Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2016 – 04:32 AM EST

PDB ID	:	5TD8
Title	:	Crystal structure of an Extended Dwarf Ndc80 Complex
Authors	:	Valverde, R.; Ingram, J.; Harrison, S.C.
Deposited on	:	2016-09-17
Resolution	:	7.53 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

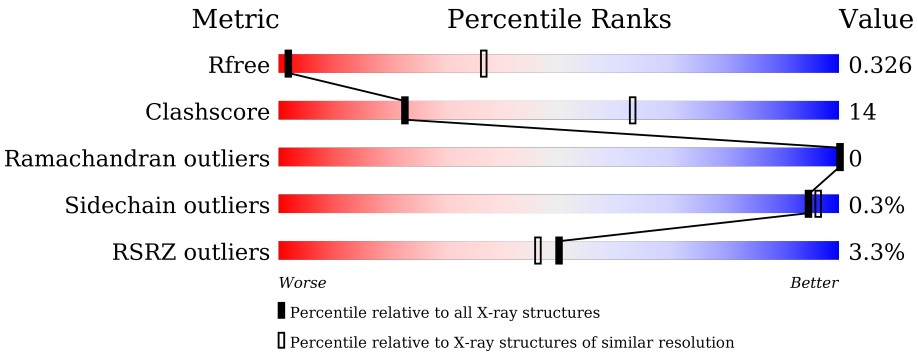
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

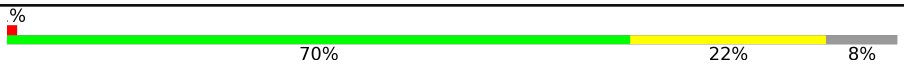
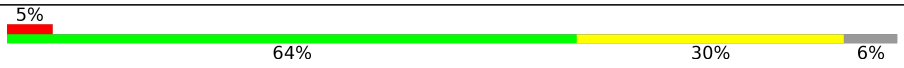
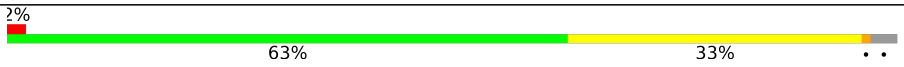
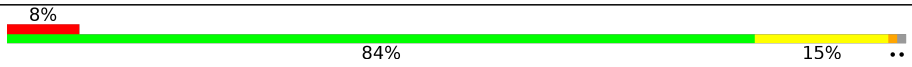
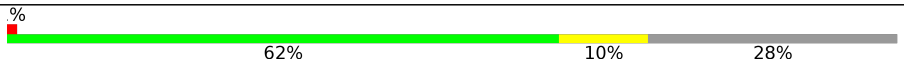
The reported resolution of this entry is 7.53 Å.

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	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 <=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	279	
2	B	198	
3	C	114	
4	D	129	
5	E	145	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12626 atoms, of which 6191 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 Kinetochore protein NDC80.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	256	Total	C	H	N	O	S	0	0	0
			4302	1385	2144	363	404	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	-	expression tag	UNP P40460
A	112	ASN	-	expression tag	UNP P40460
A	113	ALA	-	expression tag	UNP P40460

- Molecule 2 is a protein called Kinetochore protein NUF2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	186	Total	C	H	N	O	S	0	0	0
			2902	964	1376	247	303	12			

- Molecule 3 is a protein called Kinetochore protein SPC24.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	111	Total	C	H	N	O	S	0	0	0
			1839	578	917	162	181	1			

- Molecule 4 is a protein called Kinetochore protein SPC25.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	128	Total	C	H	N	O	S	0	0	0
			2011	632	998	190	186	5			

- Molecule 5 is a protein called nanobody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	105	Total	C	H	N	O	S	0	0	0
			1566	512	756	143	152	3			

