wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:09 PM BST

PDB ID	:	5A9K
EMDB ID:	:	EMD-3087
Title	:	Structural basis for DNA strand separation by a hexameric replicative helicase
Authors	:	Chaban, Y.; Stead, J.A.; Ryzhenkova, K.; Whelan, F.; Lamber, K.; Antson, F.; Sanders, C.M.; Orlova, E.V.
Deposited on	:	2015-07-21
Resolution	:	19.00 Å(reported)
Based on PDB ID	:	2V9P

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

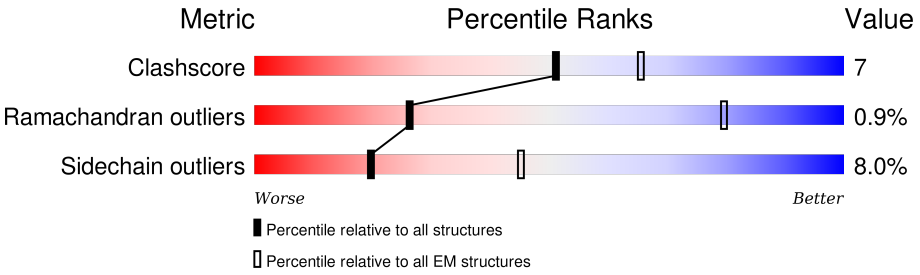
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 19.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	305	69% 19% • 11%
1	B	305	71% 14% • 12%
1	C	305	70% 16% • 12%
1	D	305	73% 14% • 10%
1	E	305	68% 20% • 11%
1	F	305	64% 22% • • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1580	-	-	X	-

2 Entry composition

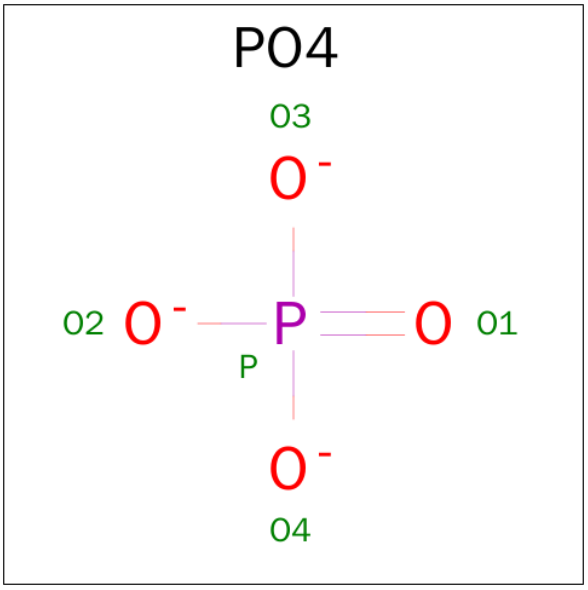
There are 4 unique types of molecules in this entry. The entry contains 13059 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 REPLICATION PROTEIN E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	272	Total	C	N	O	S	0	0
			2183	1404	375	394	10		
1	B	268	Total	C	N	O	S	0	0
			2149	1386	370	383	10		
1	C	267	Total	C	N	O	S	0	0
			2142	1382	369	381	10		
1	D	274	Total	C	N	O	S	0	0
			2191	1409	377	395	10		
1	E	270	Total	C	N	O	S	0	0
			2170	1398	373	389	10		
1	F	269	Total	C	N	O	S	0	0
			2158	1392	372	384	10		

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	O	P	0
			10	8	2	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total O P 10 8 2	0
2	B	1	Total O P 10 8 2	0
2	B	1	Total O P 10 8 2	0
2	C	1	Total O P 10 8 2	0
2	C	1	Total O P 10 8 2	0
2	D	1	Total O P 5 4 1	0
2	E	1	Total O P 5 4 1	0
2	F	1	Total O P 5 4 1	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total Mg 1 1	0
3	A	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0

- Molecule 4 is water.

