



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:41 PM UTC

PDB ID : 4R11 / pdb_00004r11
Title : A conserved phosphorylation switch controls the interaction between cadherin and beta-catenin in vitro and in vivo
Authors : Choi, H.-J.; Loveless, T.; Lynch, A.; Bang, I.; Hardin, J.; Weis, W.I.
Deposited on : 2014-08-03
Resolution : 2.79 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:

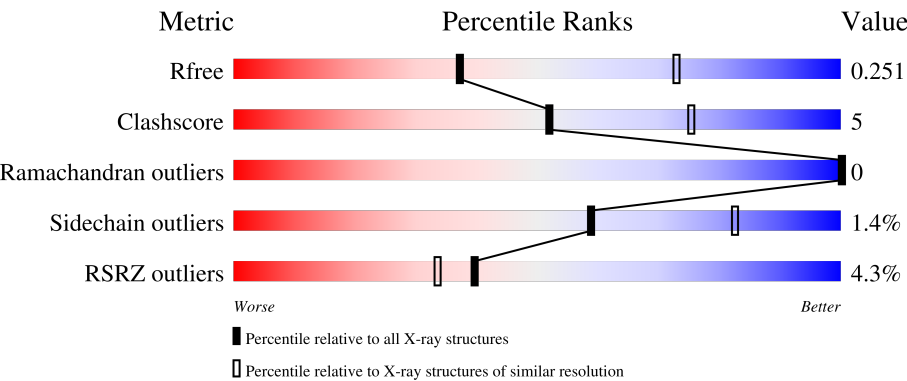
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	572	3% 82% 11% 7%
1	C	572	% 81% 12% 6%
1	E	572	6% 74% 14% 11%
2	B	84	4% 42% 10% 49%
2	D	84	6% 44% 5% 50%

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Mol	Chain	Length	Quality of chain
2	F	84	7% 33% 11% 55%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13120 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 Protein humpback-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4070	2540	733	770	27			
1	C	536	Total	C	N	O	S	0	0	0
			4087	2552	735	773	27			
1	E	508	Total	C	N	O	S	0	0	0
			3882	2423	703	729	27			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLY	-	expression tag	UNP O44326
A	51	GLY	-	expression tag	UNP O44326
A	52	ILE	-	expression tag	UNP O44326
C	50	GLY	-	expression tag	UNP O44326
C	51	GLY	-	expression tag	UNP O44326
C	52	ILE	-	expression tag	UNP O44326
E	50	GLY	-	expression tag	UNP O44326
E	51	GLY	-	expression tag	UNP O44326
E	52	ILE	-	expression tag	UNP O44326

- Molecule 2 is a protein called Cadherin-related hmr-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	43	Total	C	N	O	P	S	0	0
			355	215	61	77	1	1		
2	D	42	Total	C	N	O	P	S	0	0
			348	210	60	76	1	1		
2	F	38	Total	C	N	O	P		0	0
			317	186	46	81	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1140	GLY	-	expression tag	UNP Q967F4
B	1141	GLY	-	expression tag	UNP Q967F4
B	1142	ILE	-	expression tag	UNP Q967F4
B	1143	GLN	-	expression tag	UNP Q967F4
D	1140	GLY	-	expression tag	UNP Q967F4
D	1141	GLY	-	expression tag	UNP Q967F4
D	1142	ILE	-	expression tag	UNP Q967F4
D	1143	GLN	-	expression tag	UNP Q967F4
F	1140	GLY	-	expression tag	UNP Q967F4
F	1141	GLY	-	expression tag	UNP Q967F4
F	1142	ILE	-	expression tag	UNP Q967F4
F	1143	GLN	-	expression tag	UNP Q967F4

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total I 4 4	0	0
3	C	4	Total I 4 4	0	0
3	E	1	Total I 1 1	0	0

