



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:53 am BST

PDB ID : 5FK0
Title : Yeast delta-COP-I mu-homology domain
Authors : Suckling, R.J.; Evans, P.R.; Owen, D.J.
Deposited on : 2015-10-14
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

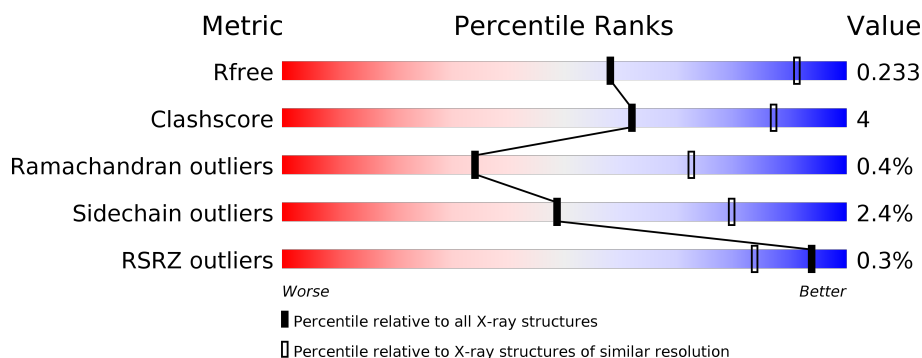
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	270	<div> <div>84%</div> <div>13%</div> <div>••</div> </div>
1	B	270	<div> <div>86%</div> <div>11%</div> <div>••</div> </div>
1	C	270	<div> <div>86%</div> <div>11%</div> <div>•</div> </div>
1	D	270	<div> <div>86%</div> <div>11%</div> <div>•</div> </div>
1	E	270	<div> <div>84%</div> <div>13%</div> <div>•</div> </div>
1	F	270	<div> <div>89%</div> <div>9%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	270	<div><div>%</div><div><div></div></div><div>87%11%•</div></div>
1	H	270	<div><div>%</div><div><div></div></div><div>89%8%••</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16818 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 COATOMER SUBUNIT DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	1	0
			2061	1296	335	424	6			
1	B	263	Total	C	N	O	S	0	2	0
			2067	1300	336	425	6			
1	C	263	Total	C	N	O	S	0	2	0
			2067	1300	336	425	6			
1	D	263	Total	C	N	O	S	0	3	0
			2073	1304	337	426	6			
1	E	263	Total	C	N	O	S	0	1	0
			2059	1295	333	424	7			
1	F	263	Total	C	N	O	S	0	2	0
			2066	1299	335	426	6			
1	G	263	Total	C	N	O	S	0	2	0
			2067	1300	336	425	6			
1	H	263	Total	C	N	O	S	0	2	0
			2068	1301	337	424	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	GLY	-	expression tag	UNP P43621
A	278	PRO	-	expression tag	UNP P43621
A	279	LEU	-	expression tag	UNP P43621
A	280	GLY	-	expression tag	UNP P43621
A	281	SER	-	expression tag	UNP P43621
B	277	GLY	-	expression tag	UNP P43621
B	278	PRO	-	expression tag	UNP P43621
B	279	LEU	-	expression tag	UNP P43621
B	280	GLY	-	expression tag	UNP P43621
B	281	SER	-	expression tag	UNP P43621
C	277	GLY	-	expression tag	UNP P43621
C	278	PRO	-	expression tag	UNP P43621
C	279	LEU	-	expression tag	UNP P43621

