Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 08:02 AM EST

PDB ID	:	3RV0
Title	:	Crystal structure of K. polysporus Dcr1 without the C-terminal dsRBD
Authors	:	Nakanishi, K.; Weinberg, D.E.; Bartel, D.P.; Patel, D.J.
Deposited on	:	2011-05-05
Resolution	:	2.29 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

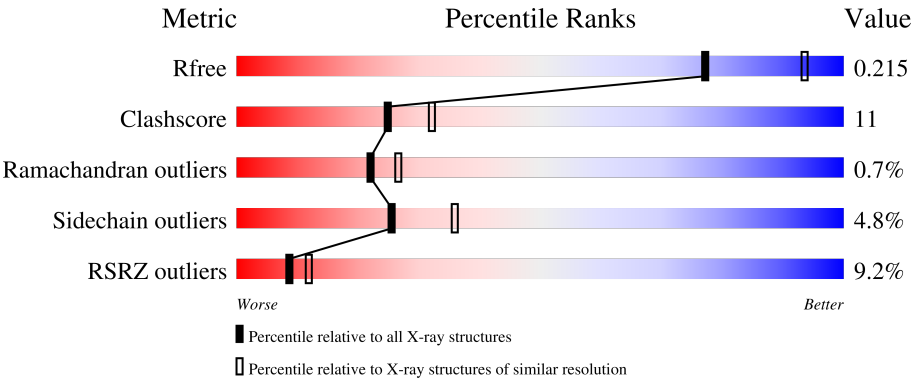
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	341	4% 54% 15% • 30%
1	B	341	13% 66% 21% • 11%
1	C	341	6% 51% 13% • 33%
1	D	341	4% 53% 14% • 32%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8628 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 K. polysporus Dcr1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1939	1236	321	374	8			
1	B	304	Total	C	N	O	S	0	0	0
			2477	1577	417	474	9			
1	C	228	Total	C	N	O	S	0	0	0
			1856	1186	307	356	7			
1	D	232	Total	C	N	O	S	0	0	0
			1885	1204	311	363	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

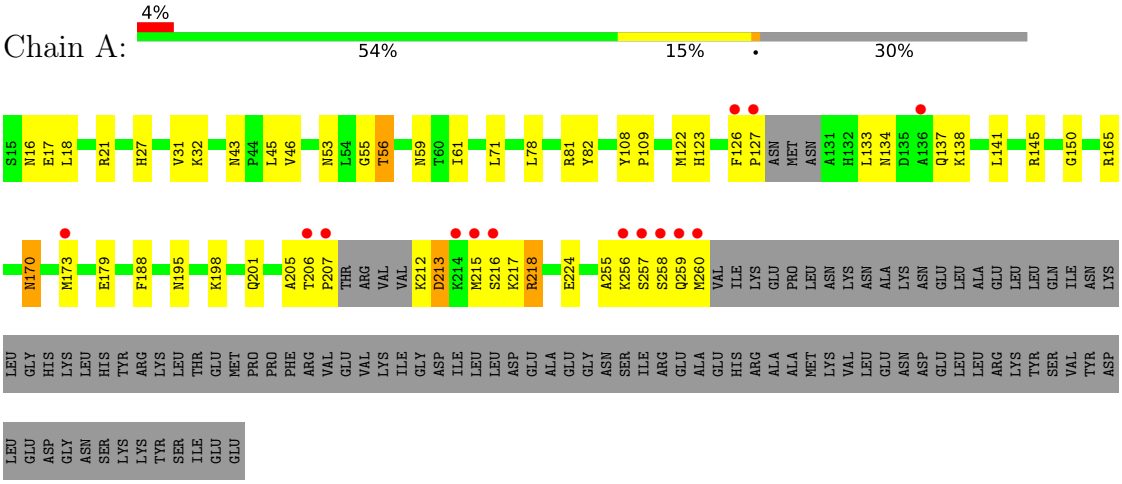
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	141	Total	O	0	0
			141	141		
3	C	98	Total	O	0	0
			98	98		
3	D	98	Total	O	0	0
			98	98		