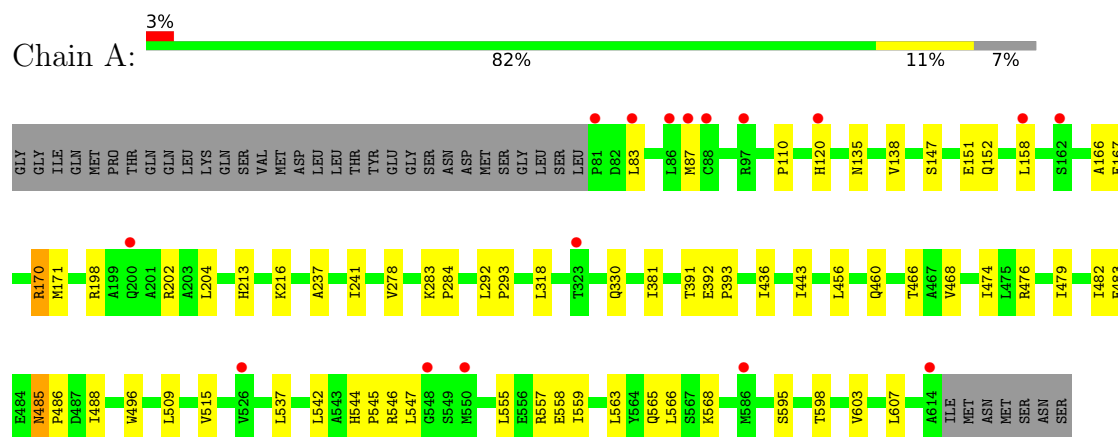
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	2	Total O 2 2	0	0
4	C	22	Total O 22 22	0	0
4	D	4	Total O 4 4	0	0
4	E	11	Total O 11 11	0	0
4	F	1	Total O 1 1	0	0

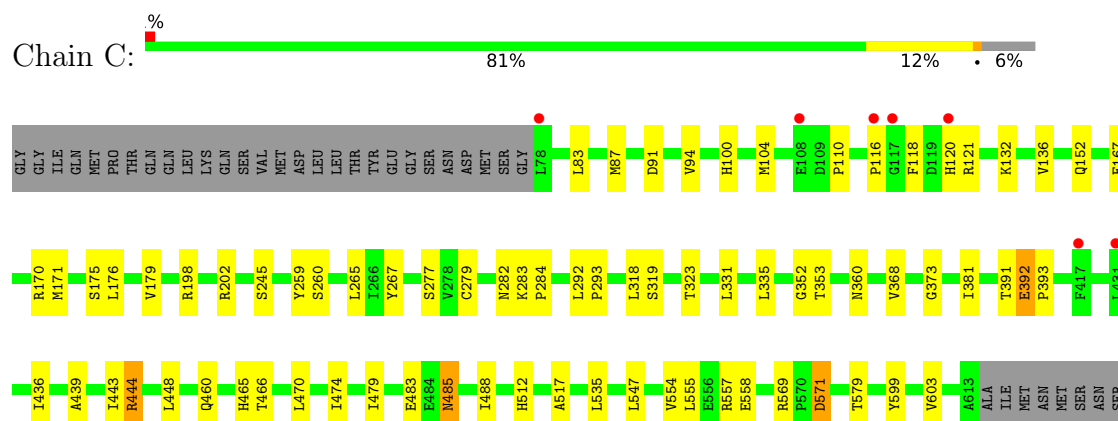
3 Residue-property plots [i](#)

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.