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Chain	Residue	Modelled	Actual	Comment	Reference
C	280	GLY	-	expression tag	UNP P43621
C	281	SER	-	expression tag	UNP P43621
D	277	GLY	-	expression tag	UNP P43621
D	278	PRO	-	expression tag	UNP P43621
D	279	LEU	-	expression tag	UNP P43621
D	280	GLY	-	expression tag	UNP P43621
D	281	SER	-	expression tag	UNP P43621
E	277	GLY	-	expression tag	UNP P43621
E	278	PRO	-	expression tag	UNP P43621
E	279	LEU	-	expression tag	UNP P43621
E	280	GLY	-	expression tag	UNP P43621
E	281	SER	-	expression tag	UNP P43621
F	277	GLY	-	expression tag	UNP P43621
F	278	PRO	-	expression tag	UNP P43621
F	279	LEU	-	expression tag	UNP P43621
F	280	GLY	-	expression tag	UNP P43621
F	281	SER	-	expression tag	UNP P43621
G	277	GLY	-	expression tag	UNP P43621
G	278	PRO	-	expression tag	UNP P43621
G	279	LEU	-	expression tag	UNP P43621
G	280	GLY	-	expression tag	UNP P43621
G	281	SER	-	expression tag	UNP P43621
H	277	GLY	-	expression tag	UNP P43621
H	278	PRO	-	expression tag	UNP P43621
H	279	LEU	-	expression tag	UNP P43621
H	280	GLY	-	expression tag	UNP P43621
H	281	SER	-	expression tag	UNP P43621

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	58	Total O 58 58	0	0

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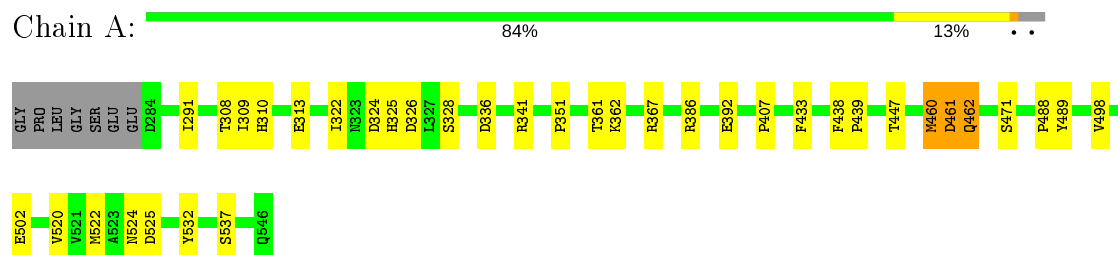
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	53	Total 53	O 53	0	0
3	C	38	Total 38	O 38	0	0
3	D	28	Total 28	O 28	0	0
3	E	36	Total 36	O 36	0	0
3	F	26	Total 26	O 26	0	0
3	G	27	Total 27	O 27	0	0
3	H	22	Total 22	O 22	0	0

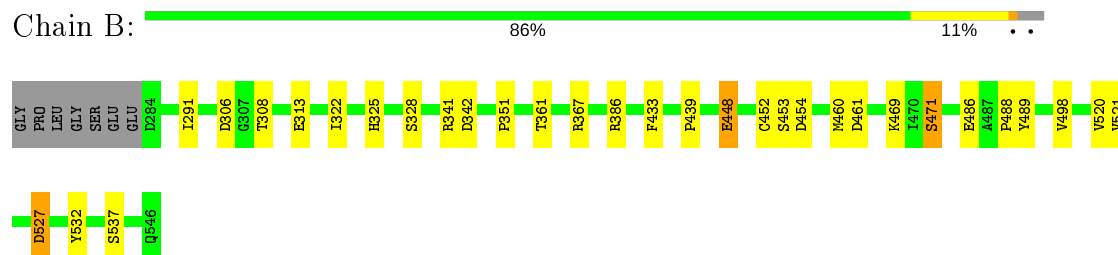
3 Residue-property plots [i](#)

