Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 07:24 AM EDT

PDB ID	:	6E29
Title	:	Crystal structure of Myceliophteria_thermophila Cps50 (Swd1) beta-propeller domain
Authors	:	Joshi, M.; Yang, Y.; Brunzelle, J.S.; Couture, J.F.
Deposited on	:	2018-07-10
Resolution	:	1.82 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:

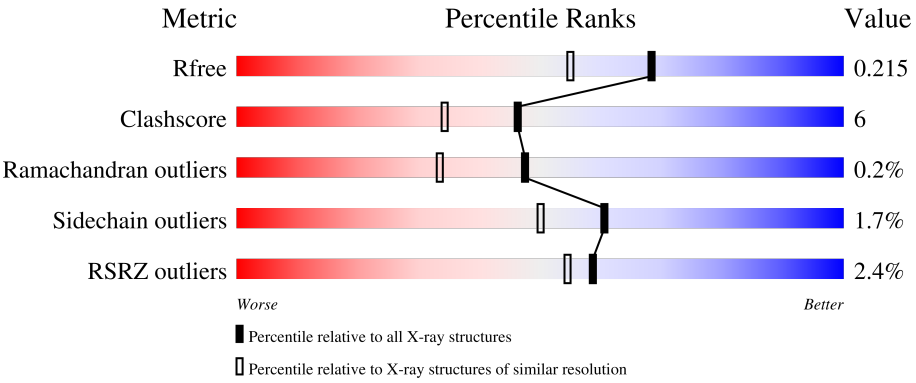
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	345	3% 85% 9% • 5%
1	B	345	3% 75% 15% • 9%
1	C	345	2% 77% 13% • 9%
1	D	345	% 78% 11% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10930 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 SWD1-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	312	Total	C	N	O	S	3	7	0
			2514	1594	457	454	9			
1	A	327	Total	C	N	O	S	4	8	0
			2646	1672	481	484	9			
1	B	315	Total	C	N	O	S	0	8	0
			2547	1616	461	461	9			
1	C	314	Total	C	N	O	S	0	10	0
			2547	1613	463	462	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	GLY	-	expression tag	UNP G2Q1Q9
A	0	GLY	-	expression tag	UNP G2Q1Q9
B	0	GLY	-	expression tag	UNP G2Q1Q9
C	0	GLY	-	expression tag	UNP G2Q1Q9

- Molecule 2 is water.

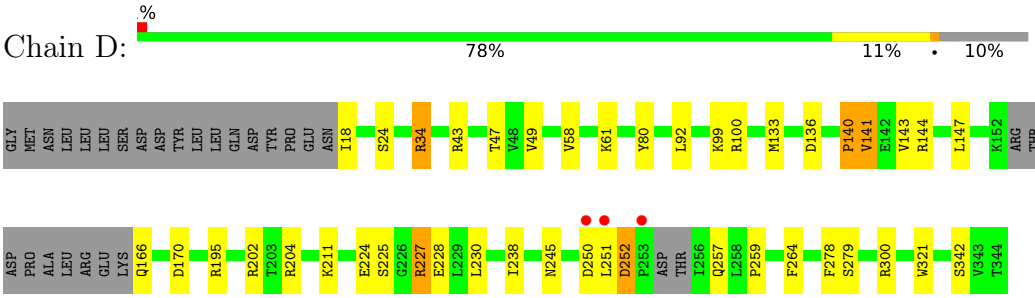
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	213	Total	O	0	0
			213	213		
2	A	126	Total	O	0	0
			126	126		
2	B	164	Total	O	0	0
			164	164		
2	C	173	Total	O	0	0
			173	173		

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.

