Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:10 PM GMT

PDB ID	:	4R11
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

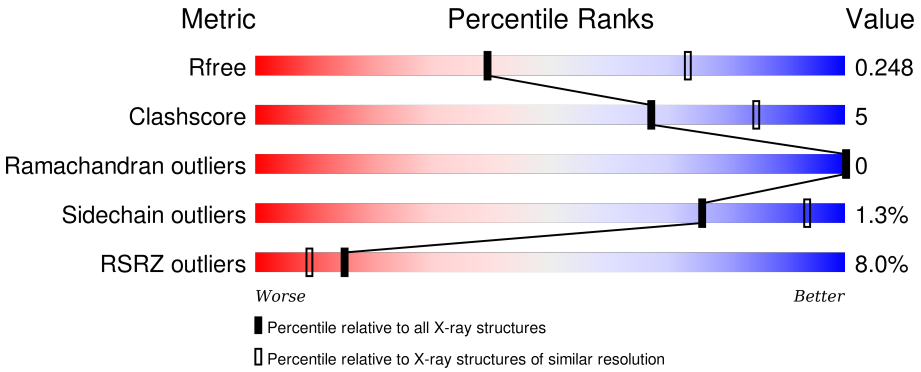
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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% 81% 12% 7%
1	C	572	% 81% 12% 6%
1	E	572	14% 76% 12% • 11%
2	B	84	17% 43% 8% 49%
2	D	84	8% 44% 6% 50%

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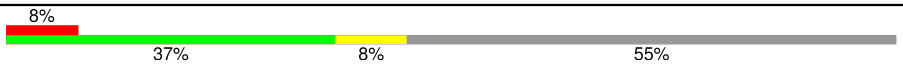
Mol	Chain	Length	Quality of chain
2	F	84	

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	0
			355	215	61	77	1	1			
2	D	42	Total	C	N	O	P	S	0	0	0
			348	210	60	76	1	1			
2	F	38	Total	C	N	O	P		0	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 (three-letter code: 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.

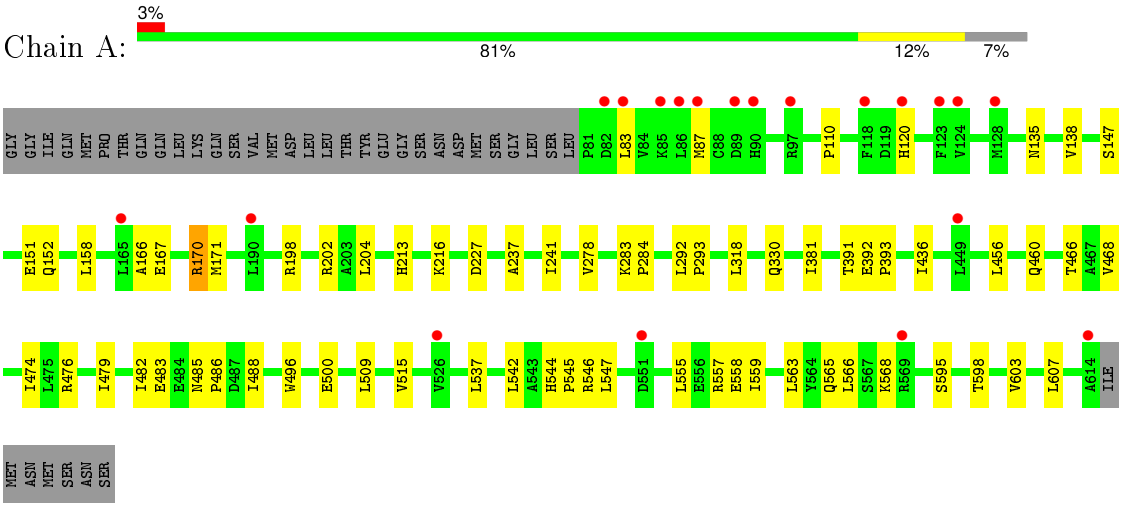
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	2	Total O 2 2	0	0
4	C	22	Total O 22 22	0	0
4	D	4	Total O 4 4	0	0
4	E	11	Total O 11 11	0	0
4	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