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

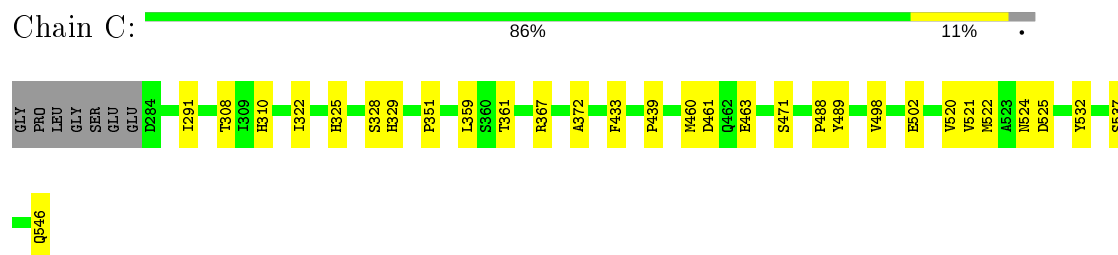
• Molecule 1: COATOMER SUBUNIT DELTA



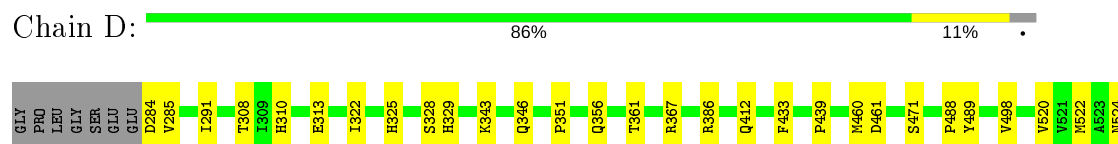
• Molecule 1: COATOMER SUBUNIT DELTA



• Molecule 1: COATOMER SUBUNIT DELTA



• Molecule 1: COATOMER SUBUNIT DELTA





• Molecule 1: COATOMER SUBUNIT DELTA

Chain E: 84% 13% .



• Molecule 1: COATOMER SUBUNIT DELTA

Chain F: 89% 9% .



• Molecule 1: COATOMER SUBUNIT DELTA

Chain G: 87% 11% .



• Molecule 1: COATOMER SUBUNIT DELTA

Chain H: 89% 8% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.90Å 148.63Å 222.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 3.00 48.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.41-3.00) 99.7 (48.36-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.233 0.199 , 0.233	Depositor DCC
R_{free} test set	2953 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	84.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16818	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.60	2/2101 (0.1%)	0.75	3/2853 (0.1%)
1	B	0.57	1/2110 (0.0%)	0.78	2/2865 (0.1%)
1	C	0.54	0/2110	0.71	0/2865
1	D	0.52	0/2119	0.69	0/2877
1	E	0.53	0/2098	0.71	1/2848 (0.0%)
1	F	0.51	0/2109	0.72	2/2864 (0.1%)
1	G	0.49	0/2110	0.69	0/2865
1	H	0.47	0/2112	0.70	1/2868 (0.0%)
All	All	0.53	3/16869 (0.0%)	0.72	9/22905 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	GLN	CD-OE1	6.41	1.38	1.24
1	A	462	GLN	CD-NE2	-6.01	1.17	1.32
1	B	527	ASP	CB-CG	5.23	1.62	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	544	LEU	CB-CG-CD1	9.20	126.63	111.00
1	B	527	ASP	CB-CG-OD2	7.76	125.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	327	LEU	CB-CG-CD1	-7.39	98.44	111.00
1	A	461	ASP	N-CA-C	7.13	130.24	111.00
1	B	448	GLU	CA-C-N	-5.91	104.20	117.20
1	E	355	LYS	CA-CB-CG	5.81	126.19	113.40
1	F	284	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	462	GLN	N-CA-CB	5.15	119.86	110.60
1	A	460	MET	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	448	GLU	Peptide

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	2061	0	2021	31	0
1	B	2067	0	2029	15	0
1	C	2067	0	2029	17	0
1	D	2073	0	2037	20	0
1	E	2059	0	2023	26	1
1	F	2066	0	2025	12	0
1	G	2067	0	2029	21	1
1	H	2068	0	2028	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	58	0	0	13	0
3	B	53	0	0	3	0
3	C	38	0	0	5	0
3	D	28	0	0	8	0
3	E	36	0	0	5	0
3	F	26	0	0	3	0
3	G	27	0	0	7	0
3	H	22	0	0	7	0
All	All	16818	0	16221	143	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 4.