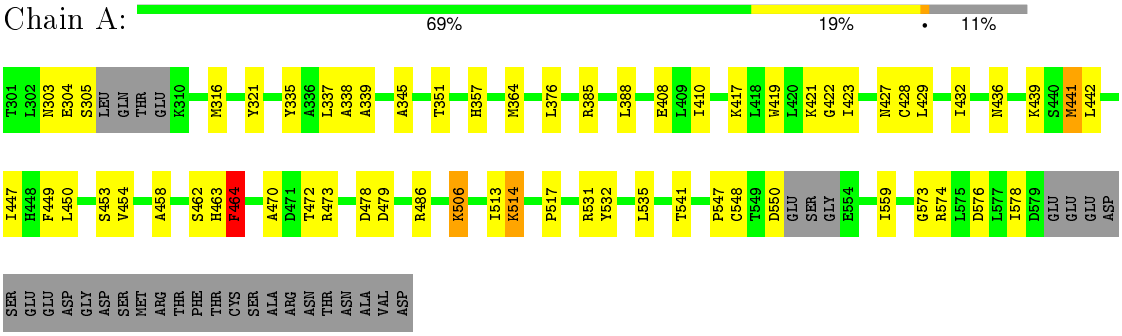
Mol	Chain	Residues	Atoms	AltConf
4	A	3	Total O 3 3	0
4	B	3	Total O 3 3	0
4	C	3	Total O 3 3	0
4	D	4	Total O 4 4	0
4	E	2	Total O 2 2	0
4	F	3	Total O 3 3	0

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. 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. 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.

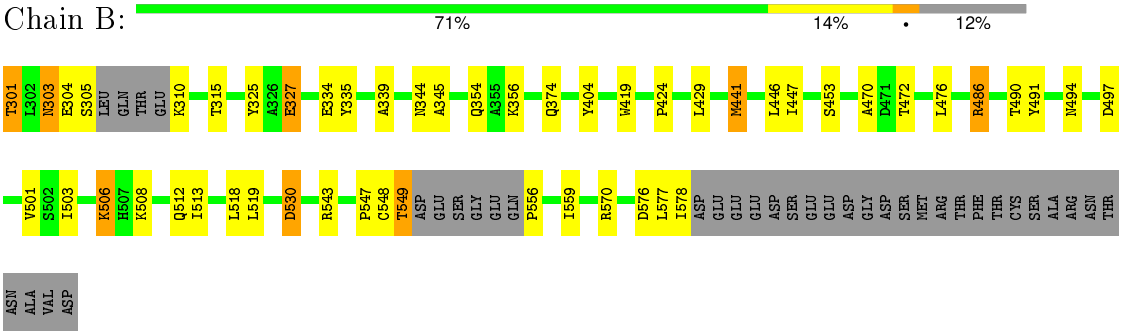
- Molecule 1: REPLICATION PROTEIN E1

Chain A:



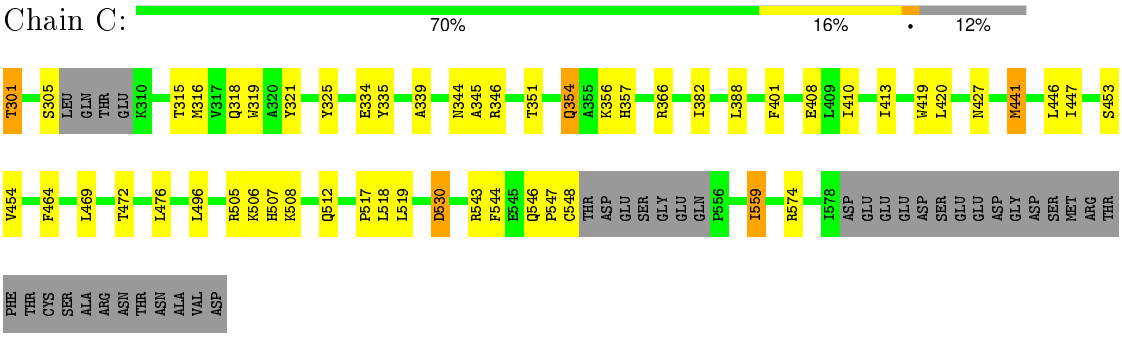
- Molecule 1: REPLICATION PROTEIN E1

Chain B:



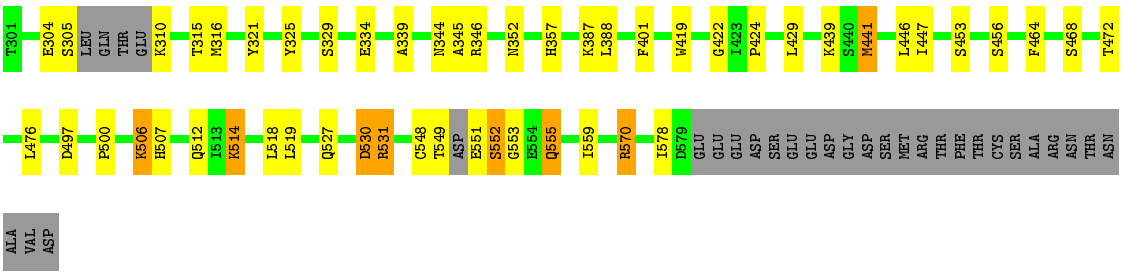
- Molecule 1: REPLICATION PROTEIN E1

Chain C:



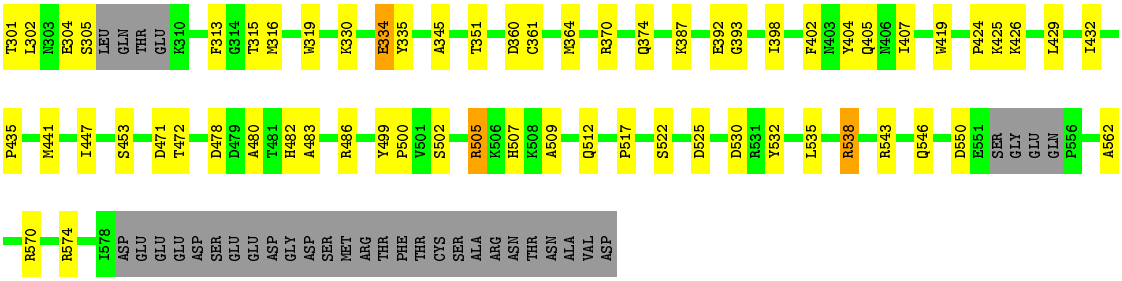
- Molecule 1: REPLICATION PROTEIN E1

Chain D:



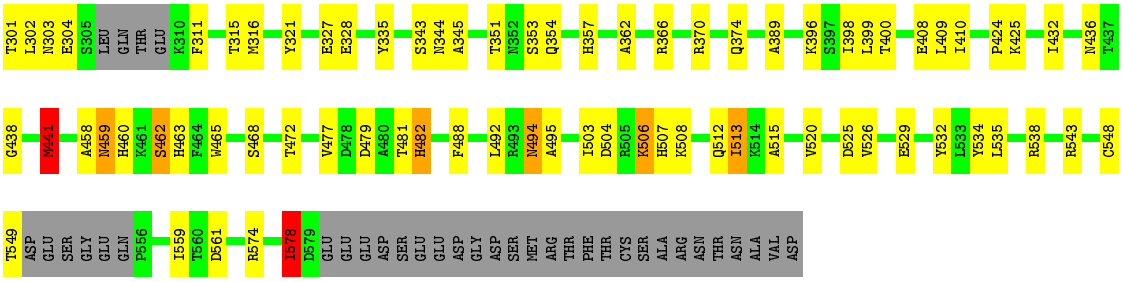
- Molecule 1: REPLICATION PROTEIN E1

Chain E:



- Molecule 1: REPLICATION PROTEIN E1

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FRAMES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	62000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.48	0/2240	0.59	0/3037
1	B	0.50	1/2206 (0.0%)	0.62	2/2990 (0.1%)
1	C	0.49	0/2199	0.61	0/2980
1	D	0.47	0/2248	0.64	4/3047 (0.1%)
1	E	0.48	0/2227	0.59	0/3017
1	F	0.49	0/2215	0.62	0/3001
All	All	0.48	1/13335 (0.0%)	0.61	6/18072 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	GLU	CD-OE1	5.96	1.32	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	486	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	486	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	531	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	570	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	531	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	570	ARG	NE-CZ-NH2	-5.46	117.57	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2183	0	2132	40	0
1	B	2149	0	2110	28	0
1	C	2142	0	2103	28	0
1	D	2191	0	2140	32	0
1	E	2170	0	2132	43	0
1	F	2158	0	2124	35	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
All	All	13059	0	12741	183	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 (183) 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:D:304:GLU:HG2	1:D:305:SER:H	1.18	1.06
1:E:453:SER:HB2	1:F:512:GLN:HE22	1.32	0.94
1:A:441:MET:HE1	1:A:559:ILE:H	1.32	0.92
1:A:304:GLU:HG2	1:A:305:SER:H	1.41	0.83
2:A:1580:PO4:O1	2:A:1581:PO4:O2	1.97	0.82
1:F:503:ILE:HD12	1:F:513:ILE:CD1	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:MET:HE3	1:C:559:ILE:H	1.51	0.74
1:A:464:PHE:HD1	1:A:464:PHE:H	1.35	0.74
1:F:370:ARG:O	1:F:374:GLN:HG2	1.88	0.73
1:A:421:LYS:HB2	1:A:423:ILE:HD12	1.71	0.71
2:B:1579:PO4:O1	2:B:1580:PO4:O2	2.09	0.71
1:A:376:LEU:O	1:A:473:ARG:NH2	2.24	0.71
1:A:458:ALA:HA	1:B:491:TYR:CD1	2.26	0.70
1:E:505:ARG:HH11	1:E:505:ARG:HB2	1.56	0.70
1:A:573:GLY:HA2	1:A:578:ILE:HD11	1.73	0.69
1:D:352:ASN:OD1	1:E:313:PHE:HB2	1.93	0.69
1:D:439:LYS:NZ	2:D:1580:PO4:O4	2.24	0.68
1:D:304:GLU:HG2	1:D:305:SER:N	1.98	0.68
1:B:303:ASN:HD22	1:C:318:GLN:HA	1.57	0.67
1:B:549:THR:HB	1:B:556:PRO:HD2	1.78	0.66
1:F:462:SER:O	1:F:465:TRP:HD1	1.81	0.63
1:F:482:HIS:ND1	1:F:532:TYR:OH	2.32	0.62
1:A:453:SER:HA	1:B:512:GLN:HE22	1.65	0.62
1:A:385:ARG:HD3	1:A:449:PHE:O	2.00	0.61
1:B:303:ASN:ND2	1:C:318:GLN:HA	2.15	0.61
1:F:503:ILE:HD12	1:F:513:ILE:HD11	1.84	0.59
1:D:507:HIS:HE1	1:E:507:HIS:O	1.85	0.59
1:F:462:SER:O	1:F:465:TRP:CD1	2.56	0.59
1:F:362:ALA:O	1:F:366:ARG:HG2	2.02	0.59
1:C:453:SER:HA	1:D:512:GLN:HE22	1.68	0.58
1:A:532:TYR:HB3	1:A:535:LEU:HD12	1.85	0.58
1:A:432:ILE:CD1	1:A:541:THR:HG23	2.34	0.58
1:E:419:TRP:CD1	1:E:429:LEU:HG	2.39	0.57
1:B:506:LYS:NZ	1:C:508:LYS:O	2.36	0.57
1:F:399:LEU:HD13	1:F:409:LEU:HD22	1.86	0.57
1:D:441:MET:HE3	1:D:559:ILE:H	1.68	0.57
1:A:316:MET:HE1	1:A:357:HIS:HB3	1.86	0.57
1:D:419:TRP:CD1	1:D:429:LEU:HG	2.40	0.56
1:D:441:MET:HA	1:E:499:TYR:OH	2.06	0.56
1:D:401:PHE:HE1	1:D:548:CYS:HG	1.52	0.56
1:E:453:SER:HB3	1:E:472:THR:HG21	1.88	0.56
1:A:464:PHE:N	1:A:464:PHE:CD1	2.73	0.55