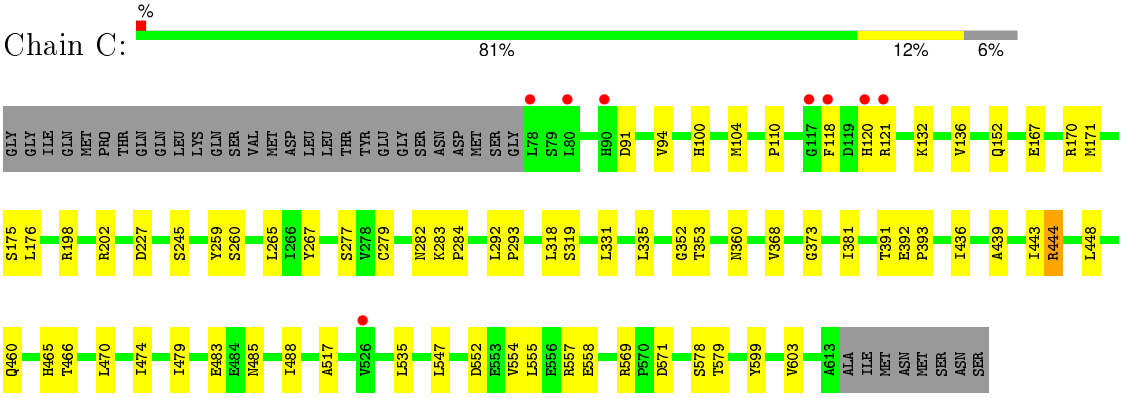
- Molecule 1: Protein humpback-2

Chain A:



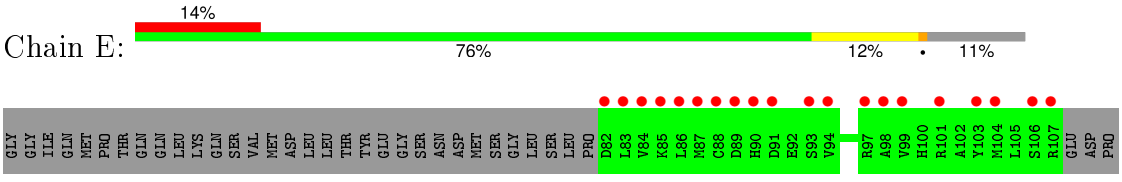
- Molecule 1: Protein humpback-2

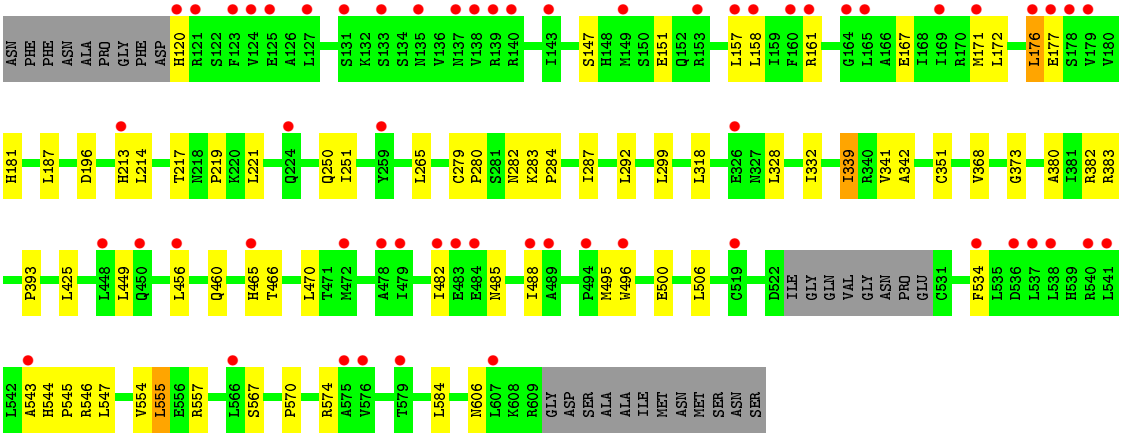
Chain C:



- Molecule 1: Protein humpback-2

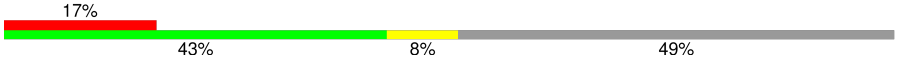
Chain E:

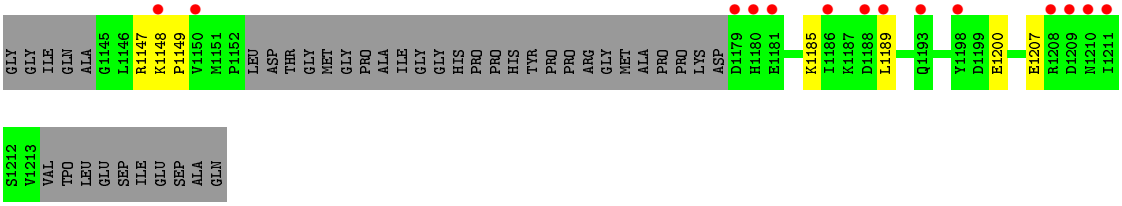




• Molecule 2: Cadherin-related hmr-1

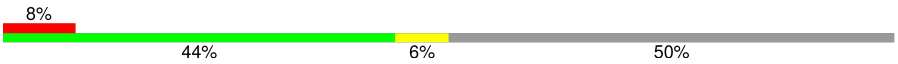
Chain B:





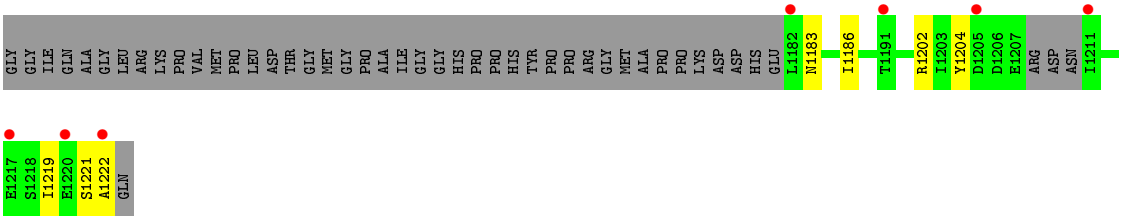
• Molecule 2: Cadherin-related hmr-1

Chain D:



• Molecule 2: Cadherin-related hmr-1

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.20 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.199 , 0.249 0.200 , 0.248	Depositor DCC
R_{free} test set	4260 reflections (7.78%)	DCC
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 , 49.2	EDS
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 54770 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, IOD, SEP

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	0.22	0/4131	0.41	0/5611
1	C	0.25	0/4148	0.43	0/5635
1	E	0.23	0/3934	0.41	0/5338
2	B	0.23	0/348	0.41	0/467
2	D	0.25	0/342	0.38	0/460
2	F	0.24	0/273	0.41	0/362
All	All	0.23	0/13176	0.42	0/17873

There are no bond length outliers.

There are no bond angle outliers.