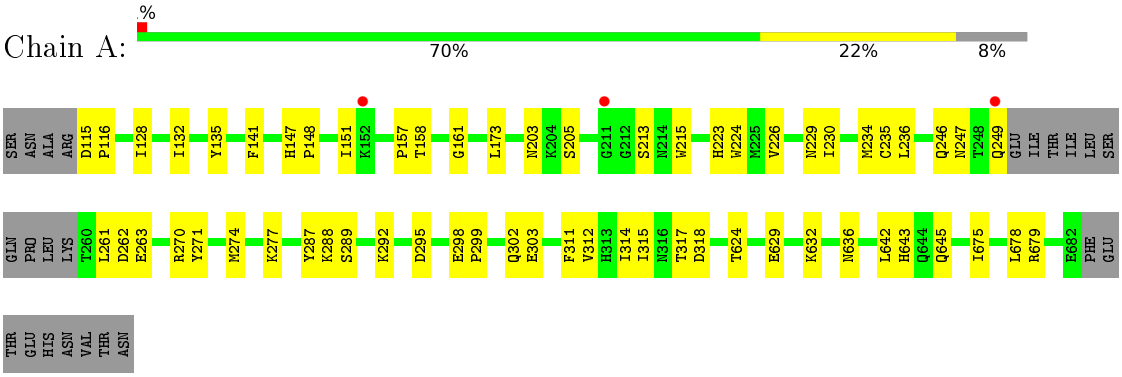
- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Hg	0	0
			2	2		
6	A	2	Total	Hg	0	0
			2	2		
6	D	2	Total	Hg	0	0
			2	2		

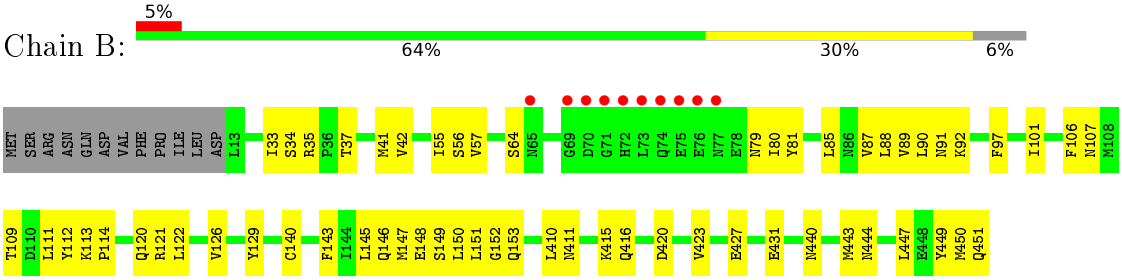
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

