



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2016 – 02:20 PM EDT

PDB ID : 4XGC
Title : Crystal structure of the eukaryotic origin recognition complex
Authors : Bleichert, F.; Botchan, M.R.; Berger, J.M.
Deposited on : 2014-12-30
Resolution : 3.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027674
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) : rb-20027674

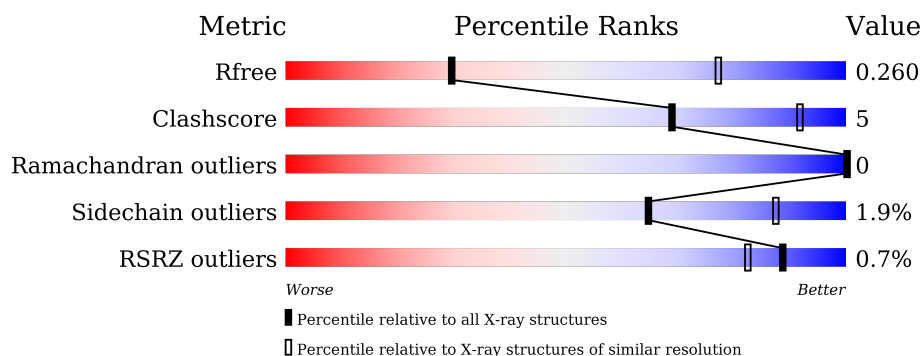
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 $\leq 5\%$. 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	B	354	<div> <div></div> <div>69%11%21%</div> </div>
2	C	676	<div> <div>%</div> <div>75%9%16%</div> </div>
3	E	460	<div> <div></div> <div>73%14%13%</div> </div>
4	A	393	<div> <div>2%</div> <div>69%9%21%</div> </div>
5	G	41	<div> <div></div> <div>90%10%</div> </div>
6	F	72	<div> <div></div> <div>26%74%</div> </div>

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Mol	Chain	Length	Quality of chain
7	D	459	 87% 9% .

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
9	CL	E	501	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16338 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 Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	281	Total	C	N	O	S	0	0	0
			2242	1439	374	416	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	265	MET	-	initiating methionine	UNP Q24168

- Molecule 2 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	567	Total	C	N	O	S	0	0	0
			4581	2940	803	814	24			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	46	MET	-	initiating methionine	UNP Q7K2L1

- Molecule 3 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	402	Total	C	N	O	S	0	0	0
			3190	2036	542	594	18			

- Molecule 4 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	310	Total	C	N	O	S	0	0	0
			2435	1535	435	450	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	532	MET	-	initiating methionine	UNP O16810

- Molecule 5 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	37	Total	C	N	O	0	0	0
			185	111	37	37			

- Molecule 6 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	19	Total	C	N	O	S	0	0	0
			160	104	28	27	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	186	MET	-	initiating methionine	UNP Q9Y1B2

- Molecule 7 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	440	Total	C	N	O	S	0	0	0
			3543	2260	624	643	16			

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	K	0	0
			1	1		

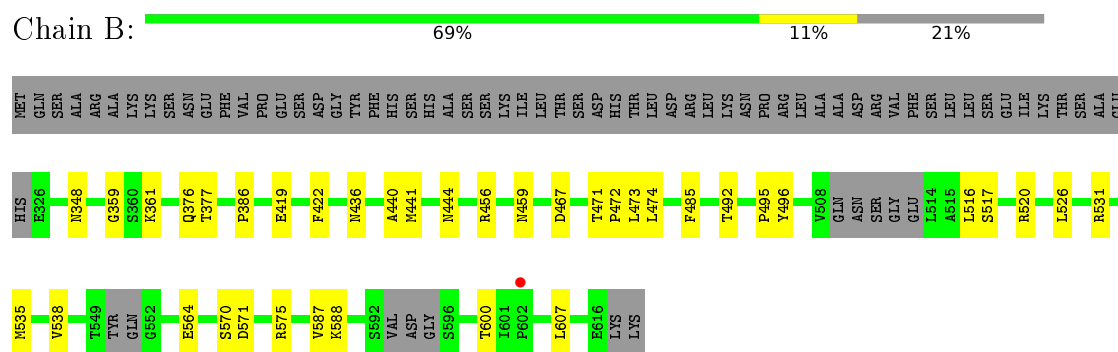
- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total	Cl	0	0
			1	1		