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	44	0
1	E	3882	0	3985	41	0
2	B	355	0	332	5	0
2	D	348	0	323	4	0
2	F	317	0	281	4	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	13232	126	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 (126) 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:C:381:ILE:HG23	1:C:391:THR:HG22	1.77	0.65
1:A:485:ASN:HB3	1:A:488:ILE:HB	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: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
1:C:118:PHE:HE2	1:C:120:HIS:HA	1.67	0.60
1:A:83:LEU:HG	1:A:87:MET:HE3	1.85	0.59
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:E:547:LEU:HD13	1:E:555:LEU:HD12	1.87	0.56
1:A:476:ARG:HG2	1:A:537:LEU:HD21	1.86	0.56
2:F:1221:SEP:HA	2:F:1222:ALA:HB3	1.88	0.55
1:C:599:TYR:O	1:C:603:VAL:HG23	2.05	0.55
1:A:460:GLN:HG2	1:A:466:THR:HG22	1.88	0.55
1:A:292:LEU:HB2	1:A:293:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:571:ASP:OD1	1:C:571:ASP:N	2.38	0.49
1:C:167:GLU:O	1:C:171:MET:HG3	2.13	0.49
1:E:544:HIS:HE1	1:E:546:ARG:HG2	1.76	0.49
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:100:HIS:O	1:C:104:MET:HG2	2.13	0.48
1:C:91:ASP:HB3	1:C:94:VAL:HG12	1.95	0.48
1:C:479:ILE:O	1:C:483:GLU:HG2	2.13	0.48
1:A:147:SER:O	1:A:151:GLU:HG2	2.13	0.48
1:E:147:SER:O	1:E:151:GLU:HG2	2.13	0.48
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: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: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:C:260:SER:HB2	4:C:812:HOH:O	2.14	0.47
1:A:198:ARG:O	1:A:202:ARG:HG3	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:425:LEU:HD22	1:E:470:LEU:HD12	1.97	0.46
1:C:331:LEU:O	1:C:335:LEU:HG	2.16	0.46
1:C:368:VAL:HG13	1:C:373:GLY:HA3	1.98	0.46
1:A:563:LEU:HD23	1:A:566:LEU:HD12	1.98	0.46
1:A:542:LEU:HD13	1:A:559:ILE:HG21	1.98	0.46
1:E:157:LEU:O	1:E:161:ARG:HG2	2.16	0.46
1:A:213:HIS:ND1	1:A:216:LYS:HE2	2.31	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: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:E:214:LEU:HB3	1:E:251:ILE:HG21	1.97	0.45
1:C:535:LEU:HB3	1:C:579:THR:HG21	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:C:110:PRO:HB3	1:C:152:GLN:CD	2.38	0.44
1:C:120:HIS:CD2	1:C:121:ARG:HG3	2.54	0.43
1:A:544:HIS:HA	1:A:545:PRO:HD3	1.89	0.43
1:C:436:ILE:HG23	1:C:474:ILE:HD13	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:E:176:LEU:HA	1:E:176:LEU:HD23	1.82	0.42
1:C:465:HIS:HB3	1:C:470:LEU:HG	2.00	0.42
1:A:120:HIS:HB3	1:A:158:LEU:HD13	2.01	0.42
1:A:482:ILE:HA	1:A:485:ASN:O	2.19	0.42
1:A:237:ALA:O	1:A:241:ILE:HG12	2.18	0.42
1:E:570:PRO:O	1:E:574:ARG:HG3	2.19	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: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:598:THR:HG21	2:B:1185:LYS:HB3	2.01	0.42
1:A:330:GLN:HG3	1:C:245:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:436:ILE:HG23	1:A:474:ILE:HD13	2.01	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:HH11	1:A:170:ARG:HG2	1.85	0.41
2:D:1207:GLU:HA	4:D:1302:HOH:O	2.21	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: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:E:485:ASN:HB3	1:E:488:ILE:HB	2.03	0.41
1:A:392:GLU:HB3	1:A:393:PRO:HD3	2.03	0.41
1:E:449:LEU:HD23	1:E:449:LEU:HA	1.93	0.40
1:E:217:THR:O	1:E:219:PRO:HD3	2.22	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 (i)

5.3.1 Protein backbone (i)

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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 (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	449/483 (93%)	445 (99%)	4 (1%)	84 96
1	C	452/483 (94%)	448 (99%)	4 (1%)	84 96
1	E	430/483 (89%)	420 (98%)	10 (2%)	58 87
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%)	1421 (99%)	18 (1%)	76 93

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

Mol	Chain	Res	Type
1	A	170	ARG
1	A	227	ASP
1	A	500	GLU
1	A	595	SER
1	C	227	ASP
1	C	444	ARG
1	C	552	ASP
1	C	578	SER
1	E	176	LEU
1	E	187	LEU
1	E	196	ASP
1	E	265	LEU
1	E	292	LEU

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Mol	Chain	Res	Type
1	E	299	LEU
1	E	339	ILE
1	E	456	LEU
1	E	495	MET
1	E	555	LEU

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	135	ASN
2	B	1210	ASN
1	E	141	ASN

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	1.53	1 (12%)	8,12,14	1.77	1 (12%)
2	SEP	D	1212	2	8,9,10	1.51	1 (12%)	8,12,14	1.21	1 (12%)
2	SEP	F	1212	2	8,9,10	1.51	1 (12%)	8,12,14	1.70	1 (12%)
2	TPO	F	1215	2	8,10,11	1.13	0	7,14,16	1.41	1 (14%)
2	SEP	F	1218	2	8,9,10	1.53	1 (12%)	8,12,14	1.45	1 (12%)
2	SEP	F	1221	2	8,9,10	1.53	1 (12%)	8,12,14	1.73	2 (25%)