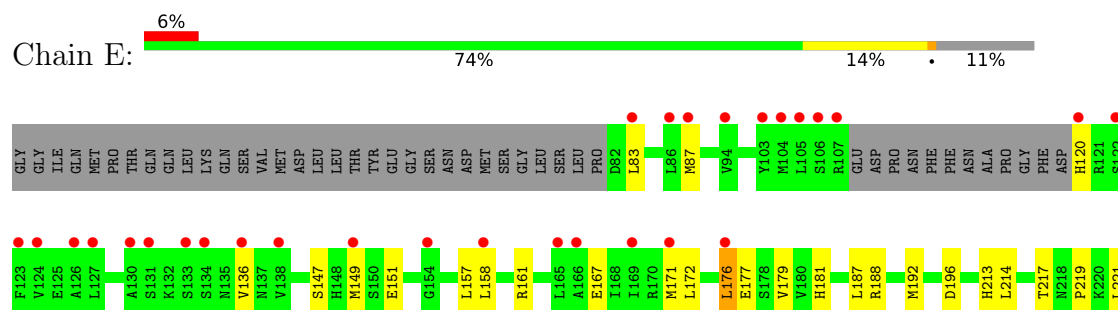
• Molecule 1: Protein humpback-2

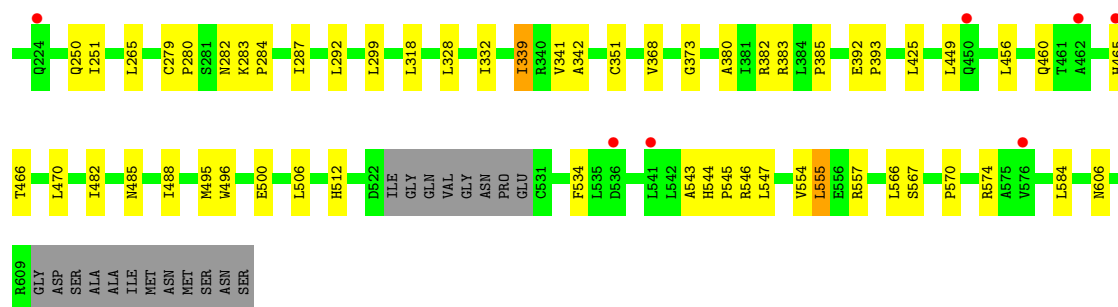


• Molecule 1: Protein humpback-2

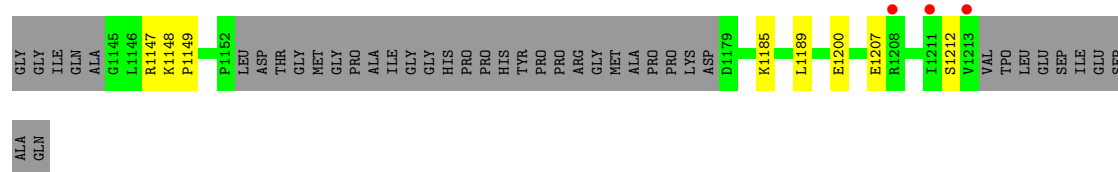


• Molecule 1: Protein humpback-2

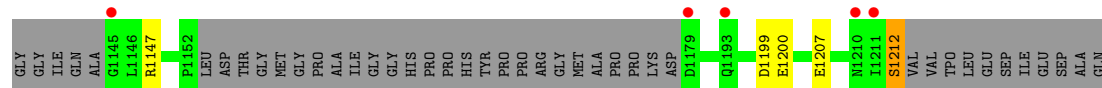




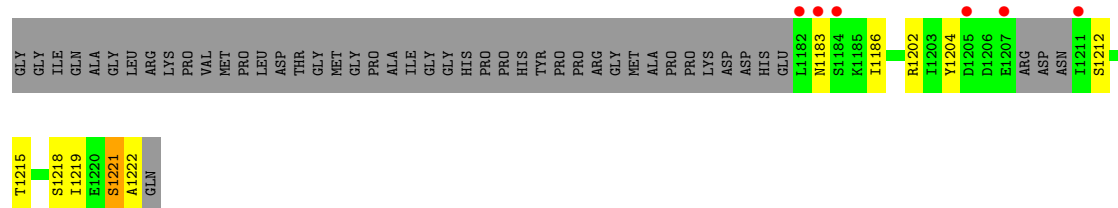
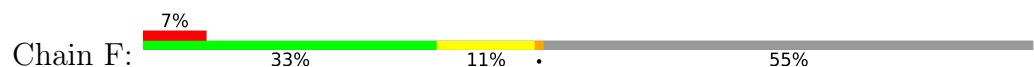
• Molecule 2: Cadherin-related hmr-1



• Molecule 2: Cadherin-related hmr-1



• Molecule 2: Cadherin-related hmr-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.06Å 157.72Å 84.82Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	44.69 – 2.79 44.69 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.69-2.79) 98.7 (44.69-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.249 0.204 , 0.251	Depositor DCC
R_{free} test set	4262 reflections (7.78%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13120	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: TPO, SEP, IOD

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	0.32	0/4131	0.79	2/5611 (0.0%)
1	C	0.36	1/4148 (0.0%)	0.80	4/5635 (0.1%)
1	E	0.32	0/3934	0.78	2/5338 (0.0%)
2	B	0.31	0/348	0.69	0/467
2	D	0.29	0/342	0.65	0/460
2	F	0.28	0/273	0.59	0/362
All	All	0.33	1/13176 (0.0%)	0.78	8/17873 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	PRO	CA-C	7.34	1.60	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CA-C-N	6.42	126.18	119.05
1	A	485	ASN	C-N-CA	6.42	126.18	119.05
1	E	512	HIS	CA-C-N	5.30	124.75	119.24
1	E	512	HIS	C-N-CA	5.30	124.75	119.24
1	C	485	ASN	CA-C-N	5.23	124.85	119.05
1	C	485	ASN	C-N-CA	5.23	124.85	119.05
1	C	512	HIS	CA-C-N	5.07	124.51	119.24
1	C	512	HIS	C-N-CA	5.07	124.51	119.24

There are no chirality outliers.