All (143) 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:F:310[B]:HIS:CD2	3:F:2001:HOH:O	2.08	1.07
1:B:454:ASP:HB3	1:B:471:SER:OG	1.61	1.01
1:A:310[B]:HIS:CD2	3:A:2007:HOH:O	2.13	0.98
1:E:392:GLU:OE1	1:G:386:ARG:NH2	1.97	0.98
1:G:346[A]:GLN:OE1	3:G:2006:HOH:O	1.80	0.97
1:H:325[A]:HIS:NE2	3:H:2005:HOH:O	1.97	0.97
1:D:346[A]:GLN:OE1	3:D:2007:HOH:O	1.84	0.94
1:A:532:TYR:HE1	3:A:2053:HOH:O	1.51	0.93
1:A:310[B]:HIS:HD2	3:A:2007:HOH:O	1.55	0.87
1:F:310[B]:HIS:HD2	3:F:2001:HOH:O	1.51	0.84
1:D:522:MET:CE	3:D:2027:HOH:O	2.31	0.79
1:A:438:PHE:CE1	1:A:460:MET:O	2.39	0.76
1:A:522:MET:HE3	3:A:2017:HOH:O	1.85	0.74
1:G:427:GLU:HG2	1:G:474:ALA:HA	1.69	0.73
1:B:454:ASP:HB3	1:B:471:SER:HG	1.53	0.73
1:H:325[A]:HIS:CE1	3:H:2005:HOH:O	2.37	0.72
1:H:539:LYS:HG3	3:H:2001:HOH:O	1.89	0.72
1:C:463:GLU:HG2	3:C:2032:HOH:O	1.90	0.72
1:A:438:PHE:CD1	1:A:460:MET:O	2.44	0.71
1:B:486:GLU:HB3	3:B:2049:HOH:O	1.88	0.71
1:H:351:PRO:O	1:H:367:ARG:NH2	2.24	0.71
1:B:342:ASP:OD2	3:B:2013:HOH:O	2.09	0.70
1:F:351:PRO:O	1:F:367:ARG:NH2	2.24	0.70
1:F:338:ILE:HA	3:F:2007:HOH:O	1.91	0.70
1:C:329:HIS:CD2	1:C:372:ALA:HB2	2.27	0.70
1:G:351:PRO:O	1:G:367:ARG:NH2	2.25	0.70
1:B:351:PRO:O	1:B:367:ARG:NH2	2.25	0.70
1:A:351:PRO:O	1:A:367:ARG:NH2	2.25	0.70
1:A:392:GLU:OE1	1:E:386:ARG:NH2	2.24	0.70
1:C:351:PRO:O	1:C:367:ARG:NH2	2.25	0.70
1:D:522:MET:HE2	3:D:2027:HOH:O	1.92	0.69
1:D:351:PRO:O	1:D:367:ARG:NH2	2.25	0.69
1:E:351:PRO:O	1:E:367:ARG:NH2	2.25	0.69
1:H:444:ASP:OD1	3:H:2017:HOH:O	2.12	0.69
1:A:326:ASP:OD2	3:A:2014:HOH:O	2.11	0.68
1:H:324:ASP:HB3	1:H:327:LEU:CD1	2.24	0.67
1:E:444:ASP:OD1	3:E:2028:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:450:SER:CB	3:G:2024:HOH:O	2.44	0.65
1:E:362:LYS:HE2	3:E:2012:HOH:O	1.97	0.64
1:E:419:GLU:CG	1:G:351:PRO:HG3	2.29	0.62
1:A:309:ILE:HD12	3:A:2006:HOH:O	2.00	0.61
1:C:502:GLU:HG2	3:C:2026:HOH:O	2.00	0.60
1:B:306:ASP:OD2	1:F:315:LYS:NZ	2.22	0.60
3:A:2051:HOH:O	1:B:341:ARG:NH1	2.36	0.59
1:A:502:GLU:HG2	3:A:2037:HOH:O	2.03	0.59
1:A:367:ARG:NH1	3:A:2023:HOH:O	2.34	0.59
1:A:532:TYR:CE1	3:A:2053:HOH:O	2.37	0.58
1:B:469:LYS:HE2	3:B:2046:HOH:O	2.02	0.58
1:A:341:ARG:NE	1:G:488:PRO:HB3	2.20	0.57
1:C:524:ASN:OD1	1:C:525:ASP:N	2.37	0.57
1:G:450:SER:HB3	3:G:2024:HOH:O	2.05	0.55
1:H:325[B]:HIS:CE1	3:H:2004:HOH:O	2.58	0.55
1:A:439:PRO:HD2	1:A:460:MET:HE2	1.88	0.54
1:A:488:PRO:HB2	1:A:489:TYR:CD1	2.43	0.54
1:F:339:ASP:HB3	1:F:342[B]:ASP:OD2	2.07	0.54
1:B:488:PRO:HB2	1:B:489:TYR:CD1	2.43	0.54
1:E:402:THR:HG22	1:G:384:ARG:HH12	1.72	0.54
1:E:488:PRO:HB2	1:E:489:TYR:CD1	2.43	0.53
1:E:367:ARG:NH1	3:E:2018:HOH:O	2.42	0.53
1:A:524:ASN:OD1	1:A:525:ASP:N	2.38	0.53
1:D:522:MET:HE3	3:D:2027:HOH:O	2.00	0.52
1:D:524:ASN:ND2	3:D:2027:HOH:O	2.29	0.52
1:E:334:LEU:HD22	1:E:515[B]:MET:CE	2.40	0.52
1:E:419:GLU:HG3	1:G:351:PRO:HG3	1.92	0.52
1:E:419:GLU:CD	1:G:351:PRO:HG3	2.29	0.52
1:A:407:PRO:O	1:E:378:GLN:NE2	2.43	0.52
1:C:488:PRO:HB2	1:C:489:TYR:CD1	2.45	0.52
1:C:546:GLN:HB3	3:C:2003:HOH:O	2.09	0.52
1:D:439:PRO:HG2	1:D:460:MET:HE1	1.92	0.52
1:F:439:PRO:HG2	1:F:460:MET:HE1	1.91	0.51
1:A:447:THR:HG23	3:A:2044:HOH:O	2.11	0.51
1:F:520:VAL:HG23	1:F:532:TYR:CD2	2.46	0.50
1:E:325:HIS:HA	1:E:328:SER:OG	2.12	0.50