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	-	0/6/8/10	0/0/0/0
2	SEP	D	1212	2	-	0/6/8/10	0/0/0/0
2	SEP	F	1212	2	-	0/6/8/10	0/0/0/0
2	TPO	F	1215	2	-	0/8/11/13	0/0/0/0
2	SEP	F	1218	2	-	0/6/8/10	0/0/0/0
2	SEP	F	1221	2	-	0/6/8/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1212	SEP	P-O1P	3.07	1.61	1.51
2	F	1212	SEP	P-O1P	3.11	1.61	1.51
2	B	1212	SEP	P-O1P	3.14	1.61	1.51
2	F	1218	SEP	P-O1P	3.16	1.61	1.51
2	F	1221	SEP	P-O1P	3.18	1.61	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1215	TPO	CG2-CB-CA	-2.95	107.16	113.17
2	F	1221	SEP	O-C-CA	-2.65	118.58	125.49
2	D	1212	SEP	OG-CB-CA	2.60	110.49	108.27
2	F	1218	SEP	OG-CB-CA	3.29	111.08	108.27
2	F	1221	SEP	OG-CB-CA	3.70	111.43	108.27
2	F	1212	SEP	OG-CB-CA	4.09	111.76	108.27
2	B	1212	SEP	OG-CB-CA	4.20	111.85	108.27

