



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 03:30 pm GMT

PDB ID : 2W99
Title : Crystal Structure of CDK4 in complex with a D-type cyclin
Authors : Day, P.J.; Cleasby, A.; Tickle, I.J.; Reilly, M.O.; Coyle, J.E.; Holding, F.P.;
McMenamin, R.L.; Yon, J.; Chopra, R.; Lengauer, C.; Jhoti, H.
Deposited on : 2009-01-22
Resolution : 2.80 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

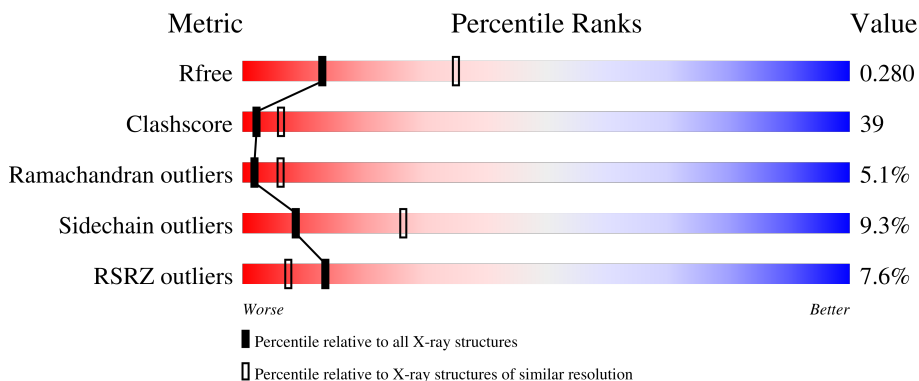
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. 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	271	 12% 57% 30% 9%
2	B	306	 30% 54% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4385 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 G1/S-SPECIFIC CYCLIN-D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1960	1246	333	360	21	0	0	0

- Molecule 2 is a protein called CELL DIVISION PROTEIN KINASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	291	2299	1472	403	413	11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	43	GLU	GLY	engineered mutation	UNP P11802
B	44	GLU	GLY	engineered mutation	UNP P11802
B	172	ALA	THR	engineered mutation	UNP P11802

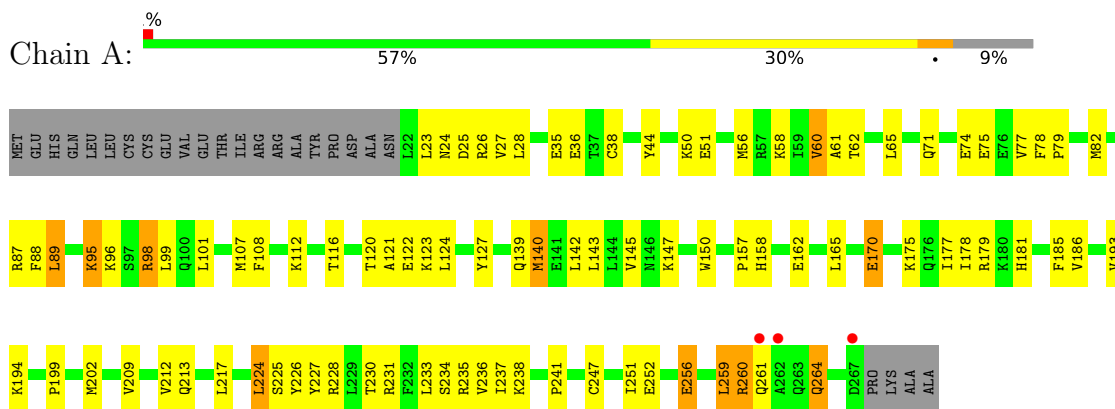
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total 100	O 100	0	0
3	B	26	Total 26	O 26	0	0