1:A:453:SER:HB3	1:A:472:THR:HG21	1.87	0.55
1:A:304:GLU:HG2	1:A:305:SER:N	2.17	0.55
1:F:424:PRO:O	1:F:425:LYS:HB2	2.06	0.55
1:F:578:ILE:O	1:F:578:ILE:HG13	2.06	0.55
1:D:551:GLU:HG3	1:D:552:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:PHE:HA	1:F:492:LEU:HB2	1.89	0.55
1:E:478:ASP:OD2	1:F:494:ASN:ND2	2.40	0.54
1:A:432:ILE:HD12	1:A:541:THR:HG23	1.90	0.54
1:F:438:GLY:O	1:F:441:MET:HB3	2.08	0.54
1:D:304:GLU:CG	1:D:305:SER:H	2.02	0.54
1:B:447:ILE:HG13	1:B:476:LEU:HB2	1.89	0.54
1:B:453:SER:HB3	1:B:472:THR:HG21	1.90	0.54
1:C:325:TYR:CE2	1:C:334:GLU:HG2	2.43	0.54
1:F:432:ILE:HD13	1:F:525:ASP:HA	1.90	0.53
1:F:353:SER:O	1:F:357:HIS:CD2	2.60	0.53
1:B:301:THR:HG22	1:C:321:TYR:CE2	2.43	0.53
1:C:453:SER:HB3	1:C:472:THR:HG21	1.91	0.53
1:E:505:ARG:HH11	1:E:505:ARG:CB	2.22	0.53
1:A:436:ASN:O	1:A:547:PRO:HA	2.08	0.53
1:A:385:ARG:HD2	1:A:450:LEU:O	2.08	0.53
1:B:453:SER:HA	1:C:512:GLN:HE22	1.74	0.53
1:B:304:GLU:HG2	1:B:305:SER:H	1.74	0.52
1:E:319:TRP:HH2	1:E:334:GLU:HB3	1.74	0.52
1:E:425:LYS:HG2	1:E:538:ARG:HG3	1.92	0.52
1:E:505:ARG:NH1	1:E:509:ALA:O	2.44	0.51
1:A:486:ARG:NH2	1:A:531:ARG:HH11	2.09	0.51
1:D:453:SER:HB2	1:E:512:GLN:OE1	2.10	0.50
1:A:321:TYR:CE2	1:F:301:THR:HG22	2.46	0.50
1:F:389:ALA:HB1	1:F:561:ASP:HB3	1.94	0.50
1:D:315:THR:HB	1:D:344:ASN:ND2	2.28	0.49
1:C:351:THR:O	1:C:354:GLN:HG2	2.13	0.49
1:E:335:TYR:CE2	1:E:345:ALA:HA	2.48	0.49
1:A:385:ARG:HD2	1:A:450:LEU:C	2.34	0.49
1:A:419:TRP:CD1	1:A:429:LEU:HG	2.48	0.48
1:C:316:MET:HE1	1:C:357:HIS:HB3	1.94	0.48
1:D:441:MET:CE	1:D:559:ILE:H	2.26	0.48
1:E:505:ARG:HH11	1:E:505:ARG:CG	2.26	0.48
1:B:424:PRO:HA	1:B:497:ASP:O	2.14	0.48
1:A:441:MET:HE1	1:A:559:ILE:N	2.14	0.48
1:A:513:ILE:HG22	1:A:514:LYS:O	2.13	0.48
1:B:325:TYR:CE2	1:B:334:GLU:HG2	2.49	0.48
1:C:446:LEU:HD23	1:C:519:LEU:HD11	1.96	0.48
1:B:530:ASP:OD1	1:B:530:ASP:N	2.43	0.48
1:E:393:GLY:H	1:E:562:ALA:HB1	1.79	0.47
1:D:464:PHE:CE1	1:D:506:LYS:HA	2.49	0.47
1:F:311:PHE:HZ	1:F:316:MET:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ASN:HB3	1:C:496:LEU:O	2.14	0.47
1:F:503:ILE:HD12	1:F:513:ILE:HD13	1.92	0.47
1:B:304:GLU:HG3	1:C:315:THR:HA	1.97	0.47
1:A:486:ARG:HH22	1:A:531:ARG:HH11	1.62	0.47
1:C:301:THR:HG22	1:D:321:TYR:CE2	2.50	0.47
1:D:316:MET:HE1	1:D:357:HIS:HB3	1.96	0.47
1:E:532:TYR:HB3	1:E:535:LEU:HD12	1.96	0.47
1:B:315:THR:HB	1:B:344:ASN:ND2	2.30	0.47
1:E:313:PHE:CZ	1:E:360:ASP:HB3	2.49	0.47
1:C:546:GLN:HA	1:C:547:PRO:HD3	1.71	0.46
1:F:315:THR:HB	1:F:344:ASN:ND2	2.30	0.46
1:F:335:TYR:CE2	1:F:345:ALA:HA	2.51	0.46
1:E:480:ALA:HB3	1:E:522:SER:HB2	1.97	0.46
1:A:304:GLU:CG	1:A:305:SER:H	2.22	0.46
1:A:470:ALA:HA	1:A:513:ILE:HD12	1.97	0.46
1:F:351:THR:O	1:F:354:GLN:HG3	2.15	0.46
1:C:447:ILE:HG13	1:C:476:LEU:HB2	1.97	0.46
1:D:447:ILE:HG13	1:D:476:LEU:HB2	1.97	0.46
1:C:530:ASP:OD1	1:C:530:ASP:N	2.44	0.46
1:D:551:GLU:CG	1:D:552:SER:N	2.79	0.46
1:A:417:LYS:HD2	1:A:576:ASP:HB2	1.97	0.45
1:C:382:ILE:HD11	1:C:420:LEU:HD22	1.98	0.45
1:D:555:GLN:HG3	1:D:555:GLN:O	2.16	0.45
1:A:422:GLY:HA2	1:A:427:ASN:HD22	1.81	0.45
1:D:422:GLY:HA3	1:D:514:LYS:NZ	2.32	0.45
1:E:404:TYR:O	1:E:546:GLN:HG3	2.16	0.45