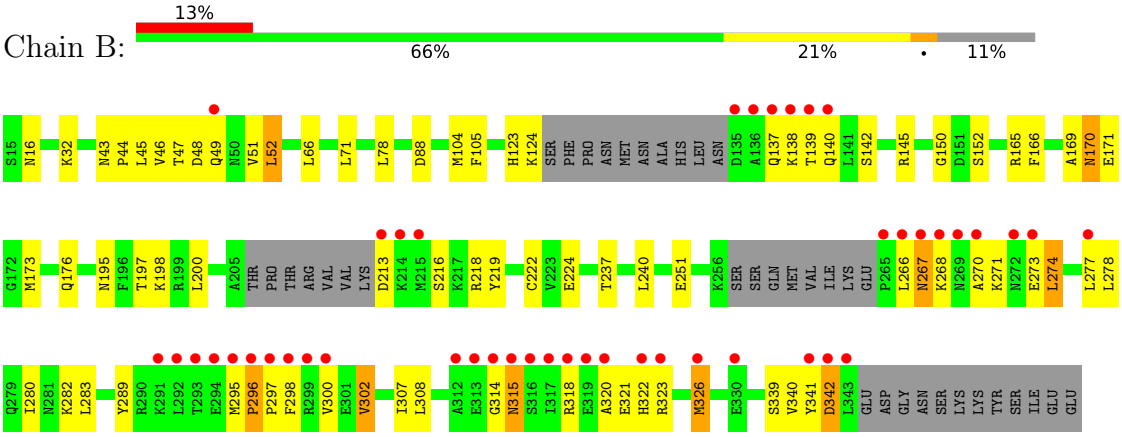
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