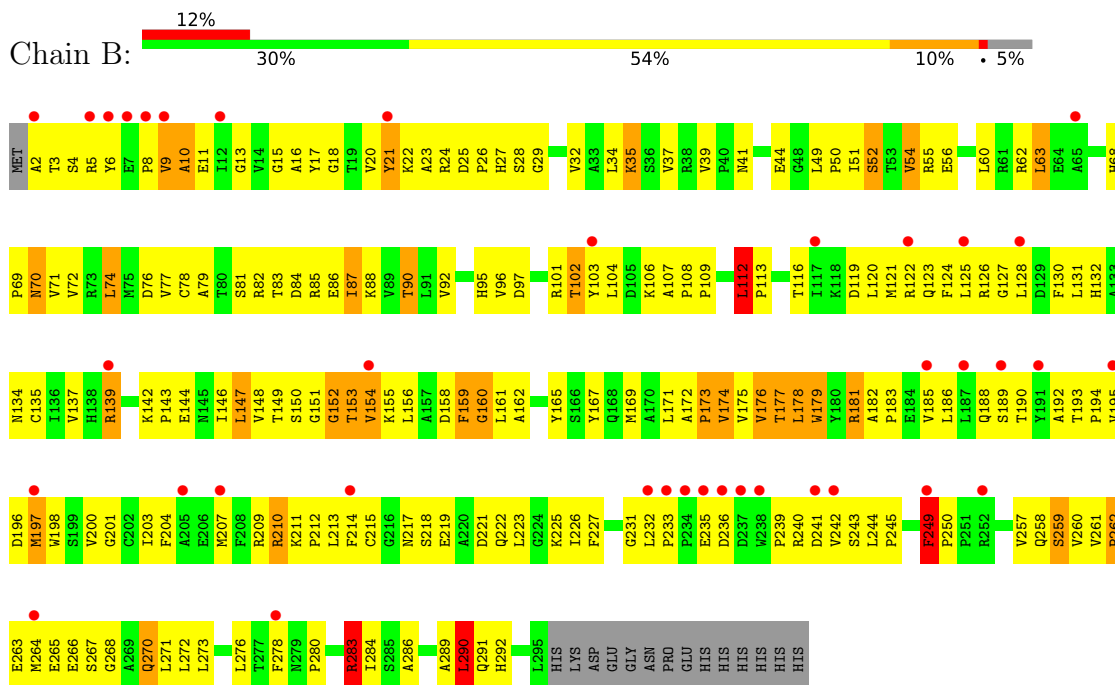
3 Residue-property plots [i](#)

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: G1/S-SPECIFIC CYCLIN-D1



- Molecule 2: CELL DIVISION PROTEIN KINASE 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.02Å 64.68Å 188.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.49 – 2.80 94.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (94.49-2.80) 98.4 (94.37-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.82Å)	Xtrriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.213 , 0.270 0.221 , 0.280	Depositor DCC
R_{free} test set	845 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 105.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4385	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/1993	0.44	0/2691
2	B	0.24	0/2358	0.48	0/3209
All	All	0.26	0/4351	0.46	0/5900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1960	0	2014	86	0
2	B	2299	0	2310	255	0
3	A	100	0	0	5	0
3	B	26	0	0	5	0
All	All	4385	0	4324	332	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 39.