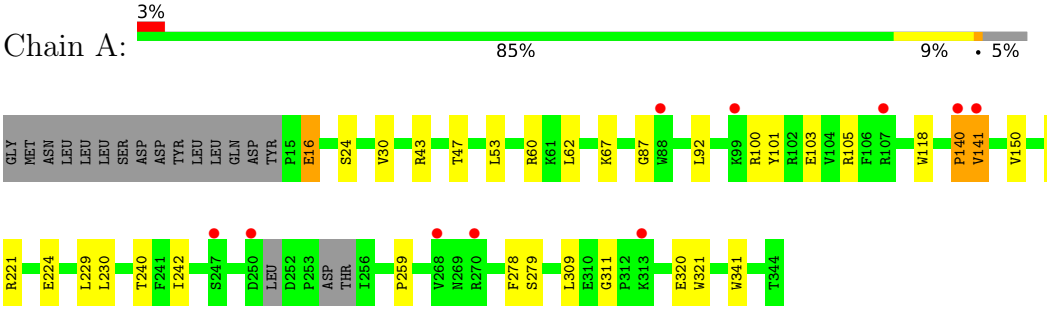
• Molecule 1: SWD1-like protein

Chain D:



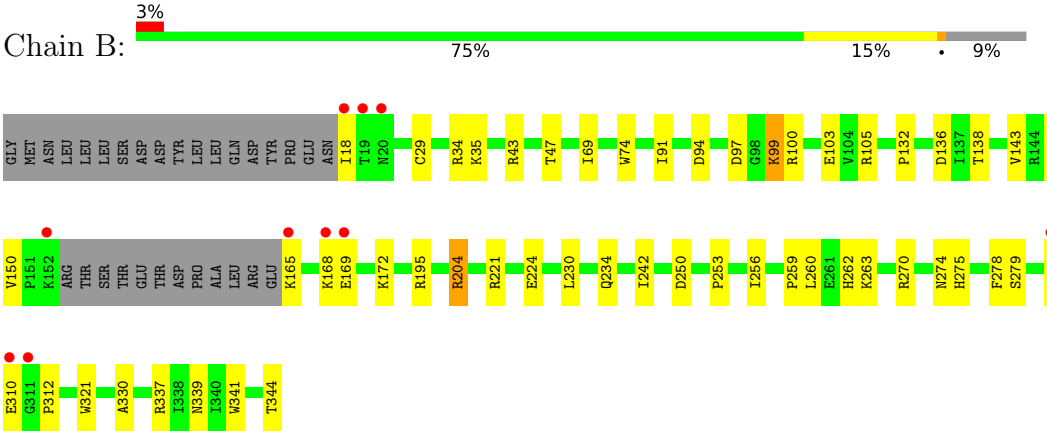
• Molecule 1: SWD1-like protein

Chain A:



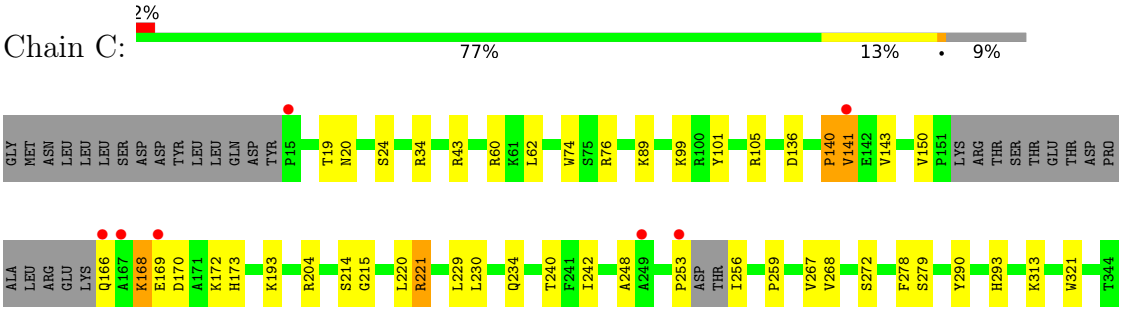
• Molecule 1: SWD1-like protein

Chain B:



• Molecule 1: SWD1-like protein

Chain C:


2%
77%
13%
9%
GLY MET ASN LEU LEU LEU SER ASP ASP TYR LEU LEU LEU GLN ASP TYR P15 T19 N20 S24 R34 R43 R60 K61 L62 W74 S75 R76 K89 K99 R100 Y101 R105 D136 P140 V141 E142 V143 V150 P151 LYS ARG THR SER THR GLU THR ASP PRO
ALA LEU ARG GLU LYS Q166 A167 K168 E169 D170 A171 K172 H173 K193 R204 S214 G215 L220 R221 L229 L230 Q234 T240 F241 I242 A248 A249 P253 ASP THR I256 P259 V267 V268 S272 F278 S279 Y290 H293 K313 W321 T344