1:D:488:PRO:HB2	1:D:489:TYR:CD1	2.47	0.50
1:C:439:PRO:HD2	1:C:460:MET:HE3	1.94	0.49
1:C:489:TYR:CB	1:E:341:ARG:HD3	2.43	0.49
1:H:537:SER:OG	3:H:2001:HOH:O	2.19	0.49
1:D:325:HIS:HA	1:D:328:SER:OG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:520:VAL:HG23	1:G:532:TYR:CD2	2.47	0.49
1:H:520:VAL:HG23	1:H:532:TYR:CD2	2.47	0.49
1:A:520:VAL:HG23	1:A:532:TYR:CD2	2.48	0.49
1:A:325:HIS:HA	1:A:328:SER:OG	2.13	0.49
1:B:439:PRO:HD2	1:B:460:MET:HE3	1.95	0.49
1:E:334:LEU:HD22	1:E:515[B]:MET:HE1	1.95	0.48
1:G:325:HIS:HA	1:G:328:SER:OG	2.13	0.48
1:E:520:VAL:HG23	1:E:532:TYR:CD2	2.48	0.48
1:G:371:LYS:HG3	3:G:2010:HOH:O	2.12	0.48
1:B:325:HIS:HA	1:B:328:SER:OG	2.13	0.48
1:C:433:PHE:CD2	1:C:498:VAL:HG22	2.49	0.48
1:A:336:ASP:OD1	1:A:362:LYS:NZ	2.45	0.48
1:A:433:PHE:CD2	1:A:498:VAL:HG22	2.49	0.48
1:D:520:VAL:HG23	1:D:532:TYR:CD2	2.49	0.47
1:E:433:PHE:CD2	1:E:498:VAL:HG22	2.49	0.47
1:E:439:PRO:HD2	1:E:460:MET:HE3	1.97	0.47
1:B:520:VAL:HG23	1:B:532:TYR:CD2	2.50	0.47
1:F:325:HIS:HA	1:F:328:SER:OG	2.14	0.47
1:A:309:ILE:HD11	3:A:2025:HOH:O	2.15	0.46
1:A:439:PRO:HG2	1:A:460:MET:HE3	1.97	0.46
1:E:486:GLU:HB3	3:E:2027:HOH:O	2.14	0.46
1:D:412[B]:GLN:OE1	1:D:412[B]:GLN:HA	2.16	0.46
1:D:433:PHE:CD2	1:D:498:VAL:HG22	2.50	0.46
1:B:433:PHE:CD2	1:B:498:VAL:HG22	2.51	0.45
1:C:520:VAL:HG23	1:C:532:TYR:CD2	2.52	0.45
1:F:433:PHE:CD2	1:F:498:VAL:HG22	2.52	0.45
1:G:433:PHE:CD2	1:G:498:VAL:HG22	2.52	0.45
1:G:450:SER:HB2	3:G:2024:HOH:O	2.11	0.45
1:H:433:PHE:CD2	1:H:498:VAL:HG22	2.52	0.44
1:D:343:LYS:HE3	1:D:343:LYS:HB3	1.85	0.44
1:D:329:HIS:CE1	3:D:2005:HOH:O	2.70	0.44
1:A:438:PHE:HE1	1:A:460:MET:O	1.96	0.44
1:D:284:ASP:O	1:D:285:VAL:C	2.56	0.44
1:E:439:PRO:HG2	1:E:460:MET:HE1	2.00	0.44
1:C:325:HIS:HA	1:C:328:SER:OG	2.18	0.43
1:D:439:PRO:HD2	1:D:460:MET:HE3	1.99	0.43
1:F:291:ILE:HG12	1:F:322:ILE:HG12	2.01	0.43
1:H:291:ILE:HG12	1:H:322:ILE:HG12	2.01	0.43
1:B:291:ILE:HG12	1:B:322:ILE:HG12	2.01	0.42
1:C:488:PRO:HB2	1:E:359:LEU:HD13	2.01	0.42
1:D:310[B]:HIS:ND1	3:D:2002:HOH:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:ILE:HD12	1:G:350:HIS:CE1	2.55	0.42
1:C:291:ILE:HG12	1:C:322:ILE:HG12	2.02	0.42
1:H:328:SER:OG	1:H:373:PHE:O	2.35	0.42
1:A:313:GLU:OE2	1:A:386:ARG:NH1	2.52	0.42
1:E:486:GLU:OE1	3:E:2027:HOH:O	2.21	0.42
1:G:451:THR:N	3:G:2024:HOH:O	2.52	0.42
1:A:291:ILE:HG12	1:A:322:ILE:HG12	2.01	0.42
1:C:522:MET:HE1	3:C:2038:HOH:O	2.20	0.42
1:A:336:ASP:OD1	1:A:362:LYS:HE3	2.20	0.41
1:E:359:LEU:HA	1:E:359:LEU:HD23	1.93	0.41
1:F:439:PRO:HD2	1:F:460:MET:HE3	2.01	0.41
1:G:291:ILE:HG12	1:G:322:ILE:HG12	2.02	0.41
1:D:313:GLU:OE2	1:D:386:ARG:NH1	2.53	0.41
1:D:291:ILE:HG12	1:D:322:ILE:HG12	2.01	0.41
1:E:291:ILE:HG12	1:E:322:ILE:HG12	2.01	0.41
1:H:365:SER:N	3:H:2009:HOH:O	2.50	0.41
1:G:427:GLU:HA	3:G:2018:HOH:O	2.20	0.41
1:A:324:ASP:HA	3:A:2013:HOH:O	2.20	0.41
1:B:313:GLU:OE2	1:B:386:ARG:NH1	2.52	0.41
1:C:310[B]:HIS:CE1	3:C:2004:HOH:O	2.73	0.41
1:D:367:ARG:NH1	3:D:2010:HOH:O	2.54	0.41
1:G:313:GLU:OE2	1:G:386:ARG:NH1	2.53	0.41
1:A:439:PRO:HG2	1:A:460:MET:CE	2.51	0.40
1:C:359:LEU:HD23	1:C:359:LEU:HA	1.96	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)
1:E:524:ASN:ND2	1:G:324:ASP:OD2[1_455]	1.88	0.32