All (332) 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:112:LYS:HD2	2:B:51:ILE:HD12	1.30	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:VAL:HB	2:B:147:LEU:HD12	1.32	1.11
2:B:112:LEU:HB2	2:B:113:PRO:HA	1.41	1.00
2:B:96:VAL:HG11	2:B:147:LEU:HB2	1.41	0.98
2:B:193:THR:HG22	2:B:194:PRO:HD3	1.45	0.96
2:B:32:VAL:HG11	2:B:92:VAL:HG13	1.51	0.91
2:B:182:ALA:HB3	2:B:185:VAL:HG23	1.50	0.90
2:B:173:PRO:HB2	2:B:174:VAL:HG22	1.53	0.89
1:A:259:LEU:HD13	1:A:260:ARG:N	1.90	0.86
2:B:240:ARG:HB2	2:B:241:ASP:HB2	1.59	0.85
1:A:259:LEU:HD13	1:A:260:ARG:H	1.38	0.85
2:B:173:PRO:HB2	2:B:174:VAL:CB	2.08	0.83
1:A:95:LYS:NZ	1:A:95:LYS:H	1.77	0.83
2:B:107:ALA:HB1	2:B:209:ARG:HH11	1.42	0.81
2:B:51:ILE:O	2:B:55:ARG:HG3	1.80	0.81
2:B:96:VAL:CB	2:B:147:LEU:HD12	2.11	0.81
2:B:32:VAL:CG1	2:B:92:VAL:HG13	2.11	0.81
2:B:9:VAL:HG23	2:B:10:ALA:H	1.45	0.80
2:B:63:LEU:HD21	2:B:134:ASN:HD22	1.46	0.80
2:B:123:GLN:HE21	2:B:154:VAL:HG22	1.44	0.79
2:B:173:PRO:HB2	2:B:174:VAL:CG2	2.11	0.79
2:B:172:ALA:N	2:B:173:PRO:HD3	1.99	0.78
1:A:228:ARG:HD3	1:A:231:ARG:HG3	1.65	0.78
2:B:173:PRO:HB2	2:B:174:VAL:HG13	1.66	0.77
2:B:72:VAL:HG22	2:B:156:LEU:O	1.84	0.77
2:B:112:LEU:HB2	2:B:113:PRO:CA	2.14	0.77
2:B:124:PHE:HE2	2:B:200:VAL:HG13	1.47	0.77
2:B:207:MET:O	2:B:209:ARG:HA	1.85	0.76
1:A:23:LEU:O	1:A:27:VAL:HG22	1.86	0.76
2:B:261:VAL:O	2:B:263:GLU:HA	1.87	0.75
1:A:120:THR:HG21	3:A:2057:HOH:O	1.87	0.75
1:A:228:ARG:HA	1:A:228:ARG:NE	2.02	0.75
2:B:107:ALA:HB1	2:B:209:ARG:NH1	2.01	0.75
2:B:102:THR:O	2:B:106:LYS:HG2	1.87	0.74
1:A:112:LYS:HD2	2:B:51:ILE:CD1	2.14	0.73
2:B:173:PRO:CB	2:B:174:VAL:HG22	2.18	0.73
2:B:9:VAL:HG23	2:B:10:ALA:N	2.05	0.72
2:B:186:LEU:HD23	2:B:219:GLU:HG3	1.70	0.71
2:B:186:LEU:HD23	2:B:219:GLU:CG	2.21	0.71
2:B:87:ILE:HD12	2:B:88:LYS:N	2.06	0.70
2:B:173:PRO:HB2	2:B:174:VAL:CG1	2.20	0.70
2:B:69:PRO:O	2:B:155:LYS:HD3	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ALA:HB1	2:B:3:THR:HA	1.72	0.69
2:B:146:ILE:C	2:B:147:LEU:HD23	2.12	0.69
2:B:203:ILE:O	2:B:207:MET:HG3	1.91	0.69
1:A:58:LYS:O	1:A:62:THR:HG23	1.93	0.69
2:B:68:HIS:ND1	2:B:69:PRO:HD2	2.08	0.69
2:B:153:THR:O	2:B:154:VAL:HG22	1.93	0.69
2:B:143:PRO:HD3	2:B:203:ILE:HD11	1.75	0.68
2:B:265:GLU:HG2	2:B:266:GLU:H	1.59	0.68
1:A:88:PHE:CE1	1:A:147:LYS:HG3	2.28	0.68
1:A:260:ARG:HD3	1:A:261:GLN:N	2.09	0.68
1:A:112:LYS:O	2:B:55:ARG:NH1	2.27	0.67
