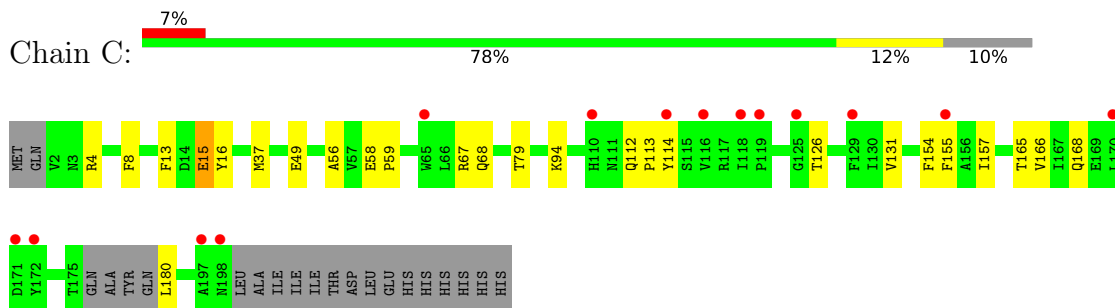
• Molecule 1: Protocadherin-15



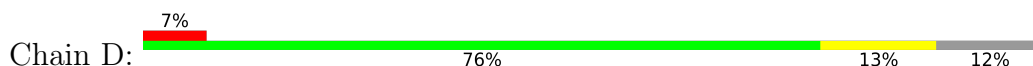
• Molecule 1: Protocadherin-15

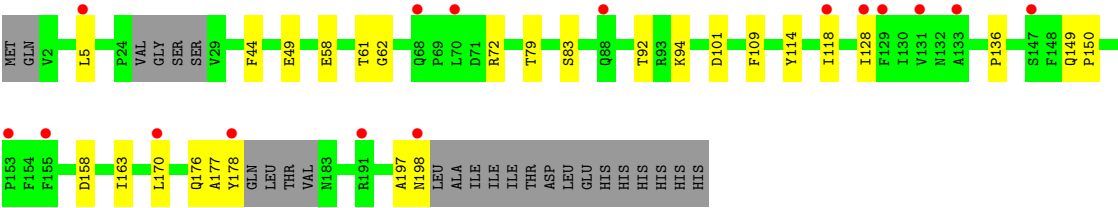


• Molecule 2: Cadherin-23



• 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 – 2.89	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.52-2.90) 92.4 (49.52-2.89)	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 (4.90%)	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 , 49.0	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	0.77	2/2866 (0.1%)	0.90	1/3915 (0.0%)
1	B	0.82	3/2965 (0.1%)	0.89	1/4053 (0.0%)
2	C	0.69	0/1543	0.80	0/2112
2	D	0.67	0/1524	0.78	0/2084
All	All	0.76	5/8898 (0.1%)	0.86	2/12164 (0.0%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	GLU	CD-OE2	10.12	1.36	1.25
1	A	202	GLU	CD-OE2	6.45	1.32	1.25
1	A	311	GLU	CD-OE1	6.31	1.32	1.25
1	B	311	GLU	CD-OE2	6.30	1.32	1.25
1	B	202	GLU	CD-OE1	5.21	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	269	ARG	CG-CD-NE	-5.13	101.03	111.80

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	43	0
1	B	2899	0	2832	30	0
2	C	1507	0	1444	17	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	104	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 6.