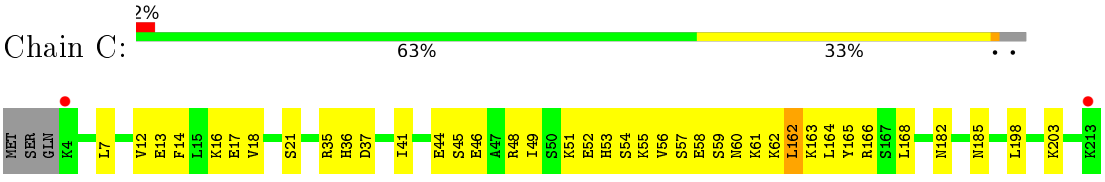
- Molecule 1: Kinetochore protein NDC80



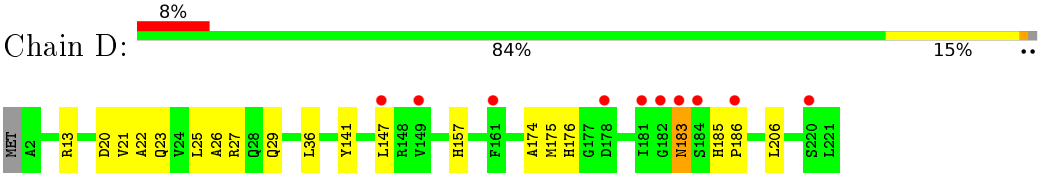
- Molecule 2: Kinetochore protein NUF2



- Molecule 3: Kinetochore protein SPC24

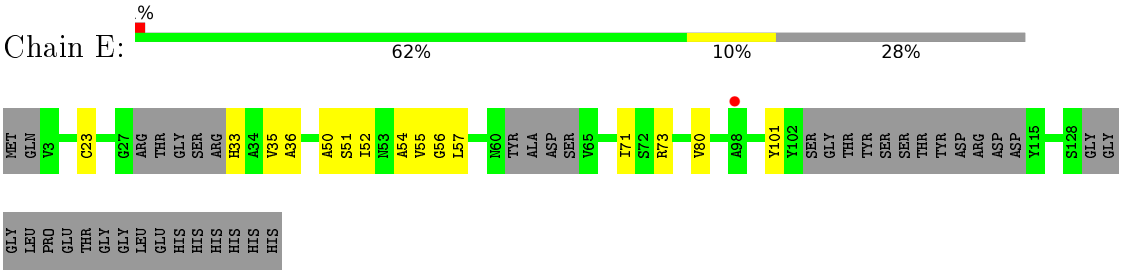


- Molecule 4: Kinetochore protein SPC25



- Molecule 5: nanobody

Chain E:


%
62%
10%
28%
MET GLN V3 C23 G27 ARG THR GLY SER ARG H33 A34 V35 A36 A50 S51 I52 N53 A54 V55 G56 L57 N60 TYR ALA ASP SER V65 I71 S72 R73 V80 A98 Y101 Y102 SER GLY THR TYR SER SER THR TYR ASP ARG ASP ASP Y115 S123 GLY GLY
GLY LEU PRO GLU THR GLY GLY LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	226.82Å 226.82Å 237.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.41 – 7.53 163.96 – 7.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (113.41-7.53) 99.7 (163.96-7.53)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 7.45Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.312 , 0.328 0.302 , 0.326	Depositor DCC
R_{free} test set	203 reflections (4.91%)	DCC
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , -8.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.016 for -l,-k,-h 0.013 for -h,l,k	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	12626	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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: HG

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	0.30	0/2199	0.45	0/2958
2	B	0.28	0/1547	0.47	0/2083
3	C	0.30	0/933	0.62	1/1251 (0.1%)
4	D	0.26	0/1030	0.44	0/1392
5	E	0.26	0/826	0.49	0/1116
All	All	0.28	0/6535	0.49	1/8800 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	162	LEU	CA-CB-CG	7.90	133.48	115.30

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	2158	2144	2171	52	2
2	B	1526	1376	1493	56	0
3	C	922	917	932	68	2
4	D	1013	998	999	15	0
5	E	810	756	771	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
All	All	6435	6191	6366	175	2

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 14.