2:B:218:SER:HB3	2:B:221:ASP:HB2	1.77	0.67
1:A:228:ARG:CD	1:A:231:ARG:HG3	2.25	0.67
2:B:211:LYS:HB3	2:B:212:PRO:CD	2.24	0.67
2:B:271:LEU:HD13	2:B:292:HIS:ND1	2.10	0.67
2:B:124:PHE:CE2	2:B:200:VAL:HG13	2.29	0.67
2:B:160:GLY:O	2:B:162:ALA:N	2.28	0.67
2:B:235:GLU:HB3	2:B:236:ASP:HA	1.76	0.66
2:B:257:VAL:HG21	2:B:273:LEU:HG	1.77	0.66
2:B:235:GLU:OE1	2:B:235:GLU:N	2.29	0.65
2:B:173:PRO:HB2	2:B:174:VAL:CA	2.26	0.65
2:B:213:LEU:O	2:B:213:LEU:HD22	1.96	0.65
2:B:8:PRO:HA	2:B:23:ALA:HB2	1.77	0.65
2:B:15:GLY:O	2:B:18:GLY:N	2.30	0.65
2:B:193:THR:CG2	2:B:194:PRO:HD3	2.22	0.64
2:B:178:LEU:O	2:B:222:GLN:NE2	2.28	0.64
2:B:123:GLN:NE2	2:B:153:THR:O	2.30	0.64
2:B:176:VAL:O	2:B:178:LEU:N	2.30	0.63
2:B:284:ILE:HD13	2:B:289:ALA:HB2	1.80	0.63
2:B:173:PRO:CB	2:B:174:VAL:HG13	2.28	0.63
2:B:192:ALA:HB1	2:B:194:PRO:HD2	1.81	0.63
1:A:108:PHE:O	1:A:112:LYS:HG3	1.98	0.63
2:B:76:ASP:OD1	2:B:77:VAL:N	2.30	0.63
2:B:173:PRO:HG2	2:B:174:VAL:HG22	1.81	0.62
2:B:79:ALA:HB1	2:B:87:ILE:CD1	2.29	0.62
2:B:218:SER:HB3	2:B:221:ASP:CB	2.30	0.62
2:B:63:LEU:CD2	2:B:134:ASN:HD22	2.10	0.62
1:A:256:GLU:O	1:A:259:LEU:HD12	2.00	0.62
2:B:6:TYR:CE2	2:B:92:VAL:HG21	2.34	0.62
2:B:81:SER:O	2:B:87:ILE:HA	1.99	0.62
2:B:34:LEU:CD2	2:B:92:VAL:HG22	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PRO:HG3	1:A:158:HIS:CE1	2.35	0.61
1:A:120:THR:HG22	1:A:123:LYS:H	1.65	0.61
2:B:127:GLY:O	2:B:131:LEU:HD13	1.99	0.61
2:B:79:ALA:HB1	2:B:87:ILE:HD11	1.81	0.61
2:B:171:LEU:HB3	2:B:173:PRO:HG3	1.82	0.61
2:B:171:LEU:HD23	2:B:171:LEU:O	2.00	0.61
1:A:228:ARG:HA	1:A:228:ARG:HE	1.65	0.61
2:B:85:ARG:O	2:B:86:GLU:HG3	2.00	0.61
1:A:56:MET:O	1:A:60:VAL:HG23	2.01	0.60
2:B:181:ARG:HG3	2:B:185:VAL:HG11	1.83	0.60
1:A:193:VAL:HG22	3:A:2080:HOH:O	2.02	0.60
2:B:51:ILE:N	2:B:51:ILE:HD13	2.17	0.60
1:A:71:GLN:NE2	1:A:127:TYR:OH	2.30	0.60
2:B:210:ARG:NH1	3:B:2025:HOH:O	2.27	0.59
2:B:123:GLN:NE2	2:B:154:VAL:HG22	2.17	0.59
2:B:52:SER:O	2:B:56:GLU:HG2	2.03	0.59
2:B:209:ARG:H	2:B:210:ARG:HG3	1.68	0.59
1:A:170:GLU:OE1	1:A:225:SER:HB2	2.02	0.59
2:B:25:ASP:O	2:B:29:GLY:N	2.28	0.59
2:B:70:ASN:ND2	2:B:127:GLY:N	2.50	0.59
2:B:150:SER:O	2:B:152:GLY:N	2.36	0.59
2:B:242:VAL:HG22	2:B:243:SER:H	1.68	0.58
2:B:34:LEU:HD22	2:B:92:VAL:HG22	1.84	0.58
1:A:162:GLU:OE2	1:A:179:ARG:HD3	2.03	0.58
2:B:125:LEU:HB3	2:B:290:LEU:HD12	1.86	0.58
1:A:60:VAL:HG21	1:A:99:LEU:HG	1.85	0.58