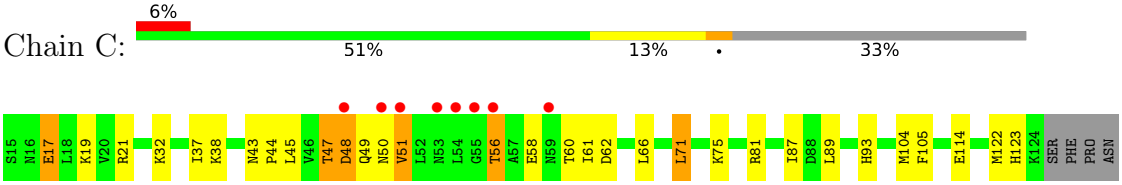
• Molecule 1: K. polysporus Dcr1

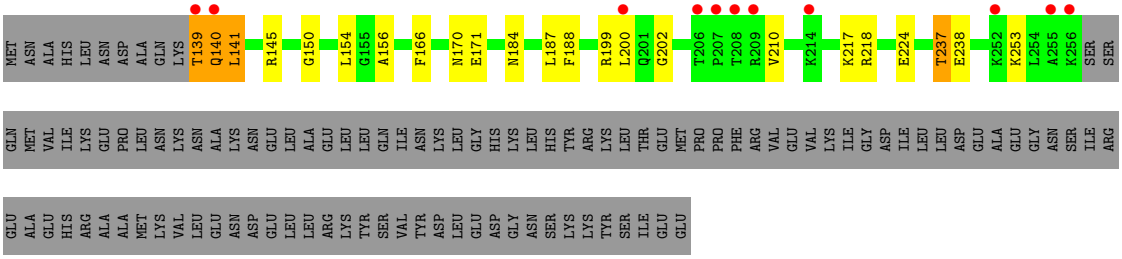


• Molecule 1: K. polysporus Dcr1

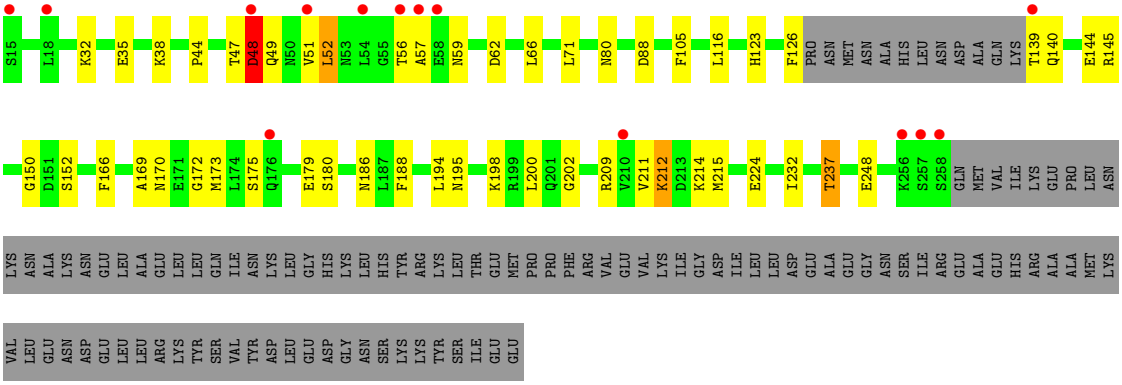


• Molecule 1: K. polysporus Dcr1





• Molecule 1: K. polysporus Dcr1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.04Å 112.97Å 135.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.41 – 2.29 43.41 – 2.29	Depositor EDS
% Data completeness (in resolution range)	92.4 (43.41-2.29) 92.4 (43.41-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.64 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_538	Depositor
R, R_{free}	0.175 , 0.220 0.172 , 0.215	Depositor DCC
R_{free} test set	3303 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8628	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.95% 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, 0.333 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: 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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/1974	0.52	0/2666
1	B	0.38	0/2517	0.50	0/3392
1	C	0.38	0/1889	0.51	0/2554
1	D	0.37	0/1919	0.52	0/2594
All	All	0.38	0/8299	0.51	0/11206

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	1939	0	1920	46	0
1	B	2477	0	2480	60	0
1	C	1856	0	1852	47	0
1	D	1885	0	1876	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	130	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	141	0	0	3	0
3	C	98	0	0	3	0
3	D	98	0	0	4	0
All	All	8628	0	8128	176	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 11.