There are no planarity outliers.

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	4070	0	4145	38	0
1	C	4087	0	4166	46	0
1	E	3882	0	3985	46	0
2	B	355	0	332	5	0
2	D	348	0	323	4	0
2	F	317	0	282	4	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
3	E	1	0	0	1	0
4	A	12	0	0	0	0
4	B	2	0	0	0	0
4	C	22	0	0	1	0
4	D	4	0	0	1	0
4	E	11	0	0	0	0
4	F	1	0	0	0	0
All	All	13120	0	13233	133	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 5.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HD13	1:A:555:LEU:HD23	1.66	0.75
1:C:259:TYR:HB3	1:C:265:LEU:HD23	1.70	0.72
1:A:278:VAL:HG11	2:B:1207:GLU:HB3	1.73	0.69
1:A:485:ASN:HB3	1:A:488:ILE:HB	1.79	0.65
1:C:381:ILE:HG23	1:C:391:THR:HG22	1.77	0.65
1:A:83:LEU:HG	1:A:87:MET:HE3	1.79	0.65
1:C:118:PHE:CE2	1:C:120:HIS:HA	2.32	0.65
1:E:460:GLN:HG2	1:E:466:THR:HG22	1.79	0.64
1:E:83:LEU:HG	1:E:87:MET:HE3	1.79	0.63
1:E:120:HIS:HB2	1:E:158:LEU:HD21	1.81	0.63
1:C:485:ASN:HB3	1:C:488:ILE:HB	1.80	0.62
1:C:132:LYS:HG2	1:E:341:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:PHE:HE2	1:C:120:HIS:HA	1.67	0.60
1:E:500:GLU:HA	1:E:555:LEU:HD23	1.86	0.58
1:C:547:LEU:HD13	1:C:555:LEU:HD23	1.86	0.57
2:B:1147:ARG:HB3	2:B:1200:GLU:HB3	1.87	0.57
1:C:267:TYR:OH	2:D:1212:SEP:O2P	2.23	0.56
1:A:110:PRO:HB3	1:A:152:GLN:HG3	1.86	0.56
1:A:456:LEU:HD21	1:A:509:LEU:HD21	1.87	0.56
1:E:465:HIS:HB3	1:E:470:LEU:HG	1.88	0.56
1:A:476:ARG:HG2	1:A:537:LEU:HD21	1.86	0.56
1:E:547:LEU:HD13	1:E:555:LEU:HD12	1.87	0.56
2:F:1221:SEP:HA	2:F:1222:ALA:HB3	1.88	0.55
1:A:460:GLN:HG2	1:A:466:THR:HG22	1.88	0.55
1:C:599:TYR:O	1:C:603:VAL:HG23	2.05	0.55
1:A:292:LEU:HB2	1:A:293:PRO:HD3	1.89	0.55
1:E:172:LEU:HB3	1:E:213:HIS:HE2	1.72	0.54
1:C:175:SER:HB3	1:E:382:ARG:HH12	1.74	0.53
1:E:279:CYS:HB3	1:E:282:ASN:HB2	1.91	0.53
1:E:283:LYS:HB3	1:E:284:PRO:HD3	1.90	0.53
1:C:554:VAL:HG22	1:C:557:ARG:HH21	1.73	0.53
1:C:170:ARG:HD3	1:E:341:VAL:HA	1.90	0.53
1:E:177:GLU:HG3	1:E:181:HIS:NE2	2.23	0.53
1:E:283:LYS:HG3	1:E:318:LEU:HD23	1.91	0.52
1:E:283:LYS:O	1:E:287:ILE:HG12	2.10	0.52
1:E:351:CYS:HB3	1:E:393:PRO:HB2	1.92	0.52
1:A:456:LEU:CD2	1:A:509:LEU:HD21	2.39	0.51
1:C:557:ARG:NH1	1:C:558:GLU:OE2	2.44	0.51
1:A:283:LYS:HB3	1:A:284:PRO:HD3	1.93	0.50
1:A:598:THR:HB	2:B:1189:LEU:HD11	1.92	0.50
1:E:339:ILE:HG23	1:E:380:ALA:HB2	1.91	0.50
1:C:360:ASN:ND2	2:D:1199:ASP:HB2	2.27	0.50