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates 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, 95^{th} 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%)	0.30	20 (3%) 45 37	39, 68, 124, 175	0
1	C	536/572 (93%)	0.16	8 (1%) 76 71	37, 58, 108, 189	0
1	E	508/572 (88%)	0.83	79 (15%) 3 2	38, 90, 177, 250	0
2	B	42/84 (50%)	1.50	14 (33%) 0 0	57, 106, 149, 169	0
2	D	41/84 (48%)	0.89	7 (17%) 2 1	52, 99, 135, 171	0
2	F	34/84 (40%)	1.26	7 (20%) 1 1	63, 104, 130, 144	0
All	All	1695/1968 (86%)	0.48	135 (7%) 15 9	37, 69, 148, 250	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	MET	10.4
1	E	83	LEU	7.7
1	E	107	ARG	7.1
1	E	87	MET	6.9
2	F	1205	ASP	6.7
1	A	86	LEU	6.5
1	E	84	VAL	6.4
1	E	124	VAL	6.3
2	B	1211	ILE	6.2
2	D	1180	HIS	6.1
1	C	78	LEU	6.1
1	E	106	SER	5.9
1	E	131	SER	5.8
1	E	120	HIS	5.6
1	E	91	ASP	5.6
1	E	94	VAL	5.5
1	E	138	VAL	5.5
1	E	82	ASP	5.4
2	F	1222	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	137	ASN	5.2
1	A	90	HIS	5.2
1	E	123	PHE	5.1
1	E	178	SER	5.1
2	B	1180	HIS	4.7
1	E	536	ASP	4.6
1	E	97	ARG	4.6
1	E	158	LEU	4.5
1	A	85	LYS	4.5
1	E	161	ARG	4.3
1	E	176	LEU	4.3
1	E	541	LEU	4.2
1	E	121	ARG	4.2
2	B	1208	ARG	4.1
1	E	86	LEU	4.1
2	D	1208	ARG	4.0
1	E	171	MET	4.0
1	E	99	VAL	4.0
1	E	93	SER	4.0
1	E	179	VAL	4.0
1	E	90	HIS	3.9
1	E	89	ASP	3.9
1	E	98	ALA	3.9
1	E	101	ARG	3.9
1	C	118	PHE	3.6
1	E	576	VAL	3.5
1	E	127	LEU	3.4
2	B	1189	LEU	3.4
2	F	1191	THR	3.4
2	F	1211	ILE	3.3
1	E	85	LYS	3.3
2	B	1188	ASP	3.3
1	C	121	ARG	3.2
1	E	165	LEU	3.2
1	E	133	SER	3.2
2	F	1217	GLU	3.1
1	E	489	ALA	3.1
1	E	482	ILE	3.1
1	C	526	VAL	3.1
1	E	143	ILE	3.1
1	E	534	PHE	3.1
1	E	575	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	124	VAL	3.0
1	E	125	GLU	3.0
1	E	103	TYR	3.0
1	E	607	LEU	3.0
1	E	139	ARG	3.0
1	A	89	ASP	2.9
1	A	83	LEU	2.9
1	C	90	HIS	2.9
1	E	224	GLN	2.9
2	B	1150	VAL	2.9
1	E	483	GLU	2.9
2	B	1181	GLU	2.9
1	A	118	PHE	2.8
1	E	213	HIS	2.8
2	B	1209	ASP	2.8
1	E	543	ALA	2.8
2	B	1210	ASN	2.8
2	B	1179	ASP	2.7
1	E	488	ILE	2.7
1	A	551	ASP	2.6
1	A	449	LEU	2.6
2	B	1148	LYS	2.6
1	E	169	ILE	2.6
1	A	123	PHE	2.6
2	F	1220	GLU	2.6
1	E	149	MET	2.6
1	E	537	LEU	2.6
2	B	1198	TYR	2.6
2	D	1211	ILE	2.6
1	E	478	ALA	2.5
1	E	538	LEU	2.5
1	A	165	LEU	2.5
1	E	177	GLU	2.5
1	E	465	HIS	2.5
1	E	164	GLY	2.5
1	E	160	PHE	2.5
1	C	117	GLY	2.5
1	E	135	ASN	2.5
1	E	494	PRO	2.5
1	A	120	HIS	2.5
1	C	120	HIS	2.5
1	E	484	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	579	THR	2.5
1	E	326	GLU	2.4
1	E	88	CYS	2.4
1	A	614	ALA	2.4
1	E	456	LEU	2.4
1	C	80	LEU	2.4
1	E	472	MET	2.4
1	A	82	ASP	2.4
1	A	190	LEU	2.3
1	E	157	LEU	2.3
1	A	97	ARG	2.3
2	B	1193	GLN	2.3
1	E	104	MET	2.3
1	E	540	ARG	2.2
2	D	1181	GLU	2.2
1	A	569	ARG	2.2
1	E	153	ARG	2.2
1	E	479	ILE	2.2
1	E	566	LEU	2.1
2	D	1209	ASP	2.1
1	A	128	MET	2.1
2	F	1182	LEU	2.1
1	E	140	ARG	2.1
1	E	450	GLN	2.1
1	E	519	CYS	2.1
2	B	1186	ILE	2.1
1	E	259	TYR	2.1
1	E	496	TRP	2.0
1	A	526	VAL	2.0
2	D	1187	LYS	2.0
2	D	1145	GLY	2.0
1	E	448	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SEP	F	1212	10/11	0.95	0.15	-	63,104,116,140	0
2	SEP	D	1212	10/11	0.88	0.21	-	59,118,131,172	0
2	TPO	F	1215	11/12	0.86	0.15	-	84,110,134,143	0
2	SEP	F	1221	10/11	0.80	0.15	-	75,125,131,189	0
2	SEP	F	1218	10/11	0.71	0.19	-	78,145,164,172	0
2	SEP	B	1212	10/11	0.87	0.16	-	102,128,133,134	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	IOD	C	703	1/1	0.99	0.19	-1.22	92,92,92,92	0
3	IOD	A	701	1/1	0.98	0.12	-1.27	89,89,89,89	0
3	IOD	E	701	1/1	0.99	0.14	-1.41	94,94,94,94	0
3	IOD	C	701	1/1	0.98	0.08	-1.75	109,109,109,109	0
3	IOD	C	704	1/1	0.97	0.09	-1.86	94,94,94,94	0
3	IOD	A	704	1/1	0.97	0.07	-1.90	142,142,142,142	0
3	IOD	C	702	1/1	0.98	0.06	-4.12	131,131,131,131	0
3	IOD	A	703	1/1	0.99	0.07	-4.71	138,138,138,138	0
3	IOD	A	702	1/1	0.95	0.10	-	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.