All (176) 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:122:MET:HE1	1:A:141:LEU:HA	1.51	0.90
1:B:277:LEU:HD22	1:B:341:TYR:OH	1.75	0.85
1:C:140:GLN:O	1:C:140:GLN:HG2	1.83	0.77
1:B:124:LYS:HE2	1:B:138:LYS:HG2	1.66	0.76
1:B:197:THR:HA	1:B:219:TYR:HE2	1.51	0.75
1:B:198:LYS:HD2	1:B:198:LYS:H	1.55	0.72
1:B:195:ASN:HB3	1:B:198:LYS:HD3	1.70	0.72
1:C:71:LEU:HD13	1:C:75:LYS:HE2	1.70	0.71
1:B:200:LEU:HD21	1:B:222:CYS:SG	2.30	0.71
1:A:122:MET:CE	1:A:141:LEU:HA	2.20	0.71
1:B:289:TYR:CE2	1:B:302:VAL:HG13	2.25	0.69
1:B:213:ASP:HA	1:B:216:SER:HB3	1.73	0.69
1:B:137:GLN:HA	1:B:140:GLN:HE21	1.58	0.68
1:A:126:PHE:HB3	1:A:127:PRO:HD2	1.75	0.67
1:C:19:LYS:HE2	1:D:52:LEU:O	1.94	0.67
1:C:166:PHE:O	1:D:145:ARG:NH2	2.27	0.67
1:C:238:GLU:HG3	1:D:32:LYS:HE2	1.76	0.67
1:C:237:THR:HB	1:D:35:GLU:OE1	1.95	0.66
1:C:184:ASN:HD22	1:C:217:LYS:NZ	1.94	0.66
1:B:66:LEU:HA	1:B:71:LEU:HD12	1.78	0.65
1:A:206:THR:N	1:A:207:PRO:HD3	2.11	0.65
1:A:145:ARG:NH2	1:B:166:PHE:O	2.30	0.65
1:A:78:LEU:HD12	1:A:81:ARG:HD2	1.78	0.64
1:D:49:GLN:NE2	1:D:52:LEU:HD23	2.11	0.64
1:A:134:ASN:H	1:A:137:GLN:HE21	1.46	0.64
1:D:80:ASN:ND2	3:D:380:HOH:O	2.30	0.64
1:C:43:ASN:HD22	1:C:45:LEU:H	1.45	0.64
1:B:295:MET:HB3	1:B:296:PRO:HD2	1.80	0.64
1:C:17:GLU:HG3	1:C:21:ARG:HE	1.63	0.63
1:B:46:VAL:HG12	1:B:78:LEU:HD22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LYS:HE2	1:D:32:LYS:HD3	1.80	0.63
1:B:169:ALA:HA	1:B:173:MET:HE1	1.80	0.62
1:C:156:ALA:HA	1:D:152:SER:OG	1.98	0.62
1:C:114:GLU:HG2	3:C:441:HOH:O	1.98	0.62
1:C:145:ARG:NH2	1:D:166:PHE:O	2.34	0.61
1:C:123:HIS:HE1	1:C:200:LEU:HD22	1.65	0.61
1:D:47:THR:HG22	1:D:48:ASP:N	2.16	0.60
1:B:124:LYS:HG3	1:B:142:SER:HB3	1.85	0.59
1:B:51:VAL:HG23	1:B:52:LEU:HD13	1.84	0.59
1:A:46:VAL:HG12	1:A:78:LEU:HD22	1.84	0.58
1:D:170:ASN:ND2	1:D:172:GLY:H	2.00	0.58
1:A:260:MET:HA	1:B:173:MET:HE3	1.84	0.58
1:D:44:PRO:HA	1:D:48:ASP:HB2	1.85	0.58
1:C:43:ASN:ND2	1:C:45:LEU:H	2.01	0.58
1:B:47:THR:CG2	1:B:49:GLN:HG2	2.34	0.58
1:D:47:THR:O	1:D:49:GLN:N	2.37	0.57