1:C:136:VAL:HG22	1:C:176:LEU:HD11	1.94	0.50
1:E:328:LEU:O	1:E:332:ILE:HG12	2.12	0.49
1:E:250:GLN:HB2	3:E:701:IOD:I	2.82	0.49
1:C:283:LYS:HB3	1:C:284:PRO:HD3	1.93	0.49
1:C:167:GLU:O	1:C:171:MET:HG3	2.13	0.49
1:C:571:ASP:OD1	1:C:571:ASP:N	2.38	0.49
1:E:544:HIS:HE1	1:E:546:ARG:HG2	1.76	0.49
1:C:100:HIS:O	1:C:104:MET:HG2	2.13	0.48
1:C:259:TYR:CB	1:C:265:LEU:HD23	2.39	0.48
1:E:544:HIS:CE1	1:E:546:ARG:HG2	2.47	0.48
1:C:110:PRO:HB3	1:C:152:GLN:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASP:HB3	1:C:94:VAL:HG12	1.95	0.48
1:A:147:SER:O	1:A:151:GLU:HG2	2.13	0.48
1:C:479:ILE:O	1:C:483:GLU:HG2	2.13	0.48
1:E:147:SER:O	1:E:151:GLU:HG2	2.13	0.48
1:E:188:ARG:CZ	1:E:192:MET:HE1	2.44	0.47
1:A:557:ARG:NH1	1:A:558:GLU:OE2	2.47	0.47
1:A:565:GLN:HA	1:A:568:LYS:HD3	1.96	0.47
1:C:283:LYS:HG3	1:C:318:LEU:HD23	1.96	0.47
1:E:554:VAL:HG22	1:E:557:ARG:HH21	1.79	0.47
1:C:460:GLN:HG2	1:C:466:THR:HG22	1.96	0.47
1:E:181:HIS:CE1	1:E:221:LEU:HD22	2.50	0.47
1:A:198:ARG:O	1:A:202:ARG:HG3	2.15	0.47
1:C:260:SER:HB2	4:C:812:HOH:O	2.14	0.47
1:A:381:ILE:HG23	1:A:391:THR:HG22	1.96	0.46
1:C:279:CYS:HB3	1:C:282:ASN:HB2	1.97	0.46
1:C:517:ALA:HA	1:C:569:ARG:NH2	2.29	0.46
1:A:135:ASN:HD22	1:A:138:VAL:HG23	1.80	0.46
1:A:167:GLU:O	1:A:171:MET:HG3	2.15	0.46
1:C:331:LEU:O	1:C:335:LEU:HG	2.16	0.46
1:E:425:LEU:HD22	1:E:470:LEU:HD12	1.97	0.46
1:A:563:LEU:HD23	1:A:566:LEU:HD12	1.98	0.46
1:C:368:VAL:HG13	1:C:373:GLY:HA3	1.98	0.46
1:A:542:LEU:HD13	1:A:559:ILE:HG21	1.98	0.46
1:A:213:HIS:ND1	1:A:216:LYS:HE2	2.31	0.46
1:E:157:LEU:O	1:E:161:ARG:HG2	2.16	0.46
1:E:342:ALA:O	1:E:383:ARG:NH2	2.41	0.45
1:E:567:SER:O	1:E:606:ASN:HB3	2.16	0.45
1:A:166:ALA:HA	1:A:204:LEU:HD13	1.98	0.45
1:C:83:LEU:HG	1:C:87:MET:HE3	1.98	0.45
1:C:292:LEU:HB2	1:C:293:PRO:HD3	1.98	0.45
1:E:167:GLU:O	1:E:171:MET:HG3	2.17	0.45
1:C:535:LEU:HB3	1:C:579:THR:HG21	1.99	0.45
1:E:214:LEU:HB3	1:E:251:ILE:HG21	1.97	0.45
1:C:171:MET:HE2	1:C:179:VAL:HG13	1.99	0.45
1:C:277:SER:O	1:C:283:LYS:HE2	2.17	0.44
1:A:485:ASN:HA	1:A:486:PRO:HD3	1.73	0.44
1:A:496:TRP:NE1	1:A:546:ARG:HD3	2.32	0.44
1:C:319:SER:HB3	1:C:353:THR:HG23	2.00	0.44
2:D:1147:ARG:HB3	2:D:1200:GLU:HB3	1.98	0.44
1:E:279:CYS:HA	1:E:280:PRO:HD3	1.90	0.44
1:A:544:HIS:HA	1:A:545:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:HIS:CD2	1:C:121:ARG:HG3	2.54	0.43