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.78Å 88.90Å 124.32Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	45.03 – 1.82 45.03 – 1.82	Depositor EDS
% Data completeness (in resolution range)	91.0 (45.03-1.82) 91.0 (45.03-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.82Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.168 , 0.216 0.169 , 0.215	Depositor DCC
R_{free} test set	5197 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10930	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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

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	0.65	1/2727 (0.0%)	0.80	2/3701 (0.1%)
1	B	0.65	0/2630	0.79	1/3571 (0.0%)
1	C	0.73	0/2633	0.86	2/3575 (0.1%)
1	D	0.74	1/2592 (0.0%)	0.87	5/3518 (0.1%)
All	All	0.69	2/10582 (0.0%)	0.83	10/14365 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	252	ASP	N-CA	-7.28	1.31	1.46
1	A	16	GLU	CB-CG	-5.80	1.41	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	141	VAL	N-CA-C	-12.29	77.81	111.00
1	A	140	PRO	N-CA-C	12.28	144.04	112.10
1	C	141	VAL	N-CA-C	-10.83	81.75	111.00
1	D	141	VAL	N-CA-C	-10.37	82.99	111.00
1	C	140	PRO	N-CA-C	10.27	138.79	112.10
1	D	140	PRO	N-CA-C	8.59	134.43	112.10
1	D	251	LEU	O-C-N	7.50	134.69	122.70
1	D	251	LEU	CA-C-N	-6.99	101.81	117.20
1	B	310	GLU	CB-CA-C	-6.48	97.44	110.40
1	D	252	ASP	N-CA-C	-6.21	94.23	111.00

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	2646	0	2639	34	0
1	B	2547	0	2552	38	0
1	C	2547	0	2542	32	1
1	D	2514	0	2518	40	1
2	A	126	0	0	1	0
2	B	164	0	0	6	0
2	C	173	0	0	10	0
2	D	213	0	0	6	0
All	All	10930	0	10251	128	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 6.