1:B:283:LEU:CD2	1:B:307:ILE:HD12	2.34	0.57
1:B:280:ILE:HG22	1:B:340:VAL:HG21	1.86	0.57
1:C:44:PRO:HA	1:C:47:THR:HG22	1.87	0.57
1:A:32:LYS:NZ	3:B:449:HOH:O	2.36	0.56
1:B:123:HIS:CE1	1:B:218:ARG:HD2	2.40	0.56
1:B:318:ARG:O	1:B:322:HIS:HD2	1.88	0.56
1:B:273:GLU:O	1:B:277:LEU:HG	2.05	0.56
1:C:150:GLY:HA3	1:C:224:GLU:O	2.04	0.56
1:A:55:GLY:O	1:D:80:ASN:HA	2.06	0.55
1:C:237:THR:HG22	1:D:32:LYS:HG2	1.87	0.55
1:B:170:ASN:C	1:B:170:ASN:HD22	2.10	0.55
1:B:267:ASN:HB3	1:B:270:ALA:HB2	1.88	0.55
1:C:32:LYS:HA	1:D:237:THR:HG21	1.89	0.55
1:B:282:LYS:HE3	1:B:339:SER:O	2.07	0.55
3:C:449:HOH:O	1:D:237:THR:HG23	2.06	0.54
1:C:184:ASN:ND2	1:C:217:LYS:NZ	2.56	0.54
1:B:197:THR:HA	1:B:219:TYR:CE2	2.40	0.54
1:B:300:VAL:HG22	1:B:320:ALA:HB1	1.89	0.54
1:A:165:ARG:NH2	1:B:251:GLU:OE2	2.41	0.53
1:B:298:PHE:HD1	1:B:315:ASN:O	1.90	0.53
1:C:60:THR:HG22	1:C:62:ASP:H	1.73	0.53
1:B:170:ASN:ND2	1:B:173:MET:H	2.06	0.53
1:C:145:ARG:HD3	3:D:410:HOH:O	2.09	0.53
1:A:134:ASN:N	1:A:137:GLN:HE21	2.07	0.53
1:A:133:LEU:O	1:A:138:LYS:HE3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:THR:HG22	1:B:49:GLN:HG2	1.90	0.53
1:A:150:GLY:HA3	1:A:224:GLU:O	2.09	0.52
1:C:184:ASN:ND2	1:C:217:LYS:HZ2	2.08	0.52
1:C:199:ARG:HG2	1:C:200:LEU:HD12	1.92	0.52
1:D:150:GLY:HA3	1:D:224:GLU:O	2.10	0.52
1:A:170:ASN:ND2	1:A:173:MET:H	2.08	0.52
1:A:145:ARG:HD3	3:B:474:HOH:O	2.10	0.52
1:B:150:GLY:HA3	1:B:224:GLU:O	2.10	0.51
1:D:126:PHE:CE2	1:D:214:LYS:HB3	2.45	0.51
1:C:66:LEU:HA	1:C:71:LEU:HD12	1.93	0.51
1:C:122:MET:HE2	1:C:141:LEU:O	2.11	0.51
1:C:253:LYS:HE3	1:D:186:ASN:OD1	2.11	0.51
1:A:43:ASN:ND2	1:A:45:LEU:H	2.09	0.51
1:A:213:ASP:N	1:A:213:ASP:OD1	2.44	0.51
1:C:93:HIS:HE1	3:D:367:HOH:O	1.93	0.51
1:A:260:MET:HA	1:B:173:MET:CE	2.41	0.50
1:B:44:PRO:HB2	1:B:52:LEU:HD22	1.93	0.50
1:B:43:ASN:ND2	1:B:45:LEU:H	2.10	0.50
1:B:123:HIS:NE2	1:B:200:LEU:HD22	2.26	0.50
1:A:27:HIS:O	1:A:31:VAL:HG23	2.11	0.50
1:C:61:ILE:HG13	1:D:105:PHE:CE2	2.46	0.50
1:C:139:THR:HG22	1:C:140:GLN:H	1.76	0.50