All (175) 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:249:GLN:OE1	1:A:270:ARG:NH1	2.07	0.88
3:C:21:SER:HB3	5:E:57:LEU:HG	1.57	0.86
2:B:148:GLU:O	2:B:152:GLY:N	2.13	0.81
3:C:61:LYS:O	3:C:164:LEU:HB2	1.81	0.80
3:C:61:LYS:O	3:C:164:LEU:CB	2.32	0.78
3:C:21:SER:CB	5:E:57:LEU:HG	2.15	0.76
2:B:143:PHE:O	2:B:147:MET:N	2.19	0.76
1:A:298:GLU:OE1	1:A:302:GLN:NE2	2.22	0.73
3:C:56:VAL:O	3:C:60:ASN:HB2	1.88	0.73
3:C:46:GLU:O	3:C:49:ILE:N	2.18	0.72
3:C:165:TYR:OH	4:D:147:LEU:O	2.09	0.71
1:A:235:CYS:SG	2:B:64:SER:OG	2.51	0.67
3:C:45:SER:O	3:C:49:ILE:HG23	1.93	0.67
1:A:262:ASP:OD1	1:A:263:GLU:N	2.29	0.66
3:C:55:LYS:O	3:C:59:SER:OG	2.13	0.65
2:B:431:GLU:CD	3:C:16:LYS:HG2	2.16	0.65
2:B:34:SER:O	2:B:37:THR:OG1	2.13	0.64
3:C:59:SER:O	3:C:162:LEU:CB	2.45	0.64
3:C:18:VAL:HA	5:E:55:VAL:HG13	1.80	0.64
3:C:55:LYS:O	3:C:59:SER:CB	2.46	0.63
1:A:230:ILE:O	1:A:234:MET:HG2	1.98	0.63
1:A:147:HIS:HB2	1:A:148:PRO:HD3	1.81	0.63
1:A:148:PRO:HB2	1:A:151:ILE:HB	1.80	0.63
3:C:59:SER:O	3:C:162:LEU:HG	2.00	0.62
1:A:173:LEU:O	2:B:92:LYS:NZ	2.30	0.62
3:C:54:SER:O	3:C:58:GLU:HB2	2.01	0.61
3:C:62:LYS:O	3:C:165:TYR:CG	2.54	0.61
3:C:62:LYS:O	3:C:165:TYR:CD2	2.54	0.60
1:A:224:TRP:HE1	2:B:80:ILE:HG22	1.66	0.60
3:C:59:SER:O	3:C:162:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASN:OD1	1:A:205:SER:OG	2.20	0.59
2:B:88:LEU:O	2:B:92:LYS:HG2	2.01	0.59
3:C:164:LEU:HG	4:D:206:LEU:CD2	2.33	0.59
3:C:46:GLU:O	3:C:49:ILE:HG12	2.03	0.59
2:B:440:ASN:OD1	4:D:13:ARG:NH2	2.35	0.58
1:A:287:TYR:CZ	2:B:129:TYR:HB2	2.37	0.58
4:D:23:GLN:O	4:D:27:ARG:N	2.31	0.58
2:B:140:CYS:O	2:B:143:PHE:HB3	2.04	0.57
1:A:128:ILE:HB	1:A:223:HIS:CG	2.40	0.57
2:B:147:MET:O	2:B:151:LEU:N	2.25	0.57
2:B:450:MET:O	2:B:451:GLN:HB2	2.05	0.57
1:A:289:SER:O	1:A:292:LYS:N	2.37	0.56
1:A:311:PHE:CE2	2:B:150:LEU:HD12	2.40	0.56
2:B:97:PHE:HZ	2:B:126:VAL:HG11	1.69	0.56
1:A:299:PRO:O	1:A:303:GLU:HB2	2.06	0.56
3:C:61:LYS:O	3:C:164:LEU:HB3	2.04	0.56
1:A:271:TYR:OH	1:A:318:ASP:OD2	2.20	0.56
3:C:18:VAL:HA	5:E:55:VAL:CG1	2.36	0.55
1:A:157:PRO:HG3	1:A:215:TRP:CE2	2.41	0.55
3:C:62:LYS:HA	3:C:164:LEU:HB3	1.89	0.55
3:C:164:LEU:O	3:C:168:LEU:HG	2.07	0.54
2:B:42:VAL:HG13	2:B:90:LEU:HD21	1.89	0.54
1:A:629:GLU:O	1:A:632:LYS:HB2	2.08	0.54
3:C:21:SER:HB2	5:E:55:VAL:CG1	2.38	0.54
2:B:85:LEU:O	2:B:89:VAL:HG23	2.07	0.54
5:E:50:ALA:HB3	5:E:71:ILE:HD12	1.88	0.53
2:B:145:LEU:O	2:B:149:SER:N	2.28	0.53
3:C:12:VAL:O	3:C:16:LYS:HG3	2.09	0.53