1:D:453:SER:HB3	1:D:472:THR:HG21	1.99	0.45
1:E:419:TRP:CE2	1:E:517:PRO:HB3	2.51	0.45
1:E:316:MET:HE3	1:E:361:CYS:HB2	1.98	0.45
1:E:301:THR:O	1:E:302:LEU:C	2.55	0.45
1:B:419:TRP:CD1	1:B:429:LEU:HG	2.52	0.45
1:E:432:ILE:HD13	1:E:525:ASP:HA	1.99	0.45
1:C:319:TRP:HH2	1:C:334:GLU:HB3	1.81	0.45
1:B:339:ALA:HA	1:B:345:ALA:HB3	1.98	0.45
1:F:463:HIS:HE1	1:F:504:ASP:OD2	2.00	0.44
1:E:402:PHE:HD1	1:E:407:ILE:HD11	1.82	0.44
1:E:301:THR:HG22	1:F:321:TYR:CZ	2.53	0.44
1:C:419:TRP:CE2	1:C:517:PRO:HB3	2.53	0.44
1:E:435:PRO:HB3	1:F:534:TYR:CE1	2.53	0.44
1:E:370:ARG:O	1:E:374:GLN:HG2	2.18	0.44
1:B:490:THR:HB	1:B:491:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LYS:HB2	1:A:423:ILE:CD1	2.44	0.44
1:C:464:PHE:CE1	1:C:506:LYS:HA	2.53	0.44
1:D:346:ARG:HB2	1:D:346:ARG:HE	1.65	0.44
1:D:530:ASP:OD1	1:D:530:ASP:N	2.49	0.44
1:C:339:ALA:HA	1:C:345:ALA:HB3	2.00	0.44
1:E:304:GLU:HB3	1:E:305:SER:H	1.65	0.44
1:C:454:VAL:HG21	1:D:500:PRO:HB2	2.00	0.43
1:F:327:GLU:O	1:F:328:GLU:C	2.56	0.43
1:E:330:LYS:O	1:E:334:GLU:HB2	2.19	0.43
1:D:339:ALA:HA	1:D:345:ALA:HB3	2.00	0.43
1:C:346:ARG:HB2	1:C:346:ARG:HE	1.50	0.43
1:E:499:TYR:HB3	1:E:500:PRO:CD	2.49	0.43
1:A:432:ILE:HD13	1:A:541:THR:HG23	2.00	0.43
1:E:447:ILE:HA	1:E:447:ILE:HD13	1.93	0.43
1:D:424:PRO:HA	1:D:497:ASP:O	2.19	0.43
1:A:464:PHE:HE2	1:A:506:LYS:HA	1.84	0.42
1:E:405:GLN:NE2	1:E:546:GLN:HB2	2.34	0.42
1:B:470:ALA:HB2	1:B:503:ILE:HG21	2.01	0.42
1:E:482:HIS:O	1:E:483:ALA:C	2.56	0.42
1:B:404:TYR:OH	1:B:547:PRO:O	2.31	0.42
1:F:534:TYR:CE2	1:F:538:ARG:CZ	3.02	0.42
1:C:410:ILE:HA	1:C:413:ILE:HD12	2.02	0.42
1:D:325:TYR:CE2	1:D:334:GLU:HG2	2.54	0.42
1:B:441:MET:CE	1:B:559:ILE:H	2.32	0.42
1:D:456:SER:HB2	1:E:502:SER:HB3	2.00	0.42
1:A:478:ASP:HB3	1:B:494:ASN:HD22	1.83	0.42
1:F:459:ASN:HB3	1:F:460:HIS:H	1.54	0.42
1:F:532:TYR:HB3	1:F:535:LEU:HD12	2.00	0.42
1:E:301:THR:HG22	1:F:321:TYR:CE2	2.54	0.42
1:C:335:TYR:OH	1:C:344:ASN:ND2	2.52	0.42
1:B:374:GLN:HE22	1:B:513:ILE:HD11	1.85	0.41
1:B:577:LEU:O	1:B:578:ILE:C	2.59	0.41
1:A:458:ALA:HB2	1:B:491:TYR:HB3	2.03	0.41
1:E:424:PRO:O	1:E:425:LYS:HB2	2.20	0.41
1:E:374:GLN:NE2	1:E:471:ASP:HA	2.35	0.41
1:F:398:ILE:HG12	1:F:559:ILE:HD12	2.02	0.41
1:D:446:LEU:HD23	1:D:519:LEU:HD11	2.02	0.41
1:F:477:VAL:HB	1:F:520:VAL:HG13	2.02	0.41
1:A:337:LEU:C	1:A:339:ALA:H	2.23	0.41
1:A:439:LYS:N	2:A:1580:PO4:O3	2.53	0.41
1:B:335:TYR:OH	1:B:344:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:ALA:HB1	1:F:515:ALA:CB	2.50	0.41
1:A:473:ARG:O	1:A:517:PRO:HD2	2.21	0.41
1:E:478:ASP:OD2	1:F:494:ASN:CG	2.60	0.41
1:D:555:GLN:HB2	1:D:555:GLN:HE21	1.66	0.41
1:E:374:GLN:HE22	1:E:471:ASP:HA	1.85	0.41
1:B:446:LEU:HD23	1:B:519:LEU:HD11	2.03	0.41
1:C:401:PHE:HE2	1:C:544:PHE:CE2	2.38	0.41
1:E:301:THR:O	1:E:301:THR:HG23	2.21	0.41
1:A:335:TYR:CE2	1:A:345:ALA:HA	2.55	0.40
1:E:453:SER:HB3	1:E:472:THR:CG2	2.50	0.40
1:A:447:ILE:HD13	1:A:447:ILE:HA	1.93	0.40
1:E:398:ILE:CG2	1:E:402:PHE:HE2	2.35	0.40
1:A:316:MET:CE	1:A:357:HIS:HB3	2.50	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 PDB entries followed by that with respect to all EM entries.