1:D:47:THR:O	1:D:48:ASP:C	2.50	0.49
1:B:315:ASN:OD1	1:B:315:ASN:N	2.41	0.49
1:C:17:GLU:CG	1:C:21:ARG:HE	2.24	0.48
1:D:126:PHE:CZ	1:D:215:MET:CE	2.96	0.48
1:C:184:ASN:HD22	1:C:217:LYS:HZ3	1.60	0.48
1:C:38:LYS:HA	1:C:87:ILE:HD11	1.96	0.48
1:D:38:LYS:HE3	3:D:432:HOH:O	2.12	0.48
1:B:47:THR:HG22	1:B:49:GLN:H	1.79	0.48
1:A:179:GLU:HB3	3:A:476:HOH:O	2.14	0.47
1:D:116:LEU:HD21	1:D:232:ILE:HG21	1.95	0.47
1:A:53:ASN:O	1:A:56:THR:HB	2.14	0.47
1:B:323:ARG:O	1:B:326:MET:HB2	2.14	0.47
1:D:56:THR:HG22	1:D:57:ALA:N	2.29	0.47
1:C:56:THR:HG21	1:C:60:THR:HG21	1.96	0.47
1:A:212:LYS:HB3	1:A:215:MET:CB	2.44	0.46
1:D:169:ALA:HB1	1:D:173:MET:HB2	1.98	0.46
1:A:170:ASN:HD22	1:A:170:ASN:C	2.18	0.46
3:A:453:HOH:O	1:B:171:GLU:HG3	2.14	0.46
1:B:268:LYS:O	1:B:322:HIS:HE1	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:GLN:HG3	1:D:52:LEU:HB2	1.97	0.46
1:A:134:ASN:O	1:A:137:GLN:HG2	2.16	0.46
1:D:52:LEU:O	1:D:52:LEU:HD13	2.16	0.46
1:A:17:GLU:O	1:A:21:ARG:HG3	2.16	0.46
1:B:237:THR:HA	1:B:240:LEU:HB2	1.98	0.45
1:A:205:ALA:C	1:A:207:PRO:HD3	2.36	0.45
1:A:123:HIS:CD2	1:A:218:ARG:HD3	2.52	0.45
1:B:300:VAL:HG21	1:B:321:GLU:N	2.32	0.45
1:D:123:HIS:NE2	1:D:200:LEU:HD13	2.31	0.45
1:D:126:PHE:HZ	1:D:215:MET:CE	2.29	0.45
1:D:175:SER:O	1:D:179:GLU:HG2	2.17	0.45
1:B:298:PHE:CD1	1:B:315:ASN:O	2.70	0.45
1:C:32:LYS:HE3	3:C:391:HOH:O	2.16	0.45
1:A:108:TYR:HB2	1:A:109:PRO:CD	2.47	0.44
1:A:256:LYS:C	1:A:258:SER:H	2.20	0.44
1:A:43:ASN:ND2	1:A:45:LEU:HB2	2.32	0.44
1:C:49:GLN:HB3	1:C:51:VAL:HG12	1.97	0.44
1:D:188:PHE:CZ	1:D:211:VAL:HG11	2.53	0.44
1:A:126:PHE:O	1:A:127:PRO:C	2.55	0.44
1:B:124:LYS:CE	1:B:138:LYS:HG2	2.42	0.44
1:B:145:ARG:NH1	3:B:366:HOH:O	2.45	0.44
1:A:32:LYS:HE3	1:B:32:LYS:HE2	2.00	0.44
1:A:188:PHE:CD1	1:A:216:SER:HA	2.53	0.44
1:D:126:PHE:CZ	1:D:215:MET:HE2	2.52	0.44
1:D:212:LYS:HB3	1:D:215:MET:HG2	1.99	0.44
1:B:314:GLY:HA3	1:B:320:ALA:HB2	1.99	0.43
1:C:154:LEU:HD21	1:C:187:LEU:HD21	2.00	0.43
1:D:56:THR:H	1:D:59:ASN:HD22	1.65	0.43
1:B:200:LEU:HD11	1:B:222:CYS:SG	2.59	0.43