1:C:436:ILE:HG23	1:C:474:ILE:HD13	2.00	0.43
1:E:171:MET:HE2	1:E:179:VAL:HG13	2.00	0.43
1:A:468:VAL:HG21	1:A:515:VAL:HG22	2.01	0.43
1:C:198:ARG:O	1:C:202:ARG:HG3	2.19	0.43
1:A:120:HIS:HB3	1:A:158:LEU:HD13	2.01	0.42
1:C:465:HIS:HB3	1:C:470:LEU:HG	2.00	0.42
1:E:176:LEU:HD23	1:E:176:LEU:HA	1.82	0.42
1:A:237:ALA:O	1:A:241:ILE:HG12	2.18	0.42
1:A:482:ILE:HA	1:A:485:ASN:O	2.19	0.42
1:E:570:PRO:O	1:E:574:ARG:HG3	2.19	0.42
1:E:149:MET:HE3	1:E:149:MET:HB2	1.90	0.42
1:E:506:LEU:HD13	1:E:534:PHE:HZ	1.83	0.42
1:A:283:LYS:HG3	1:A:318:LEU:HD23	2.00	0.42
1:C:352:GLY:HA2	1:C:393:PRO:HB3	2.02	0.42
1:E:383:ARG:C	1:E:385:PRO:HD3	2.45	0.42
1:C:444:ARG:HH21	1:C:448:LEU:HD11	1.83	0.42
1:E:543:ALA:HB2	1:E:584:LEU:HD11	2.02	0.42
1:A:330:GLN:HG3	1:C:245:SER:HB2	2.01	0.42
1:A:436:ILE:HG23	1:A:474:ILE:HD13	2.01	0.42
1:A:598:THR:HG21	2:B:1185:LYS:HB3	2.01	0.42
2:B:1148:LYS:HA	2:B:1149:PRO:HD2	1.87	0.42
1:E:482:ILE:HD12	1:E:496:TRP:CZ2	2.55	0.42
1:A:603:VAL:O	1:A:607:LEU:HG	2.20	0.42
1:C:392:GLU:HB3	1:C:393:PRO:HD3	2.01	0.41
1:E:368:VAL:HG13	1:E:373:GLY:HA3	2.03	0.41
1:E:544:HIS:HA	1:E:545:PRO:HD3	1.95	0.41
1:A:170:ARG:HG2	1:A:170:ARG:HH11	1.85	0.41
1:A:479:ILE:O	1:A:483:GLU:HG2	2.20	0.41
1:C:439:ALA:O	1:C:443:ILE:HG13	2.21	0.41
2:D:1207:GLU:HA	4:D:1302:HOH:O	2.21	0.41
2:F:1183:ASN:OD1	2:F:1186:ILE:HB	2.21	0.41
1:E:221:LEU:HB2	2:F:1219:ILE:CD1	2.51	0.41
1:A:392:GLU:HB3	1:A:393:PRO:HD3	2.03	0.41
1:E:485:ASN:HB3	1:E:488:ILE:HB	2.03	0.41
1:E:217:THR:O	1:E:219:PRO:HD3	2.22	0.40
1:E:449:LEU:HD23	1:E:449:LEU:HA	1.93	0.40
1:C:535:LEU:HD23	1:C:535:LEU:HA	1.89	0.40
2:F:1202:ARG:HG2	2:F:1204:TYR:CZ	2.56	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	532/572 (93%)	523 (98%)	9 (2%)	0	100	100
1	C	534/572 (93%)	525 (98%)	9 (2%)	0	100	100
1	E	502/572 (88%)	495 (99%)	7 (1%)	0	100	100
2	B	38/84 (45%)	32 (84%)	6 (16%)	0	100	100
2	D	38/84 (45%)	37 (97%)	1 (3%)	0	100	100
2	F	30/84 (36%)	29 (97%)	1 (3%)	0	100	100
All	All	1674/1968 (85%)	1641 (98%)	33 (2%)	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	449/483 (93%)	446 (99%)	3 (1%)	76	90
1	C	452/483 (94%)	448 (99%)	4 (1%)	70	87
1	E	430/483 (89%)	417 (97%)	13 (3%)	36	69
2	B	39/66 (59%)	39 (100%)	0	100	100
2	D	38/66 (58%)	38 (100%)	0	100	100
2	F	31/66 (47%)	31 (100%)	0	100	100
All	All	1439/1647 (87%)	1419 (99%)	20 (1%)	59	82