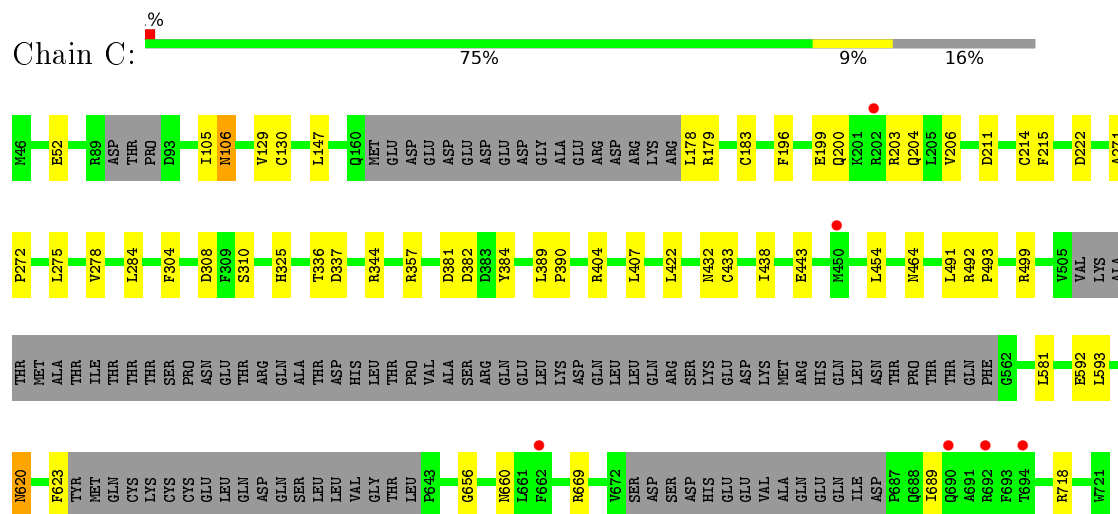
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

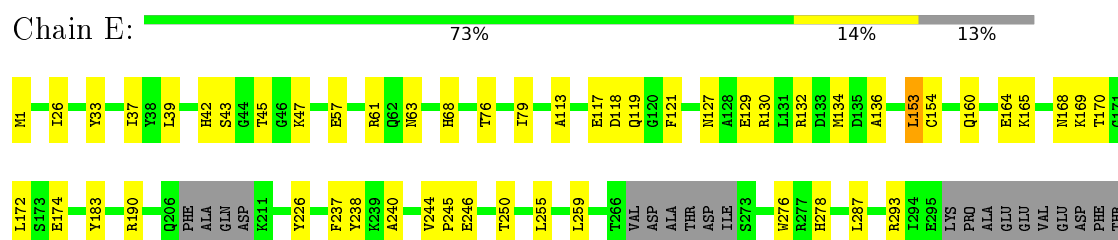
- Molecule 1: Origin recognition complex subunit 2