1:D:59:ASN:HB3	1:D:62:ASP:HB2	2.01	0.43
1:A:195:ASN:ND2	1:A:198:LYS:HD2	2.34	0.43
1:B:295:MET:C	1:B:297:PRO:HD2	2.39	0.43
1:D:126:PHE:HZ	1:D:215:MET:HE2	1.83	0.43
1:A:212:LYS:HB3	1:A:215:MET:HB3	2.01	0.42
1:A:122:MET:CE	1:A:141:LEU:CA	2.92	0.42
1:A:59:ASN:OD1	1:A:61:ILE:HG22	2.19	0.42
1:A:82:TYR:HB2	3:A:464:HOH:O	2.19	0.42
1:C:17:GLU:CD	1:C:21:ARG:HH21	2.23	0.42
1:C:170:ASN:HB2	1:D:144:GLU:OE1	2.19	0.42
1:C:188:PHE:HZ	1:C:210:VAL:HG12	1.83	0.42
1:D:126:PHE:CZ	1:D:215:MET:HE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:C	1:A:257:SER:H	2.22	0.42
1:C:122:MET:CE	1:C:141:LEU:O	2.67	0.42
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.87	0.42
1:A:217:LYS:NZ	3:A:389:HOH:O	2.51	0.42
1:C:71:LEU:HD23	1:C:71:LEU:HA	1.85	0.42
1:B:341:TYR:CD1	1:B:342:ASP:N	2.88	0.41
1:C:89:LEU:O	1:C:93:HIS:HD2	2.02	0.41
1:B:326:MET:HA	1:B:326:MET:CE	2.50	0.41
1:B:137:GLN:HA	1:B:140:GLN:NE2	2.30	0.41
1:B:271:LYS:HE2	1:B:289:TYR:CE1	2.55	0.41
1:B:277:LEU:HD22	1:B:341:TYR:HH	1.80	0.41
1:A:198:LYS:HA	1:A:201:GLN:HG2	2.03	0.41
1:D:66:LEU:HA	1:D:71:LEU:HD23	2.01	0.41
1:C:104:MET:CE	1:C:105:PHE:CZ	3.04	0.41
1:A:61:ILE:HD12	1:B:105:PHE:CD2	2.56	0.41
1:B:277:LEU:O	1:B:278:LEU:HD23	2.21	0.41
1:D:194:LEU:O	1:D:195:ASN:HB2	2.21	0.41
1:C:58:GLU:O	1:C:58:GLU:HG2	2.21	0.40
1:D:139:THR:HG22	1:D:140:GLN:N	2.36	0.40
1:C:37:ILE:HD12	1:C:37:ILE:HA	1.95	0.40
1:C:49:GLN:O	1:C:50:ASN:HB3	2.21	0.40
1:A:259:GLN:HG3	1:B:176:GLN:OE1	2.22	0.40
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.88	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	233/341 (68%)	226 (97%)	7 (3%)	0	100 100
1	B	296/341 (87%)	288 (97%)	7 (2%)	1 (0%)	41 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	224/341 (66%)	215 (96%)	7 (3%)	2 (1%)	17 20
1	D	228/341 (67%)	218 (96%)	6 (3%)	4 (2%)	8 7
All	All	981/1364 (72%)	947 (96%)	27 (3%)	7 (1%)	22 26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ASP
1	D	48	ASP
1	D	209	ARG
1	D	212	LYS
1	B	296	PRO
1	D	202	GLY
1	C	202	GLY