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ARG
1	A	443	ILE
1	A	595	SER
1	C	323	THR
1	C	392	GLU
1	C	444	ARG
1	C	571	ASP
1	E	136	VAL
1	E	176	LEU
1	E	187	LEU
1	E	196	ASP
1	E	265	LEU
1	E	292	LEU
1	E	299	LEU
1	E	339	ILE
1	E	392	GLU
1	E	456	LEU
1	E	495	MET
1	E	555	LEU
1	E	566	LEU

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	135	ASN
1	A	250	GLN
1	A	282	ASN
2	B	1193	GLN
2	B	1210	ASN
1	C	224	GLN
2	D	1194	ASN
1	E	141	ASN
1	E	193	HIS
1	E	427	GLN
1	E	565	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	B	1212	2	8,9,10	1.64	1 (12%)	7,12,14	1.67	1 (14%)
2	TPO	F	1215	2	8,10,11	1.20	0	10,14,16	1.76	2 (20%)
2	SEP	F	1218	2	8,9,10	1.62	1 (12%)	7,12,14	1.34	1 (14%)
2	SEP	D	1212	2	8,9,10	1.61	1 (12%)	7,12,14	1.13	1 (14%)
2	SEP	F	1221	2	8,9,10	1.63	1 (12%)	7,12,14	1.47	1 (14%)
2	SEP	F	1212	2	8,9,10	1.61	1 (12%)	7,12,14	1.57	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	1212	2	-	1/6/8/10	-
2	TPO	F	1215	2	-	2/9/11/13	-
2	SEP	F	1218	2	-	4/6/8/10	-
2	SEP	D	1212	2	-	2/6/8/10	-
2	SEP	F	1221	2	-	2/6/8/10	-
2	SEP	F	1212	2	-	3/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1221	SEP	P-O1P	3.59	1.61	1.50
2	F	1218	SEP	P-O1P	3.56	1.61	1.50
2	B	1212	SEP	P-O1P	3.54	1.61	1.50
2	F	1212	SEP	P-O1P	3.51	1.61	1.50
2	D	1212	SEP	P-O1P	3.47	1.61	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1215	TPO	P-OG1-CB	-3.90	112.72	123.33
2	B	1212	SEP	OG-CB-CA	3.81	111.85	108.14
2	F	1212	SEP	OG-CB-CA	3.72	111.76	108.14
2	F	1221	SEP	OG-CB-CA	3.37	111.43	108.14
2	F	1215	TPO	CG2-CB-CA	-3.13	107.16	113.26
2	F	1218	SEP	OG-CB-CA	3.02	111.08	108.14
2	D	1212	SEP	OG-CB-CA	2.41	110.49	108.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1212	SEP	CB-OG-P-O1P
2	F	1212	SEP	CB-OG-P-O2P
2	F	1218	SEP	CB-OG-P-O1P
2	F	1218	SEP	CB-OG-P-O2P
2	F	1218	SEP	CB-OG-P-O3P
2	F	1221	SEP	CB-OG-P-O1P
2	D	1212	SEP	CB-OG-P-O3P
2	F	1215	TPO	CG2-CB-OG1-P
2	B	1212	SEP	N-CA-CB-OG
2	D	1212	SEP	N-CA-CB-OG
2	F	1218	SEP	N-CA-CB-OG
2	F	1215	TPO	CB-OG1-P-O1P
2	F	1212	SEP	CB-OG-P-O3P
2	F	1221	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1212	SEP	1	0
2	F	1221	SEP	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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	534/572 (93%)	-0.02	16 (2%) 52 45	39, 68, 124, 175	0
1	C	536/572 (93%)	-0.21	7 (1%) 75 69	37, 58, 108, 189	0
1	E	508/572 (88%)	0.46	36 (7%) 22 17	38, 90, 177, 250	0