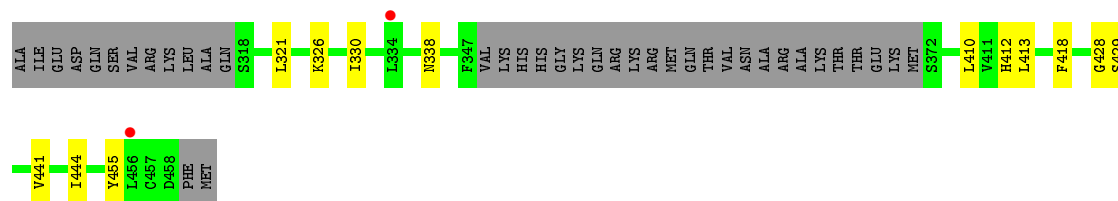


- Molecule 2: Origin recognition complex subunit 3

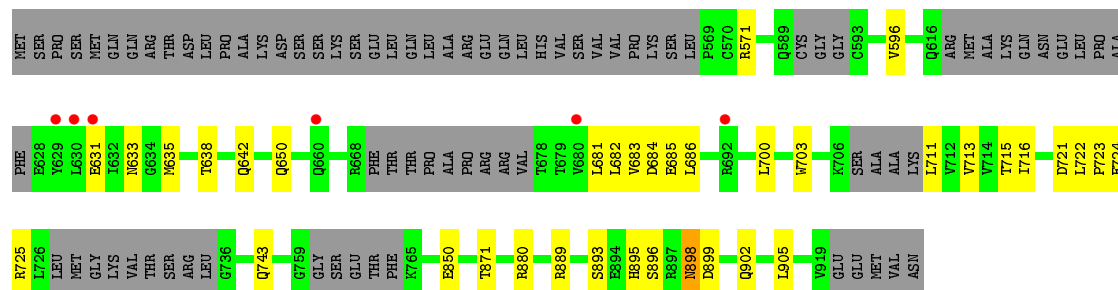


- Molecule 3: Origin recognition complex subunit 5

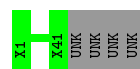




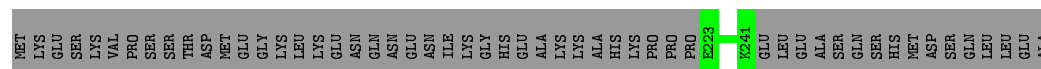
• Molecule 4: Origin recognition complex subunit 1



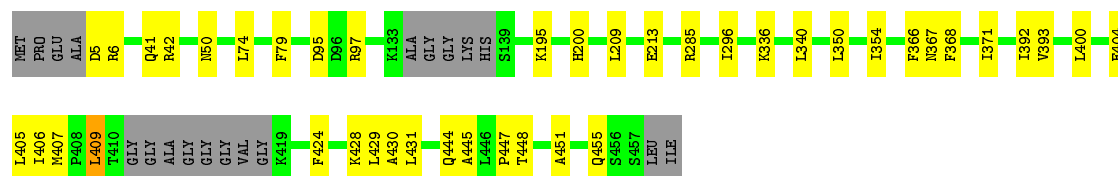
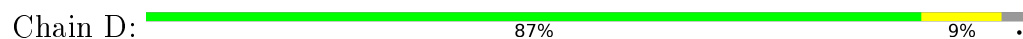
• Molecule 5: Origin recognition complex subunit 2



• Molecule 6: Origin recognition complex subunit 6



• Molecule 7: Origin recognition complex subunit 4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.54Å 258.98Å 257.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 3.50 48.80 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.80-3.50) 100.0 (48.80-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.224 , 0.258 0.225 , 0.260	Depositor DCC
R_{free} test set	1737 reflections (2.83%)	DCC
Wilson B-factor (Å ²)	118.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16338	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.25	0/2287	0.40	0/3094
2	C	0.27	0/4673	0.39	0/6319
3	E	0.31	0/3237	0.42	0/4372
4	A	0.30	0/2463	0.44	0/3325
6	F	0.20	0/162	0.26	0/214
7	D	0.32	0/3608	0.42	0/4866
All	All	0.29	0/16430	0.41	0/22190

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 [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	B	2242	0	2244	23	0
2	C	4581	0	4649	40	0
3	E	3190	0	3251	42	0
4	A	2435	0	2502	28	0
5	G	185	0	43	0	0
6	F	160	0	169	0	0
7	D	3543	0	3587	29	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	0	0
9	E	1	0	0	0	0
All	All	16338	0	16445	149	1