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	218/310 (70%)	212 (97%)	6 (3%)	43 60
1	B	275/310 (89%)	258 (94%)	17 (6%)	18 25
1	C	209/310 (67%)	196 (94%)	13 (6%)	18 25
1	D	213/310 (69%)	205 (96%)	8 (4%)	33 47
All	All	915/1240 (74%)	871 (95%)	44 (5%)	25 36

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	56	THR
1	A	71	LEU
1	A	170	ASN
1	A	213	ASP

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Mol	Chain	Res	Type
1	A	218	ARG
1	B	16	ASN
1	B	48	ASP
1	B	52	LEU
1	B	88	ASP
1	B	104	MET
1	B	139	THR
1	B	152	SER
1	B	165	ARG
1	B	170	ASN
1	B	266	LEU
1	B	267	ASN
1	B	274	LEU
1	B	302	VAL
1	B	308	LEU
1	B	315	ASN
1	B	326	MET
1	B	342	ASP
1	C	17	GLU
1	C	47	THR
1	C	48	ASP
1	C	51	VAL
1	C	56	THR
1	C	71	LEU
1	C	81	ARG
1	C	139	THR
1	C	140	GLN
1	C	141	LEU
1	C	171	GLU
1	C	218	ARG
1	C	237	THR
1	D	48	ASP
1	D	51	VAL
1	D	52	LEU
1	D	88	ASP
1	D	180	SER
1	D	198	LYS
1	D	237	THR
1	D	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	43	ASN
1	A	49	GLN
1	A	72	ASN
1	A	123	HIS
1	A	137	GLN
1	A	170	ASN
1	A	195	ASN
1	B	43	ASN
1	B	140	GLN
1	B	170	ASN
1	B	267	ASN
1	B	322	HIS
1	C	16	ASN
1	C	43	ASN
1	C	93	HIS
1	C	184	ASN
1	C	185	ASN
1	D	43	ASN
1	D	49	GLN
1	D	53	ASN
1	D	72	ASN
1	D	80	ASN
1	D	93	HIS
1	D	170	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	239/341 (70%)	-0.11	14 (5%) 22 28	14, 32, 98, 144	0
1	B	304/341 (89%)	0.40	45 (14%) 2 3	11, 38, 127, 170	0
1	C	228/341 (66%)	0.01	19 (8%) 11 15	14, 36, 105, 147	0
1	D	232/341 (68%)	-0.07	14 (6%) 21 28	15, 37, 104, 137	0
All	All	1003/1364 (73%)	0.08	92 (9%) 9 12	11, 36, 109, 170	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	TYR	11.3
1	C	54	LEU	8.5
1	B	343	LEU	8.3
1	A	206	THR	7.1
1	B	293	THR	6.7
1	D	58	GLU	6.7
1	A	215	MET	6.5
1	A	207	PRO	6.4
1	A	260	MET	6.4
1	B	323	ARG	6.4
1	B	296	PRO	6.0
1	D	56	THR	5.9
1	A	258	SER	5.9
1	B	299	ARG	5.8
1	B	215	MET	5.8
1	B	270	ALA	5.7
1	B	266	LEU	5.6
1	C	139	THR	5.4
1	C	48	ASP	5.4
1	B	298	PHE	5.4
1	B	214	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLN	5.3
1	B	295	MET	5.1
1	B	213	ASP	5.0
1	B	319	GLU	4.9
1	B	292	LEU	4.8
1	B	317	ILE	4.8
1	C	53	ASN	4.8
1	A	127	PRO	4.7
1	B	297	PRO	4.7
1	D	258	SER	4.7
1	B	136	ALA	4.7
1	B	269	ASN	4.6
1	A	214	LYS	4.6
1	B	265	PRO	4.5
1	B	342	ASP	4.5
1	B	315	ASN	4.5
1	D	15	SER	4.4
1	B	318	ARG	4.4
1	C	50	ASN	4.4
1	C	209	ARG	4.3
1	C	200	LEU	4.2
1	B	300	VAL	4.1
1	D	48	ASP	3.9
1	D	257	SER	3.9
1	B	294	GLU	3.9
1	D	139	THR	3.7
1	C	56	THR	3.7
1	C	55	GLY	3.6
1	B	268	LYS	3.6
1	C	206	THR	3.6
1	A	259	GLN	3.5
1	D	210	VAL	3.4
1	B	320	ALA	3.4
1	A	126	PHE	3.4
1	D	54	LEU	3.4
1	B	137	GLN	3.3
1	B	330	GLU	3.2
1	C	59	ASN	3.0
1	C	214	LYS	3.0
1	C	140	GLN	3.0
1	B	312	ALA	3.0
1	B	267	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	313	GLU	3.0
1	D	256	LYS	2.9
1	B	138	LYS	2.9
1	B	291	LYS	2.8
1	B	314	GLY	2.8
1	A	257	SER	2.7
1	D	57	ALA	2.7
1	C	252	LYS	2.7
1	B	322	HIS	2.7
1	A	136	ALA	2.6
1	B	316	SER	2.6
1	A	216	SER	2.4
1	B	273	GLU	2.4
1	B	277	LEU	2.4
1	C	51	VAL	2.4
1	B	272	ASN	2.4
1	A	173	MET	2.4
1	D	176	GLN	2.3
1	C	207	PRO	2.3
1	B	326	MET	2.2
1	B	139	THR	2.2
1	C	255	ALA	2.2
1	D	51	VAL	2.2
1	C	208	THR	2.2
1	C	256	LYS	2.1
1	B	135	ASP	2.1
1	A	256	LYS	2.1
1	B	49	GLN	2.0
1	D	18	LEU	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 monosaccharides in this entry.

6.4 Ligands

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, 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	B-factors(Å^2)	Q<0.9
2	MG	D	2	1/1	0.81	0.07	56,56,56,56	0
2	MG	A	1	1/1	0.93	0.07	45,45,45,45	0
2	MG	B	3	1/1	0.95	0.05	49,49,49,49	0
2	MG	C	4	1/1	0.98	0.04	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.