All (104) 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:CE	1:B:288:GLN:HG2	2.16	0.75
1:B:243:MET:HE3	1:B:288:GLN:HG2	1.76	0.65
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:243:MET:HE2	1:B:288:GLN:HG2	1.81	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:181:ASP:O	1:B:181:ASP:OD1	2.31	0.49
1:B:165:GLN:O	1:B:215:ASP:HA	2.13	0.49
1:A:10:ASP:C	1:A:12:LYS:H	2.15	0.48
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:A:313:TYR:N	1:A:314:PRO:CD	2.77	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:219:ASN:OD1	1:B:219:ASN:C	2.55	0.43
1:A:246:PRO:O	1:A:259:LEU:HD22	2.19	0.43
1:A:214:ASN:HA	1:A:224:ARG:O	2.19	0.43
1:A:138:LEU:HD22	1:B:138:LEU:HD22	1.99	0.43
1:B:53:GLU:O	1:B:99:CYS:HA	2.19	0.43
1:B:107:ILE:CG2	1:B:109:TYR:CE1	3.02	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
2:C:49:GLU:HG2	2:D:49:GLU:HB3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:GLN:HA	2:D:150:PRO:HA	1.93	0.41
1:A:196:ARG:HH21	1:A:196:ARG:HG2	1.85	0.41
2:C:180:LEU:HA	2:C:180:LEU:HD23	1.88	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:A:309:THR:HA	1:A:310:PRO:C	2.42	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 [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	321/344 (93%)	321 (100%)	0	100	100
1	B	330/344 (96%)	330 (100%)	0	100	100
2	C	172/191 (90%)	171 (99%)	1 (1%)	86	96
2	D	168/191 (88%)	168 (100%)	0	100	100
All	All	991/1070 (93%)	990 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	68	GLN

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

Mol	Chain	Res	Type
1	A	128	HIS
1	B	180	ASN
1	B	214	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 monosaccharides in this entry.

5.6 Ligand geometry

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

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, 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%)	-0.11	7 (1%) 65 63	39, 62, 129, 147	0
1	B	365/379 (96%)	-0.25	0 100 100	38, 58, 89, 127	0
2	C	193/214 (90%)	0.47	14 (7%) 15 11	82, 106, 145, 173	0
2	D	189/214 (88%)	0.55	16 (8%) 10 8	91, 113, 136, 143	0
All	All	1099/1186 (92%)	0.06	37 (3%) 45 40	38, 80, 132, 173	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	198	ASN	5.3
2	C	129	PHE	4.4
2	D	170	LEU	4.3
2	D	131	VAL	4.1
2	D	129	PHE	3.7
1	A	106	THR	3.6
2	C	197	ALA	3.6
2	C	118	ILE	3.4
2	D	178	TYR	3.2
1	A	16	ASP	3.1
1	A	54	LEU	3.0
2	C	170	LEU	3.0
2	C	116	VAL	3.0
2	C	114	TYR	2.8
2	D	68	GLN	2.8
2	D	147	SER	2.8
2	C	119	PRO	2.8
1	A	30	ARG	2.8
2	D	153	PRO	2.7
2	C	198	ASN	2.7
2	C	155	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	88	GLN	2.5
2	D	118	ILE	2.4
2	C	172	TYR	2.4
2	C	110	HIS	2.4
2	C	65	TRP	2.3
1	A	13	LEU	2.3
1	A	74	PHE	2.3
2	D	133	ALA	2.2
2	D	70	LEU	2.2
2	C	171	ASP	2.1
2	D	155	PHE	2.1
2	D	5	LEU	2.1
2	D	128	ILE	2.1
2	D	191	ARG	2.0
2	C	125	GLY	2.0
1	A	62	TYR	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 monosaccharides 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(Å ²)	Q<0.9
3	CA	D	301	1/1	0.79	0.03	139,139,139,139	0
3	CA	C	304	1/1	0.84	0.08	100,100,100,100	0
3	CA	D	303	1/1	0.86	0.04	120,120,120,120	0
3	CA	A	401	1/1	0.88	0.11	106,106,106,106	0
3	CA	C	302	1/1	0.91	0.12	102,102,102,102	0
3	CA	C	303	1/1	0.93	0.15	92,92,92,92	0
3	CA	D	302	1/1	0.94	0.10	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	B	401	1/1	0.96	0.12	64,64,64,64	0
3	CA	C	301	1/1	0.98	0.08	97,97,97,97	0
3	CA	A	402	1/1	0.98	0.12	89,89,89,89	0
3	CA	A	403	1/1	0.98	0.11	76,76,76,76	0
3	CA	A	404	1/1	0.98	0.20	38,38,38,38	0
3	CA	B	404	1/1	0.99	0.21	42,42,42,42	0
3	CA	B	405	1/1	0.99	0.18	44,44,44,44	0
3	CA	B	403	1/1	0.99	0.13	60,60,60,60	0
3	CA	B	402	1/1	0.99	0.16	58,58,58,58	0
3	CA	D	304	1/1	0.99	0.06	87,87,87,87	0
3	CA	A	405	1/1	0.99	0.15	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.