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 (149) 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)
2:C:106:ASN:HD22	2:C:106:ASN:N	1.53	0.99
2:C:129:VAL:HG12	2:C:206:VAL:HB	1.55	0.87
2:C:106:ASN:ND2	2:C:106:ASN:N	2.25	0.84
4:A:633:ASN:HD22	4:A:684:ASP:HB3	1.44	0.83
4:A:681:LEU:HB3	4:A:713:VAL:HG12	1.66	0.77
7:D:42:ARG:NH1	7:D:50:ASN:OD1	2.18	0.77
1:B:564:GLU:OE2	3:E:169:LYS:NZ	2.18	0.76
2:C:106:ASN:HD22	2:C:106:ASN:H	1.28	0.75
7:D:409:LEU:HD23	7:D:428:LYS:HE3	1.70	0.74
4:A:893:SER:OG	4:A:902:GLN:OE1	2.05	0.73
4:A:898:ASN:N	4:A:898:ASN:OD1	2.20	0.71
1:B:526:LEU:O	1:B:531:ARG:NH1	2.23	0.70
1:B:359:GLY:O	1:B:361:LYS:NZ	2.27	0.68
4:A:711:LEU:HD11	4:A:713:VAL:HG13	1.75	0.67
1:B:440:ALA:HB1	1:B:441:MET:HA	1.76	0.66
1:B:495:PRO:HA	1:B:496:TYR:HB2	1.76	0.66
4:A:711:LEU:CD1	4:A:713:VAL:HG13	2.26	0.65
3:E:57:GLU:OE1	3:E:61:ARG:NH2	2.30	0.65
2:C:357:ARG:NH2	2:C:382:ASP:OD1	2.28	0.64
4:A:682:LEU:HD11	4:A:716:ILE:CD1	2.26	0.64
3:E:113:ALA:HB2	3:E:119:GLN:HE21	1.63	0.64
1:B:436:ASN:ND2	1:B:467:ASP:OD2	2.31	0.64
2:C:199:GLU:N	2:C:200:GLN:HA	2.14	0.63
2:C:620:ASN:O	2:C:620:ASN:ND2	2.31	0.63
2:C:203:ARG:O	2:C:204:GLN:NE2	2.31	0.63
1:B:441:MET:SD	1:B:520:ARG:NH2	2.72	0.62
4:A:686:LEU:HD22	4:A:715:THR:HB	1.81	0.62
2:C:129:VAL:HG12	2:C:206:VAL:CB	2.28	0.62
3:E:165:LYS:NZ	7:D:404:GLU:O	2.32	0.62
4:A:633:ASN:OD1	4:A:635:MET:HB2	2.00	0.61
2:C:52:GLU:OE2	2:C:344:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:222:ASP:OD1	3:E:130:ARG:NH2	2.34	0.61
4:A:571:ARG:NH2	4:A:743:GLN:O	2.34	0.61
4:A:711:LEU:C	4:A:711:LEU:HD12	2.22	0.60
1:B:564:GLU:OE2	4:A:889:ARG:NH2	2.35	0.60
2:C:178:LEU:HD21	2:C:183:CYS:SG	2.42	0.60
7:D:213:GLU:OE1	7:D:285:ARG:NH2	2.35	0.59
7:D:95:ASP:O	7:D:97:ARG:N	2.34	0.58
4:A:898:ASN:O	4:A:902:GLN:N	2.36	0.58
1:B:419:GLU:OE2	1:B:456:ARG:NH2	2.36	0.58
2:C:422:LEU:O	2:C:432:ASN:ND2	2.36	0.57
3:E:132:ARG:NH2	7:D:404:GLU:OE2	2.37	0.57
4:A:631:GLU:O	4:A:650:GLN:NE2	2.38	0.57
2:C:325:HIS:NE2	2:C:593:LEU:O	2.35	0.56
7:D:296:ILE:O	7:D:296:ILE:HG23	2.06	0.56
1:B:571:ASP:OD1	1:B:575:ARG:NH1	2.38	0.56
3:E:113:ALA:HB2	3:E:119:GLN:NE2	2.21	0.56
7:D:447:PRO:O	7:D:448:THR:OG1	2.20	0.56
2:C:336:THR:HG22	2:C:337:ASP:N	2.21	0.55
7:D:350:LEU:HD21	7:D:393:VAL:HG13	1.88	0.55
3:E:168:ASN:OD1	3:E:169:LYS:N	2.39	0.54
2:C:656:GLY:O	2:C:718:ARG:NH1	2.40	0.53
4:A:683:VAL:HG21	4:A:700:LEU:HD21	1.89	0.53
4:A:682:LEU:HD11	4:A:716:ILE:HD11	1.90	0.53
7:D:5:ASP:OD1	7:D:5:ASP:N	2.40	0.53
2:C:464:ASN:OD1	2:C:499:ARG:NH1	2.42	0.53
7:D:340:LEU:HD21	7:D:431:LEU:HD11	1.90	0.53
3:E:287:LEU:HG	7:D:392:ILE:HD11	1.89	0.52
1:B:441:MET:O	1:B:444:ASN:ND2	2.43	0.52
2:C:669:ARG:HA	2:C:689:ILE:HD11	1.92	0.52
7:D:366:PHE:HB2	7:D:371:ILE:HD11	1.92	0.52
7:D:354:ILE:CG2	7:D:429:LEU:HD22	2.39	0.52
4:A:721:ASP:OD1	4:A:725:ARG:NH1	2.43	0.51
3:E:321:LEU:O	3:E:326:LYS:NZ	2.44	0.51
4:A:871:THR:HG23	4:A:871:THR:O	2.11	0.51
7:D:195:LYS:O	7:D:200:HIS:NE2	2.42	0.50
7:D:405:LEU:O	7:D:429:LEU:HD12	2.12	0.50
4:A:899:ASP:OD2	7:D:336:LYS:NZ	2.43	0.50
3:E:43:SER:OG	3:E:160:GLN:OE1	2.29	0.50
2:C:443:GLU:OE1	2:C:443:GLU:N	2.41	0.50
3:E:42:HIS:O	3:E:45:THR:OG1	2.24	0.50
3:E:39:LEU:HD11	3:E:47:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:336:THR:HG22	2:C:337:ASP:H	1.78	0.49
2:C:105:ILE:CD1	3:E:413:LEU:HD13	2.43	0.48