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	266/305 (87%)	244 (92%)	20 (8%)	2 (1%)	24 69
1	B	262/305 (86%)	251 (96%)	10 (4%)	1 (0%)	39 80
1	C	261/305 (86%)	252 (97%)	9 (3%)	0	100 100
1	D	268/305 (88%)	256 (96%)	8 (3%)	4 (2%)	13 57
1	E	264/305 (87%)	246 (93%)	18 (7%)	0	100 100
1	F	263/305 (86%)	239 (91%)	17 (6%)	7 (3%)	6 45
All	All	1584/1830 (87%)	1488 (94%)	82 (5%)	14 (1%)	26 67

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	506	LYS
1	D	553	GLY
1	F	479	ASP
1	F	506	LYS
1	B	576	ASP
1	D	552	SER
1	F	458	ALA
1	F	578	ILE
1	A	338	ALA
1	A	464	PHE
1	F	459	ASN
1	F	462	SER
1	F	441	MET
1	D	578	ILE

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 PDB entries followed by that with respect to all EM entries.

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	229/259 (88%)	210 (92%)	19 (8%)	14 49
1	B	225/259 (87%)	208 (92%)	17 (8%)	16 53
1	C	224/259 (86%)	207 (92%)	17 (8%)	16 53
1	D	229/259 (88%)	215 (94%)	14 (6%)	23 60
1	E	228/259 (88%)	212 (93%)	16 (7%)	19 56
1	F	226/259 (87%)	200 (88%)	26 (12%)	7 32
All	All	1361/1554 (88%)	1252 (92%)	109 (8%)	20 50

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	351	THR
1	A	364	MET
1	A	388	LEU
1	A	408	GLU