3:C:57:SER:O	3:C:61:LYS:HB2	2.09	0.53
3:C:13:GLU:OE1	5:E:33:HIS:NE2	2.39	0.53
1:A:287:TYR:HB2	2:B:129:TYR:CZ	2.44	0.52
2:B:91:ASN:HA	2:B:111:LEU:HD11	1.91	0.52
2:B:41:MET:HG3	2:B:114:PRO:CG	2.40	0.52
1:A:132:ILE:HA	1:A:226:VAL:HG11	1.92	0.52
2:B:87:VAL:HG13	2:B:112:TYR:OH	2.08	0.52
1:A:312:VAL:HG12	2:B:150:LEU:HD11	1.91	0.51
1:A:315:ILE:HG21	2:B:150:LEU:HD13	1.91	0.51
3:C:41:ILE:O	3:C:44:GLU:N	2.43	0.51
3:C:52:GLU:O	3:C:56:VAL:HB	2.10	0.51
1:A:632:LYS:O	1:A:636:ASN:HB2	2.11	0.50
3:C:59:SER:O	3:C:162:LEU:CG	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:LEU:O	3:C:166:ARG:HB2	2.11	0.49
3:C:60:ASN:HA	3:C:162:LEU:HB2	1.92	0.49
5:E:33:HIS:ND1	5:E:101:TYR:O	2.45	0.49
3:C:21:SER:OG	5:E:57:LEU:HG	2.12	0.49
1:A:315:ILE:HG21	2:B:150:LEU:HB3	1.93	0.49
3:C:55:LYS:O	3:C:59:SER:HB3	2.11	0.49
1:A:311:PHE:CD2	2:B:143:PHE:CE1	3.00	0.48
3:C:62:LYS:O	3:C:165:TYR:HB2	2.14	0.48
3:C:54:SER:O	3:C:58:GLU:CB	2.61	0.48
3:C:54:SER:HA	3:C:57:SER:OG	2.13	0.48
3:C:48:ARG:HA	3:C:51:LYS:HB2	1.95	0.48
1:A:148:PRO:HB2	1:A:151:ILE:CB	2.44	0.48
1:A:288:LYS:O	1:A:292:LYS:HB2	2.14	0.48
1:A:632:LYS:O	1:A:636:ASN:CB	2.62	0.48
1:A:141:PHE:CE2	1:A:148:PRO:HG3	2.50	0.47
2:B:149:SER:O	2:B:153:GLN:N	2.36	0.47
1:A:632:LYS:O	1:A:636:ASN:CG	2.53	0.47
1:A:295:ASP:O	1:A:299:PRO:HD2	2.15	0.47
2:B:101:ILE:HD11	2:B:122:LEU:HB3	1.95	0.47
1:A:236:LEU:HD11	2:B:92:LYS:HG3	1.97	0.47
1:A:315:ILE:HD13	2:B:150:LEU:HB3	1.95	0.47
1:A:642:LEU:O	1:A:645:GLN:HG2	2.14	0.47
1:A:147:HIS:CB	1:A:148:PRO:HD3	2.45	0.46
1:A:115:ASP:HB3	1:A:116:PRO:HD3	1.97	0.46
4:D:23:GLN:HA	4:D:26:ALA:HB3	1.97	0.46
2:B:57:VAL:HG11	2:B:90:LEU:HD13	1.96	0.46
2:B:79:ASN:O	2:B:79:ASN:OD1	2.32	0.46
3:C:44:GLU:O	3:C:48:ARG:HB2	2.16	0.46
3:C:14:PHE:O	3:C:18:VAL:HG23	2.15	0.46
3:C:162:LEU:O	3:C:166:ARG:CB	2.64	0.46
4:D:175:MET:HG3	4:D:176:HIS:CE1	2.50	0.46
3:C:21:SER:HB2	5:E:55:VAL:HB	1.97	0.46
3:C:53:HIS:O	3:C:57:SER:CB	2.65	0.45
1:A:246:GLN:OE1	1:A:277:LYS:NZ	2.30	0.45
2:B:81:TYR:O	2:B:85:LEU:HG	2.16	0.45
3:C:45:SER:C	3:C:49:ILE:HG23	2.37	0.45
3:C:62:LYS:O	3:C:165:TYR:CB	2.64	0.45
1:A:158:THR:HG23	1:A:161:GLY:H	1.81	0.45
3:C:165:TYR:CE2	4:D:141:TYR:HB3	2.51	0.45
2:B:126:VAL:O	2:B:129:TYR:HB3	2.16	0.45
3:C:162:LEU:O	3:C:166:ARG:CG	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:GLU:HB3	3:C:12:VAL:HG11	1.99	0.44
3:C:36:HIS:C	3:C:36:HIS:HD1	2.21	0.44
4:D:157:HIS:HA	4:D:174:ALA:HA	1.98	0.44
2:B:107:ASN:OD1	2:B:109:THR:CB	2.65	0.44