3:E:121:PHE:HB2	3:E:153:LEU:HB2	1.95	0.48
4:A:638:THR:OG1	4:A:642:GLN:OE1	2.30	0.48
7:D:451:ALA:O	7:D:455:GLN:N	2.46	0.48
1:B:386:PRO:HB3	1:B:517:SER:OG	2.14	0.48
2:C:308:ASP:OD2	2:C:310:SER:OG	2.22	0.48
2:C:130:CYS:SG	2:C:147:LEU:HD12	2.54	0.47
3:E:338:ASN:ND2	3:E:455:TYR:O	2.46	0.47
7:D:367:ASN:HD21	7:D:424:PHE:HA	1.80	0.47
3:E:246:GLU:OE2	3:E:293:ARG:NH2	2.48	0.47
2:C:433:CYS:SG	2:C:438:ILE:HD11	2.55	0.46
3:E:134:MET:O	3:E:136:ALA:N	2.46	0.46
2:C:592:GLU:N	2:C:592:GLU:OE1	2.48	0.46
1:B:516:LEU:HD13	1:B:607:LEU:HB2	1.98	0.46
3:E:240:ALA:HB1	7:D:392:ILE:HG21	1.97	0.46
3:E:76:THR:HG22	3:E:79:ILE:HG12	1.98	0.46
2:C:130:CYS:SG	2:C:147:LEU:CD1	3.04	0.45
2:C:492:ARG:N	2:C:493:PRO:HD2	2.32	0.45
4:A:895:HIS:O	4:A:896:SER:OG	2.23	0.45
3:E:117:GLU:O	3:E:117:GLU:CG	2.65	0.45
3:E:129:GLU:O	3:E:132:ARG:NH1	2.50	0.45
3:E:76:THR:CG2	3:E:79:ILE:HG12	2.47	0.45
4:A:596:VAL:CG2	4:A:716:ILE:HG12	2.47	0.45
1:B:495:PRO:CA	1:B:496:TYR:HB2	2.46	0.45
7:D:400:LEU:HB3	7:D:406:ILE:HD12	1.99	0.45
3:E:117:GLU:HG3	3:E:117:GLU:O	2.17	0.45
1:B:376:GLN:O	1:B:377:THR:OG1	2.32	0.44
1:B:359:GLY:N	1:B:492:THR:O	2.49	0.44
2:C:407:LEU:HD12	2:C:581:LEU:CD2	2.48	0.44
4:A:722:LEU:N	4:A:723:PRO:HD2	2.32	0.44
3:E:26:ILE:HG22	3:E:26:ILE:O	2.17	0.44
1:B:422:PHE:O	1:B:459:ASN:ND2	2.51	0.44
2:C:275:LEU:HD22	2:C:304:PHE:CD1	2.53	0.44
4:A:686:LEU:CD2	4:A:715:THR:HB	2.48	0.43
4:A:895:HIS:O	4:A:896:SER:CB	2.67	0.43
2:C:271:ALA:N	2:C:272:PRO:CD	2.81	0.43
7:D:74:LEU:HA	7:D:79:PHE:CD1	2.53	0.43
7:D:368:PHE:HE1	7:D:393:VAL:HG12	1.84	0.43
3:E:244:VAL:HB	3:E:245:PRO:HD3	2.00	0.43
4:A:682:LEU:HD11	4:A:716:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:THR:N	1:B:472:PRO:HD2	2.33	0.42
1:B:570:SER:OG	1:B:571:ASP:N	2.51	0.42
7:D:371:ILE:HD12	7:D:371:ILE:H	1.85	0.42
3:E:63:ASN:ND2	3:E:119:GLN:HB3	2.34	0.42
2:C:381:ASP:OD1	2:C:384:TYR:N	2.50	0.42
7:D:407:MET:HG2	7:D:430:ALA:HB2	2.02	0.42
3:E:255:LEU:O	3:E:259:LEU:N	2.53	0.42
2:C:105:ILE:HD12	3:E:413:LEU:HD13	2.02	0.42
3:E:428:GLY:HA2	3:E:429:SER:HA	1.89	0.42
3:E:121:PHE:HB2	3:E:153:LEU:CB	2.50	0.42
3:E:33:TYR:HB3	3:E:154:CYS:HB2	2.01	0.42
1:B:587:VAL:HG12	1:B:588:LYS:N	2.34	0.42
2:C:105:ILE:O	2:C:105:ILE:HG22	2.20	0.42
2:C:389:LEU:N	2:C:390:PRO:HD2	2.35	0.42
1:B:535:MET:HA	1:B:538:VAL:HG12	2.02	0.41
7:D:444:GLN:HA	7:D:445:ALA:HA	1.82	0.41
3:E:174:GLU:OE2	4:A:880:ARG:NH2	2.47	0.41
3:E:121:PHE:O	3:E:153:LEU:HA	2.21	0.41
3:E:237:PHE:CZ	3:E:250:THR:HG21	2.55	0.41
2:C:214:CYS:HG	3:E:412:HIS:CE1	2.37	0.41
3:E:170:THR:HG23	3:E:170:THR:O	2.20	0.41
2:C:178:LEU:HD23	2:C:179:ARG:N	2.36	0.41
2:C:284:LEU:O	2:C:404:ARG:NE	2.52	0.41
3:E:330:ILE:HG22	3:E:441:VAL:HG13	2.02	0.41
7:D:368:PHE:CE1	7:D:393:VAL:HG12	2.55	0.41
4:A:711:LEU:HD11	4:A:713:VAL:CG1	2.46	0.41
1:B:516:LEU:HD13	1:B:607:LEU:HD13	2.03	0.41
3:E:326:LYS:HD2	3:E:444:ILE:HG23	2.02	0.41
7:D:354:ILE:HG21	7:D:429:LEU:HD22	2.01	0.41
2:C:214:CYS:SG	3:E:412:HIS:NE2	2.94	0.40
1:B:588:LYS:O	1:B:600:THR:N	2.54	0.40
2:C:211:ASP:N	2:C:211:ASP:OD1	2.53	0.40
2:C:275:LEU:HA	2:C:278:VAL:HG12	2.04	0.40
3:E:183:TYR:O	3:E:238:TYR:OH	2.39	0.40
7:D:409:LEU:HB3	7:D:428:LYS:HE3	2.04	0.40
3:E:26:ILE:HD11	3:E:37:ILE:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:6:ARG:CD	7:D:6:ARG:CD[3_555]	1.95	0.25