All (128) 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:227:ARG:NH1	1:A:118:TRP:CZ3	2.11	1.17
1:D:227:ARG:NH1	1:A:118:TRP:CE3	2.14	1.16
1:D:195:ARG:NH1	1:D:211:LYS:HB2	1.67	1.09
1:D:227:ARG:NH1	1:A:118:TRP:CH2	2.32	0.95
1:D:227:ARG:NH1	1:A:118:TRP:CD2	2.36	0.93
1:D:252:ASP:OD2	2:D:401:HOH:O	1.96	0.82
1:D:195:ARG:HH12	1:D:211:LYS:HB2	1.45	0.81
1:B:270:ARG:NH1	2:B:401:HOH:O	2.11	0.80
1:D:227:ARG:NH1	1:A:118:TRP:CE2	2.51	0.78
1:D:136:ASP:HB3	1:D:143:VAL:HG13	1.68	0.76
1:D:227:ARG:NH1	1:A:118:TRP:CZ2	2.54	0.76
1:D:225:SER:HB3	1:A:224:GLU:HG3	1.68	0.75
1:B:136:ASP:OD1	1:B:138:THR:HG23	1.88	0.73
1:C:166:GLN:N	2:C:401:HOH:O	2.22	0.71
1:B:145:TYR:CD2	1:B:204:ARG:NH1	2.61	0.68
1:C:24:SER:O	1:C:43:ARG:HD2	1.93	0.68
1:D:224:GLU:O	2:D:403:HOH:O	2.12	0.68
1:D:227:ARG:HD3	1:A:118:TRP:CZ2	2.29	0.68
1:D:18:ILE:HG23	1:D:342[B]:SER:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:OE2	1:B:105:ARG:NH1	2.27	0.67
1:D:250:ASP:OD2	2:D:402:HOH:O	2.10	0.67
1:C:60:ARG:NH1	2:C:405:HOH:O	2.28	0.66
1:A:154:THR:HB	1:B:290[B]:TYR:OH	1.97	0.65
1:D:166:GLN:N	2:D:406:HOH:O	2.30	0.63
1:D:18:ILE:HG23	1:D:342[A]:SER:HB2	1.80	0.63
1:C:168:LYS:NZ	2:C:403:HOH:O	2.26	0.63
1:D:49:VAL:HG13	1:D:58:VAL:HG13	1.81	0.62
1:A:150[A]:VAL:HG22	1:C:268:VAL:HG13	1.81	0.62
1:B:34:ARG:NH2	1:B:74:TRP:O	2.32	0.62
1:C:60:ARG:HD3	1:C:62:LEU:HD21	1.82	0.61
1:D:49:VAL:HG22	1:D:61:LYS:HG2	1.82	0.61
1:B:145:TYR:CE2	1:B:204:ARG:NH1	2.69	0.61
1:D:133:MET:HE2	1:D:144:ARG:HB3	1.85	0.59
1:C:19:THR:HG22	1:C:20:ASN:OD1	2.03	0.59
1:D:136:ASP:HB3	1:D:143:VAL:CG1	2.32	0.59
1:D:227:ARG:HD2	2:D:450:HOH:O	2.02	0.59
1:B:145:TYR:CD2	1:B:204:ARG:CZ	2.86	0.59
1:B:262:HIS:ND1	2:B:404:HOH:O	2.32	0.59
1:A:24:SER:O	1:A:43:ARG:HD2	2.03	0.58
1:B:34:ARG:NH2	2:B:406:HOH:O	2.36	0.58
1:B:100:ARG:HD2	1:B:103:GLU:OE1	2.04	0.57
1:D:24:SER:O	1:D:43:ARG:HD2	2.05	0.57
1:A:16:GLU:OE2	1:A:311:GLY:N	2.35	0.57
1:B:221:ARG:HH22	1:B:275[B]:HIS:CE1	2.23	0.57
1:C:242:ILE:HB	1:C:259:PRO:HG2	1.87	0.57
1:A:67:LYS:HE3	1:A:87:GLY:HA2	1.88	0.56
1:C:20:ASN:ND2	2:C:407:HOH:O	2.32	0.56
1:B:132:PRO:HG2	1:B:147:LEU:HB2	1.87	0.56
1:D:227:ARG:HD3	1:A:118:TRP:CH2	2.40	0.55
1:A:60:ARG:HD3	1:A:62:LEU:HD21	1.89	0.55
1:B:253:PRO:HA	1:B:256:ILE:HD12	1.89	0.54
1:A:43:ARG:HG3	1:A:47:THR:O	2.08	0.53
1:A:163:ARG:NH1	1:B:234:GLN:OE1	2.42	0.53
1:B:18:ILE:HD11	1:B:339:ASN:HB3	1.91	0.53
1:C:172:LYS:HB3	1:C:193:LYS:NZ	2.23	0.52
1:A:103:GLU:CD	1:A:105:ARG:HH12	2.14	0.52
1:B:330:ALA:HB3	1:B:341:TRP:HZ3	1.74	0.51
1:C:136:ASP:HB3	1:C:143:VAL:HG13	1.91	0.51
1:B:253:PRO:HA	1:B:256:ILE:CD1	2.40	0.51
1:C:248:ALA:N	2:C:406:HOH:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LYS:HE3	2:B:464:HOH:O	2.11	0.50
1:A:16:GLU:HG3	1:A:309:LEU:HD22	1.94	0.50
1:C:169:GLU:OE1	1:C:169:GLU:N	2.41	0.50
1:D:34:ARG:NE	1:D:34:ARG:HA	2.25	0.50