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	262/270 (97%)	249 (95%)	12 (5%)	1 (0%)	34	72
1	B	263/270 (97%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	C	263/270 (97%)	250 (95%)	12 (5%)	1 (0%)	34	72
1	D	264/270 (98%)	251 (95%)	12 (4%)	1 (0%)	34	72
1	E	262/270 (97%)	252 (96%)	9 (3%)	1 (0%)	34	72
1	F	263/270 (97%)	250 (95%)	12 (5%)	1 (0%)	34	72
1	G	263/270 (97%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	H	263/270 (97%)	251 (95%)	11 (4%)	1 (0%)	34	72
All	All	2103/2160 (97%)	2005 (95%)	90 (4%)	8 (0%)	34	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ASP
1	B	461	ASP
1	C	461	ASP
1	D	461	ASP
1	E	461	ASP
1	F	461	ASP
1	G	461	ASP
1	H	461	ASP

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	238/242 (98%)	233 (98%)	5 (2%)	53	82
1	B	239/242 (99%)	231 (97%)	8 (3%)	38	73
1	C	239/242 (99%)	234 (98%)	5 (2%)	53	82
1	D	240/242 (99%)	235 (98%)	5 (2%)	53	82
1	E	238/242 (98%)	233 (98%)	5 (2%)	53	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	239/242 (99%)	235 (98%)	4 (2%)	60	85
1	G	239/242 (99%)	233 (98%)	6 (2%)	47	79
1	H	239/242 (99%)	232 (97%)	7 (3%)	42	76
All	All	1911/1936 (99%)	1866 (98%)	45 (2%)	49	79