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	B	273/354 (77%)	248 (91%)	25 (9%)	0	100	100
2	C	555/676 (82%)	505 (91%)	50 (9%)	0	100	100
3	E	392/460 (85%)	369 (94%)	23 (6%)	0	100	100
4	A	296/393 (75%)	277 (94%)	19 (6%)	0	100	100
6	F	17/72 (24%)	17 (100%)	0	0	100	100
7	D	434/459 (95%)	410 (94%)	24 (6%)	0	100	100
All	All	1967/2414 (82%)	1826 (93%)	141 (7%)	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	B	252/316 (80%)	248 (98%)	4 (2%)	70	89
2	C	500/601 (83%)	492 (98%)	8 (2%)	70	89
3	E	352/402 (88%)	339 (96%)	13 (4%)	41	76
4	A	263/335 (78%)	257 (98%)	6 (2%)	58	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	15/62 (24%)	15 (100%)	0	100	100
7	D	390/398 (98%)	387 (99%)	3 (1%)	86	95
All	All	1772/2114 (84%)	1738 (98%)	34 (2%)	65	87

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	348	ASN
1	B	473	LEU
1	B	474	LEU
1	B	485	PHE
2	C	106	ASN
2	C	196	PHE
2	C	215	PHE
2	C	454	LEU
2	C	491	LEU
2	C	620	ASN
2	C	623	PHE
2	C	660	ASN
3	E	1	MET
3	E	68	HIS
3	E	118	ASP
3	E	127	ASN
3	E	153	LEU
3	E	164	GLU
3	E	172	LEU
3	E	190	ARG
3	E	226	TYR
3	E	276	TRP
3	E	278	HIS
3	E	410	LEU
3	E	418	PHE
4	A	685	GLU
4	A	703	TRP
4	A	724	GLU
4	A	850	GLU
4	A	898	ASN
4	A	905	LEU
7	D	41	GLN
7	D	209	LEU
7	D	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	106	ASN
3	E	119	GLN
3	E	127	ASN
3	E	150	ASN
3	E	424	ASN
7	D	441	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 2 ligands modelled in this entry, 2 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	G	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	14:UNK	C	16:UNK	N	6.41
1	G	27:UNK	C	31:UNK	N	5.00