2:B:97:PHE:CZ	2:B:126:VAL:HG11	2.52	0.44
3:C:52:GLU:O	3:C:56:VAL:HG23	2.17	0.44
2:B:33:ILE:O	2:B:33:ILE:HG22	2.18	0.44
3:C:45:SER:O	3:C:49:ILE:N	2.51	0.44
1:A:157:PRO:HG3	1:A:215:TRP:CZ2	2.53	0.44
3:C:182:ASN:OD1	3:C:185:ASN:HA	2.17	0.44
1:A:247:ASN:O	1:A:274:MET:HE3	2.18	0.43
1:A:678:LEU:HD21	4:D:36:LEU:HD12	2.00	0.43
5:E:36:ALA:HB2	5:E:51:SER:CB	2.48	0.43
2:B:420:ASP:O	2:B:423:VAL:HB	2.18	0.43
2:B:147:MET:HG3	2:B:148:GLU:N	2.32	0.43
3:C:57:SER:O	3:C:61:LYS:CB	2.66	0.43
3:C:52:GLU:O	3:C:56:VAL:CB	2.67	0.43
3:C:59:SER:O	3:C:162:LEU:N	2.50	0.43
2:B:109:THR:HG23	2:B:113:LYS:HG3	1.99	0.43
1:A:135:TYR:CD1	1:A:230:ILE:CD1	3.01	0.43
3:C:54:SER:HA	3:C:57:SER:HG	1.84	0.43
2:B:444:ASN:O	2:B:447:LEU:HB2	2.18	0.43
1:A:226:VAL:O	1:A:230:ILE:HG12	2.18	0.42
2:B:146:GLN:O	2:B:150:LEU:HG	2.18	0.42
4:D:185:HIS:HB3	4:D:186:PRO:HD3	2.00	0.42
4:D:25:LEU:O	4:D:29:GLN:HG3	2.19	0.42
5:E:35:VAL:HG12	5:E:80:VAL:HG11	2.02	0.42
2:B:120:GLN:HG3	2:B:121:ARG:N	2.33	0.42
2:B:147:MET:CG	2:B:148:GLU:N	2.83	0.42
2:B:415:LYS:O	2:B:416:GLN:C	2.56	0.42
2:B:449:TYR:HD2	3:C:35:ARG:HD2	1.85	0.42
2:B:450:MET:HE1	4:D:20:ASP:HB3	2.01	0.42
2:B:41:MET:HG3	2:B:114:PRO:HG3	2.01	0.42
3:C:57:SER:O	3:C:61:LYS:CG	2.67	0.42
1:A:157:PRO:HD3	1:A:215:TRP:CH2	2.55	0.42
1:A:624:THR:HB	2:B:410:LEU:HD23	2.02	0.41
4:D:183:ASN:N	4:D:183:ASN:OD1	2.52	0.41
4:D:22:ALA:O	4:D:25:LEU:HB2	2.19	0.41
3:C:54:SER:O	3:C:58:GLU:CG	2.68	0.41
1:A:261:LEU:HD21	2:B:411:ASN:O	2.19	0.41
5:E:23:CYS:HB3	5:E:80:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:52:ILE:HD11	5:E:56:GLY:HA2	2.02	0.41
2:B:106:PHE:CZ	2:B:111:LEU:HG	2.56	0.41
3:C:17:GLU:C	5:E:55:VAL:HG21	2.41	0.41
5:E:55:VAL:HG12	5:E:55:VAL:O	2.21	0.41
2:B:143:PHE:HA	2:B:146:GLN:HB2	2.02	0.41
3:C:53:HIS:O	3:C:57:SER:HB3	2.20	0.41
3:C:56:VAL:O	3:C:56:VAL:HG12	2.20	0.41
5:E:54:ALA:HA	5:E:73:ARG:CZ	2.51	0.41
1:A:270:ARG:O	1:A:274:MET:HG3	2.21	0.41
1:A:643:HIS:CG	3:C:7:LEU:HD12	2.56	0.41
2:B:443:MET:O	2:B:447:LEU:HD13	2.20	0.41
3:C:198:LEU:HB2	3:C:203:LYS:HE3	2.03	0.41
3:C:60:ASN:O	3:C:163:LYS:HB2	2.21	0.40
1:A:246:GLN:HA	1:A:249:GLN:HB2	2.03	0.40
1:A:298:GLU:N	1:A:299:PRO:HD2	2.37	0.40
1:A:314:ILE:O	1:A:317:THR:HB	2.22	0.40
2:B:55:ILE:HG22	2:B:56:SER:N	2.37	0.40
3:C:52:GLU:O	3:C:56:VAL:CG2	2.69	0.40
3:C:46:GLU:C	3:C:49:ILE:H	2.17	0.40
1:A:675:ILE:CG2	1:A:679:ARG:CZ	3.00	0.40
2:B:35:ARG:O	2:B:37:THR:N	2.48	0.40
4:D:21:VAL:O	4:D:22:ALA:C	2.60	0.40