1:C:99:LYS:HE3	1:C:101:TYR:HA	1.94	0.49
1:D:257:GLN:HG2	1:D:259:PRO:HD3	1.93	0.49
1:A:103:GLU:OE1	1:A:105:ARG:NH1	2.45	0.49
1:B:312:PRO:HB3	1:B:337:ARG:HH22	1.77	0.49
1:A:30:VAL:O	1:A:320:GLU:HG3	2.13	0.49
1:B:168:LYS:HD2	1:B:168:LYS:H	1.77	0.48
1:D:225:SER:HB3	1:A:224:GLU:CG	2.41	0.48
1:D:34:ARG:NH2	2:D:417:HOH:O	2.47	0.48
1:C:173:HIS:ND1	2:C:402:HOH:O	2.25	0.48
1:A:279:SER:HA	1:A:321:TRP:CG	2.49	0.48
1:C:293[B]:HIS:HD2	1:C:313:LYS:HD2	1.80	0.47
1:B:242:ILE:HB	1:B:259:PRO:HG2	1.96	0.47
1:C:34:ARG:HH12	1:C:74:TRP:HB2	1.80	0.47
1:D:147:LEU:HD23	1:D:204:ARG:HG2	1.97	0.47
1:D:170:ASP:OD2	1:D:170:ASP:N	2.48	0.47
1:A:154:THR:HB	1:B:290[B]:TYR:HH	1.79	0.47
1:C:204:ARG:NE	2:C:409:HOH:O	2.35	0.47
1:C:230:LEU:HB2	1:C:278:PHE:CZ	2.50	0.47
1:D:43:ARG:HG3	1:D:47:THR:O	2.15	0.47
1:B:307:ARG:NH1	1:B:344:THR:H	2.13	0.47
1:C:267:VAL:HG23	2:C:454:HOH:O	2.15	0.46
1:C:293[B]:HIS:CD2	1:C:313:LYS:HD2	2.50	0.46
1:B:195:ARG:HG3	2:B:476:HOH:O	2.15	0.46
1:D:245:ASN:HB2	1:A:118:TRP:CE3	2.51	0.46
1:A:92:LEU:HD23	1:A:101:TYR:HD2	1.81	0.46
1:C:279:SER:HA	1:C:321:TRP:CG	2.51	0.46
1:B:230:LEU:HB2	1:B:278:PHE:CZ	2.51	0.45
1:B:260:LEU:HD21	1:B:263:LYS:HG3	1.97	0.45
1:B:97:ASP:OD1	1:B:99:LYS:HE2	2.16	0.45
1:B:169:GLU:OE1	1:B:172:LYS:HD2	2.17	0.45
1:C:272[A]:SER:HB3	1:C:290:TYR:HB3	1.97	0.45
1:D:202:ARG:O	1:D:204:ARG:NH2	2.50	0.44
1:D:227:ARG:CZ	1:A:118:TRP:CE2	3.00	0.44
1:D:279:SER:HA	1:D:321:TRP:CG	2.52	0.44
1:D:195:ARG:HH11	1:D:211:LYS:HB2	1.73	0.44
1:B:145:TYR:CE2	1:B:204:ARG:CZ	3.01	0.44
1:A:242:ILE:HB	1:A:259:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:HD2	1:C:76:ARG:HA	2.00	0.44
1:B:94:ASP:HB3	1:B:99:LYS:HE3	1.99	0.44
1:C:89:LYS:HG2	1:C:105:ARG:HG2	2.00	0.44
1:C:253:PRO:HA	1:C:256:ILE:HG13	1.99	0.43
1:B:274:ASN:OD1	1:B:290[A]:TYR:CE1	2.72	0.43
1:A:309:LEU:HD13	1:A:341:TRP:CD1	2.54	0.43
1:D:80:TYR:HB3	1:D:92:LEU:HD11	2.01	0.42
1:D:230:LEU:HB2	1:D:278:PHE:CZ	2.54	0.42
1:B:29[B]:CYS:SG	1:B:69:ILE:HG22	2.59	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.81	0.42
1:B:34:ARG:HG2	2:B:509:HOH:O	2.18	0.42
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.88	0.42
1:B:91:ILE:HG23	1:B:100:ARG:HG3	2.02	0.42
1:C:166:GLN:OE1	1:C:170:ASP:OD2	2.37	0.42
1:C:215:GLY:HA3	1:C:234:GLN:HG2	2.01	0.42
1:A:221:ARG:HG2	2:A:493:HOH:O	2.19	0.41
1:A:230:LEU:HB2	1:A:278:PHE:CZ	2.55	0.41
1:C:34:ARG:HG2	2:C:416:HOH:O	2.19	0.41
1:C:220:LEU:O	1:C:221:ARG:HG2	2.20	0.41
1:C:234:GLN:NE2	2:C:413:HOH:O	2.44	0.41
1:D:228:GLU:HG2	1:D:300:ARG:NH2	2.35	0.41
1:A:229:LEU:O	1:A:240:THR:HA	2.20	0.41
1:B:279:SER:HA	1:B:321:TRP:CG	2.55	0.41
1:B:43:ARG:HG3	1:B:47:THR:O	2.21	0.40
1:D:238:ILE:HB	1:D:264:PHE:HB2	2.03	0.40
1:B:136:ASP:HB3	1:B:143:VAL:HB	2.03	0.40
1:C:229:LEU:O	1:C:240:THR:HA	2.22	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:D:195:ARG:NH2	1:C:141:VAL:CB[1_545]	2.16	0.04