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	B	281/354 (79%)	-0.17	1 (0%) 93 90	73, 131, 185, 201	0
2	C	567/676 (83%)	-0.17	6 (1%) 82 73	61, 124, 188, 237	0
3	E	402/460 (87%)	-0.23	2 (0%) 91 88	49, 108, 172, 199	0
4	A	310/393 (78%)	-0.14	6 (1%) 70 60	52, 110, 186, 218	0
5	G	0/41	-	-	-	-
6	F	19/72 (26%)	0.20	0 100 100	166, 185, 201, 202	0
7	D	440/459 (95%)	-0.45	0 100 100	52, 91, 142, 182	0
All	All	2019/2455 (82%)	-0.24	15 (0%) 89 82	49, 112, 182, 237	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	630	LEU	3.7
2	C	690	GLN	3.4
4	A	660	GLN	3.0
4	A	631	GLU	2.9
4	A	629	TYR	2.6
1	B	602	PRO	2.6
3	E	334	LEU	2.5
2	C	202	ARG	2.5
2	C	692	ARG	2.4
4	A	680	VAL	2.4
3	E	456	LEU	2.4
4	A	692	ARG	2.3
2	C	694	THR	2.3
2	C	662	PHE	2.3
2	C	450	MET	2.1

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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
9	CL	E	501	1/1	0.82	0.39	7.88	108,108,108,108	0
8	K	B	701	1/1	0.92	0.23	0.55	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.