All (2) 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:A:213:SER:N	3:C:37:ASP:OD1[3_745]	2.04	0.16
1:A:213:SER:H	3:C:37:ASP:OD1[3_745]	1.54	0.06

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	252/279 (90%)	232 (92%)	20 (8%)	0	100	100
2	B	184/198 (93%)	163 (89%)	21 (11%)	0	100	100
3	C	109/114 (96%)	104 (95%)	5 (5%)	0	100	100
4	D	126/129 (98%)	112 (89%)	14 (11%)	0	100	100
5	E	97/145 (67%)	94 (97%)	3 (3%)	0	100	100
All	All	768/865 (89%)	705 (92%)	63 (8%)	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	A	246/268 (92%)	245 (100%)	1 (0%)	93	96
2	B	175/187 (94%)	175 (100%)	0	100	100
3	C	106/109 (97%)	106 (100%)	0	100	100
4	D	107/108 (99%)	106 (99%)	1 (1%)	84	93
5	E	83/115 (72%)	83 (100%)	0	100	100
All	All	717/787 (91%)	715 (100%)	2 (0%)	94	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
4	D	183	ASN

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

Mol	Chain	Res	Type
1	A	302	GLN
4	D	176	HIS

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 6 ligands modelled in this entry, 6 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

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	256/279 (91%)	0.30	3 (1%)	81	75	18, 74, 179, 213	0
2	B	186/198 (93%)	0.38	10 (5%)	29	30	42, 99, 156, 174	0
3	C	111/114 (97%)	0.48	2 (1%)	71	66	27, 69, 83, 93	0
4	D	128/129 (99%)	0.62	10 (7%)	16	19	27, 67, 113, 119	1 (0%)
5	E	105/145 (72%)	0.42	1 (0%)	84	79	30, 55, 82, 84	0
All	All	786/865 (90%)	0.41	26 (3%)	50	46	18, 72, 143, 213	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	71	GLY	6.1
2	B	70	ASP	5.5
1	A	211	GLY	4.6
2	B	72	HIS	3.9
2	B	69	GLY	3.8
4	D	183	ASN	3.4
2	B	76	GLU	3.4
2	B	77	ASN	3.2
2	B	75	GLU	2.8
4	D	186	PRO	2.8
3	C	4	LYS	2.7
4	D	184	SER	2.7
2	B	74	GLN	2.6
4	D	161	PHE	2.6
4	D	220	SER	2.5
4	D	149	VAL	2.5
1	A	152	LYS	2.5
4	D	178	ASP	2.5
2	B	65	ASN	2.4
2	B	73	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	98	ALA	2.3
4	D	182	GLY	2.2
1	A	249	GLN	2.1
3	C	213	LYS	2.1
4	D	181	ILE	2.1
4	D	147	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
6	HG	B	501	1/1	0.45	0.24	-0.15	208,208,208,208	0
6	HG	A	702	1/1	0.75	0.29	-0.72	144,144,144,144	1
6	HG	B	502	1/1	0.77	0.20	-2.15	115,115,115,115	1
6	HG	D	301	1/1	0.73	0.24	-2.71	68,68,68,68	1
6	HG	D	302	1/1	0.88	0.24	-	77,77,77,77	1
6	HG	A	701	1/1	0.93	0.20	-	81,81,81,81	1

6.5 Other polymers (i)

There are no such residues in this entry.