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	329/345 (95%)	314 (95%)	14 (4%)	1 (0%)	41	27
1	B	319/345 (92%)	308 (97%)	11 (3%)	0	100	100
1	C	318/345 (92%)	311 (98%)	6 (2%)	1 (0%)	41	27
1	D	313/345 (91%)	304 (97%)	8 (3%)	1 (0%)	41	27
All	All	1279/1380 (93%)	1237 (97%)	39 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	PRO
1	C	140	PRO
1	D	140	PRO

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	287/296 (97%)	285 (99%)	2 (1%)	84	80
1	B	276/296 (93%)	268 (97%)	8 (3%)	42	28
1	C	277/296 (94%)	272 (98%)	5 (2%)	59	48
1	D	272/296 (92%)	267 (98%)	5 (2%)	59	48
All	All	1112/1184 (94%)	1092 (98%)	20 (2%)	60	48

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	34	ARG
1	D	99	LYS
1	D	100	ARG

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Mol	Chain	Res	Type
1	D	141	VAL
1	D	227	ARG
1	A	100	ARG
1	A	141	VAL
1	B	99	LYS
1	B	150[A]	VAL
1	B	150[B]	VAL
1	B	165	LYS
1	B	204	ARG
1	B	224	GLU
1	B	250	ASP
1	B	307	ARG
1	C	150[A]	VAL
1	C	150[B]	VAL
1	C	168	LYS
1	C	214	SER
1	C	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	339	ASN
1	C	166	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	327/345 (94%)	0.07	10 (3%)	49	43	21, 39, 65, 113	0
1	B	315/345 (91%)	-0.13	10 (3%)	47	42	21, 32, 56, 102	0
1	C	314/345 (91%)	-0.14	7 (2%)	62	58	19, 31, 62, 152	0
1	D	312/345 (90%)	-0.09	3 (0%)	82	80	17, 29, 55, 129	0
All	All	1268/1380 (91%)	-0.07	30 (2%)	59	54	17, 33, 61, 152	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	THR	4.8
1	D	253	PRO	4.6
1	A	141	VAL	4.4
1	B	165	LYS	4.3
1	C	15	PRO	4.2
1	A	313	LYS	4.1
1	B	310	GLU	4.0
1	A	140	PRO	3.9
1	B	20	ASN	3.9
1	A	88	TRP	3.8
1	B	169	GLU	3.8
1	A	268	VAL	3.6
1	C	167	ALA	3.5
1	C	169	GLU	3.4
1	D	250	ASP	3.2
1	B	18	ILE	3.1
1	A	247	SER	3.1
1	C	166	GLN	3.1
1	C	249	ALA	3.0
1	A	107	ARG	2.9
1	D	251	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	152	LYS	2.7
1	A	270	ARG	2.6
1	A	99	LYS	2.5
1	B	290[A]	TYR	2.4
1	B	311	GLY	2.3
1	A	250	ASP	2.3
1	C	141	VAL	2.3
1	C	253	PRO	2.1
1	B	168	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.