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	THR
1	A	361	THR
1	A	462	GLN
1	A	471	SER
1	A	537	SER
1	B	308	THR
1	B	361	THR
1	B	452	CYS
1	B	453	SER
1	B	471	SER
1	B	521	VAL
1	B	527	ASP
1	B	537	SER
1	C	308	THR
1	C	361	THR
1	C	471	SER
1	C	521	VAL
1	C	537	SER
1	D	308	THR
1	D	356	GLN
1	D	361	THR
1	D	471	SER
1	D	537	SER
1	E	308	THR
1	E	361	THR
1	E	471	SER
1	E	521	VAL
1	E	537	SER
1	F	361	THR
1	F	471	SER
1	F	489	TYR
1	F	537	SER
1	G	284	ASP

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Mol	Chain	Res	Type
1	G	308	THR
1	G	361	THR
1	G	471	SER
1	G	489	TYR
1	G	537	SER
1	H	308	THR
1	H	356	GLN
1	H	361	THR
1	H	471	SER
1	H	489	TYR
1	H	521	VAL
1	H	537	SER

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	331	ASN
1	B	331	ASN
1	C	329	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	263/270 (97%)	-0.35	0	100	100	49, 77, 112, 146	0
1	B	263/270 (97%)	-0.34	0	100	100	45, 73, 107, 136	0
1	C	263/270 (97%)	-0.32	0	100	100	53, 78, 114, 150	0
1	D	263/270 (97%)	-0.21	0	100	100	56, 93, 134, 157	0
1	E	263/270 (97%)	-0.24	0	100	100	53, 92, 131, 154	0
1	F	263/270 (97%)	-0.22	1 (0%)	92	79	55, 96, 139, 162	0
1	G	263/270 (97%)	-0.17	2 (0%)	86	65	59, 101, 152, 177	0
1	H	263/270 (97%)	0.07	3 (1%)	80	56	76, 118, 159, 182	0
All	All	2104/2160 (97%)	-0.22	6 (0%)	94	84	45, 90, 141, 182	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	508	LEU	2.8
1	H	443	VAL	2.7
1	G	464	MET	2.2
1	H	433	PHE	2.0
1	H	467	SER	2.0
1	G	463	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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. 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(\AA^2)	Q<0.9
2	CA	B	601	1/1	0.93	0.18	64,64,64,64	0
2	CA	A	601	1/1	0.94	0.10	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.