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Mol	Chain	Res	Type
1	A	410	ILE
1	A	428	CYS
1	A	441	MET
1	A	442	LEU
1	A	454	VAL
1	A	462	SER
1	A	463	HIS
1	A	464	PHE
1	A	479	ASP
1	A	506	LYS
1	A	514	LYS
1	A	548	CYS
1	A	550	ASP
1	A	574	ARG
1	B	301	THR
1	B	303	ASN
1	B	310	LYS
1	B	327	GLU
1	B	354	GLN
1	B	356	LYS
1	B	441	MET
1	B	486	ARG
1	B	501	VAL
1	B	506	LYS
1	B	508	LYS
1	B	518	LEU
1	B	530	ASP
1	B	543	ARG
1	B	548	CYS
1	B	549	THR
1	B	570	ARG
1	C	301	THR
1	C	305	SER
1	C	354	GLN
1	C	356	LYS
1	C	366	ARG
1	C	388	LEU
1	C	408	GLU
1	C	441	MET
1	C	469	LEU
1	C	505	ARG
1	C	507	HIS

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Mol	Chain	Res	Type
1	C	518	LEU
1	C	530	ASP
1	C	543	ARG
1	C	548	CYS
1	C	559	ILE
1	C	574	ARG
1	D	310	LYS
1	D	329	SER
1	D	387	LYS
1	D	388	LEU
1	D	441	MET
1	D	468	SER
1	D	514	LYS
1	D	518	LEU
1	D	527	GLN
1	D	530	ASP
1	D	531	ARG
1	D	549	THR
1	D	555	GLN
1	D	570	ARG
1	E	315	THR
1	E	334	GLU
1	E	351	THR
1	E	364	MET
1	E	387	LYS
1	E	392	GLU
1	E	426	LYS
1	E	441	MET
1	E	486	ARG
1	E	505	ARG
1	E	530	ASP
1	E	538	ARG
1	E	543	ARG
1	E	550	ASP
1	E	570	ARG
1	E	574	ARG
1	F	302	LEU
1	F	303	ASN
1	F	304	GLU
1	F	343	SER
1	F	396	LYS
1	F	400	THR

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Mol	Chain	Res	Type
1	F	408	GLU
1	F	410	ILE
1	F	436	ASN
1	F	441	MET
1	F	468	SER
1	F	472	THR
1	F	481	THR
1	F	482	HIS
1	F	494	ASN
1	F	506	LYS
1	F	507	HIS
1	F	508	LYS
1	F	513	ILE
1	F	526	VAL
1	F	529	GLU
1	F	543	ARG
1	F	548	CYS
1	F	549	THR
1	F	574	ARG
1	F	578	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	463	HIS
1	A	512	GLN
1	A	527	GLN
1	B	303	ASN
1	B	374	GLN
1	B	527	GLN
1	C	427	ASN
1	C	459	ASN
1	D	507	HIS
1	D	527	GLN
1	D	555	GLN
1	E	523	ASN
1	F	323	HIS
1	F	427	ASN
1	F	463	HIS
1	F	512	GLN
1	F	546	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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	PO4	A	1580	3	4,4,4	0.76	0	6,6,6	0.25	0
2	PO4	A	1581	3	4,4,4	1.06	0	6,6,6	0.25	0
2	PO4	B	1579	3	4,4,4	0.84	0	6,6,6	0.28	0
2	PO4	B	1580	3	4,4,4	0.92	0	6,6,6	0.27	0
2	PO4	C	1579	3	4,4,4	1.59	1 (25%)	6,6,6	0.44	0
2	PO4	C	1580	3	4,4,4	1.52	1 (25%)	6,6,6	0.49	0
2	PO4	D	1580	-	4,4,4	0.68	0	6,6,6	0.24	0
2	PO4	E	1579	-	4,4,4	0.54	0	6,6,6	0.23	0
2	PO4	F	1580	-	4,4,4	0.71	0	6,6,6	0.23	0

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	PO4	A	1580	3	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	1581	3	-	0/0/0/0	0/0/0/0
2	PO4	B	1579	3	-	0/0/0/0	0/0/0/0
2	PO4	B	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	C	1579	3	-	0/0/0/0	0/0/0/0
2	PO4	C	1580	3	-	0/0/0/0	0/0/0/0
2	PO4	D	1580	-	-	0/0/0/0	0/0/0/0
2	PO4	E	1579	-	-	0/0/0/0	0/0/0/0
2	PO4	F	1580	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1579	PO4	P-O3	-2.53	1.45	1.53
2	C	1580	PO4	P-O2	-2.51	1.46	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1580	PO4	2	0
2	A	1581	PO4	1	0
2	B	1579	PO4	1	0
2	B	1580	PO4	1	0
2	D	1580	PO4	1	0

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.