2	B	42/84 (50%)	0.73	3 (7%) 22 17	57, 106, 149, 169	0
2	D	41/84 (48%)	0.74	5 (12%) 8 7	52, 99, 134, 171	0
2	F	34/84 (40%)	1.31	6 (17%) 4 3	63, 104, 130, 144	0
All	All	1695/1968 (86%)	0.13	73 (4%) 40 33	37, 69, 148, 250	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1182	LEU	5.1
1	A	86	LEU	4.2
1	E	106	SER	4.1
1	A	614	ALA	4.0
2	F	1205	ASP	4.0
1	A	81	PRO	3.8
2	F	1211	ILE	3.7
2	D	1145	GLY	3.5
1	E	131	SER	3.5
2	B	1213	VAL	3.5
1	A	97	ARG	3.4
1	E	124	VAL	3.4
1	E	83	LEU	3.4
1	E	127	LEU	3.3
2	F	1184	SER	3.3
1	E	86	LEU	3.2
1	E	123	PHE	3.2
1	E	120	HIS	3.1
1	A	87	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	166	ALA	3.0
1	A	526	VAL	3.0
1	E	576	VAL	3.0
1	E	165	LEU	2.9
1	E	133	SER	2.9
1	E	105	LEU	2.9
1	C	120	HIS	2.9
1	E	122	SER	2.8
2	B	1211	ILE	2.7
2	F	1207	GLU	2.7
1	E	94	VAL	2.7
1	E	107	ARG	2.7
1	A	158	LEU	2.6
1	E	134	SER	2.6
1	E	149	MET	2.6
1	E	541	LEU	2.6
1	E	536	ASP	2.5
1	A	586	MET	2.5
1	E	104	MET	2.5
1	A	550	MET	2.4
1	E	465	HIS	2.4
1	C	116	PRO	2.4
1	A	162	SER	2.4
2	F	1183	ASN	2.4
1	C	108	GLU	2.4
1	E	103	TYR	2.3
1	E	176	LEU	2.3
2	D	1210	ASN	2.3
1	C	117	GLY	2.3
1	A	83	LEU	2.3
2	D	1179	ASP	2.3
1	A	548	GLY	2.3
1	E	130	ALA	2.2
1	E	450	GLN	2.2
1	E	136	VAL	2.2
1	E	224	GLN	2.2
1	C	431	LEU	2.2
1	E	158	LEU	2.2
1	E	126	ALA	2.2
1	E	462	ALA	2.2
1	E	138	VAL	2.2
2	B	1208	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	87	MET	2.1
1	E	171	MET	2.1
1	A	120	HIS	2.1
1	A	88	CYS	2.1
1	E	154	GLY	2.1
1	E	169	ILE	2.0
2	D	1211	ILE	2.0
1	C	417	PHE	2.0
1	A	323	THR	2.0
1	A	200	GLN	2.0
1	C	78	LEU	2.0
2	D	1193	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	TPO	F	1215	11/12	0.68	0.12	84,110,134,143	0
2	SEP	F	1218	10/11	0.73	0.10	78,145,164,172	0
2	SEP	F	1221	10/11	0.78	0.08	75,125,131,189	0
2	SEP	D	1212	10/11	0.80	0.11	59,118,131,172	0
2	SEP	B	1212	10/11	0.83	0.10	102,128,133,134	0
2	SEP	F	1212	10/11	0.90	0.10	63,104,116,140	0

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
3	IOD	A	704	1/1	0.94	0.15	142,142,142,142	0
3	IOD	C	704	1/1	0.95	0.07	94,94,94,94	0
3	IOD	A	703	1/1	0.96	0.14	138,138,138,138	0
3	IOD	C	702	1/1	0.97	0.19	131,131,131,131	0
3	IOD	A	702	1/1	0.97	0.10	107,107,107,107	0
3	IOD	C	701	1/1	0.98	0.06	109,109,109,109	0
3	IOD	C	703	1/1	0.99	0.04	92,92,92,92	0
3	IOD	A	701	1/1	0.99	0.04	89,89,89,89	0
3	IOD	E	701	1/1	0.99	0.05	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.