2:B:74:LEU:HD21	2:B:77:VAL:HG22	1.87	0.57
2:B:270:GLN:HA	2:B:270:GLN:HE21	1.69	0.57
2:B:159:PHE:N	2:B:159:PHE:CD1	2.71	0.57
2:B:171:LEU:C	2:B:173:PRO:HD3	2.24	0.57
1:A:60:VAL:HG21	1:A:99:LEU:CD2	2.35	0.56
2:B:154:VAL:HG23	2:B:154:VAL:O	2.05	0.56
2:B:249:PHE:CB	2:B:250:PRO:HD3	2.36	0.56
1:A:112:LYS:CD	2:B:51:ILE:HD12	2.19	0.56
2:B:35:LYS:HE2	2:B:158:ASP:OD1	2.06	0.56
2:B:192:ALA:O	2:B:195:VAL:HG22	2.06	0.56
2:B:121:MET:CG	2:B:207:MET:HE1	2.36	0.56
2:B:173:PRO:CG	2:B:174:VAL:HG22	2.35	0.56
1:A:36:GLU:HB3	3:A:2009:HOH:O	2.06	0.55
2:B:290:LEU:HD23	2:B:290:LEU:O	2.07	0.55
1:A:25:ASP:OD2	1:A:26:ARG:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:VAL:HG23	2:B:20:VAL:O	2.07	0.54
1:A:35:GLU:CD	1:A:199:PRO:HB2	2.27	0.54
2:B:120:LEU:C	2:B:120:LEU:HD23	2.27	0.54
2:B:20:VAL:HG12	2:B:35:LYS:HG3	1.89	0.54
2:B:71:VAL:HG12	2:B:159:PHE:HE2	1.73	0.54
2:B:272:LEU:O	2:B:272:LEU:HD12	2.07	0.54
2:B:262:PRO:HA	2:B:263:GLU:CB	2.36	0.54
1:A:224:LEU:HA	1:A:226:TYR:CD1	2.43	0.54
2:B:123:GLN:HG2	2:B:154:VAL:CG2	2.38	0.54
2:B:262:PRO:HA	2:B:263:GLU:HB2	1.90	0.54
2:B:8:PRO:HA	2:B:23:ALA:CB	2.38	0.54
2:B:51:ILE:HG21	2:B:55:ARG:NH2	2.23	0.54
2:B:128:LEU:HD12	2:B:286:ALA:HB1	1.90	0.53
1:A:139:GLN:HG3	2:B:82:ARG:HH12	1.74	0.53
2:B:197:MET:HE3	2:B:197:MET:HA	1.90	0.53
1:A:75:GLU:OE1	1:A:75:GLU:N	2.36	0.53
1:A:79:PRO:HG3	1:A:158:HIS:HE1	1.73	0.53
2:B:109:PRO:HB3	2:B:112:LEU:HD12	1.90	0.53
2:B:211:LYS:HB3	2:B:212:PRO:HD2	1.90	0.53
2:B:97:ASP:H	2:B:149:THR:HA	1.74	0.52
1:A:228:ARG:HG2	1:A:231:ARG:NH1	2.24	0.52
2:B:233:PRO:HG2	2:B:278:PHE:CD2	2.44	0.52
1:A:95:LYS:H	1:A:95:LYS:CE	2.22	0.52
1:A:224:LEU:HA	1:A:226:TYR:HD1	1.75	0.52
1:A:74:GLU:O	1:A:77:VAL:HG23	2.10	0.52
2:B:171:LEU:HD22	2:B:173:PRO:HG3	1.92	0.52
2:B:188:GLN:HG2	2:B:240:ARG:O	2.10	0.52
2:B:242:VAL:HG22	2:B:243:SER:N	2.24	0.52
2:B:39:VAL:HG23	2:B:87:ILE:HG23	1.92	0.51
2:B:108:PRO:N	2:B:109:PRO:CD	2.73	0.51
2:B:214:PHE:CZ	2:B:226:ILE:HA	2.45	0.51
2:B:2:ALA:CB	2:B:3:THR:HA	2.32	0.51
2:B:128:LEU:HD11	2:B:132:HIS:CE1	2.45	0.51
2:B:289:ALA:O	2:B:291:GLN:N	2.43	0.51
1:A:27:VAL:HG23	1:A:28:LEU:N	2.26	0.51
2:B:212:PRO:HB2	2:B:215:CYS:SG	2.51	0.51
2:B:271:LEU:HD13	2:B:292:HIS:CG	2.46	0.51
2:B:212:PRO:HB2	2:B:215:CYS:HB3	1.93	0.51
2:B:240:ARG:HB2	2:B:241:ASP:CB	2.35	0.51
1:A:61:ALA:HB2	1:A:82:MET:CE	2.41	0.51
1:A:202:MET:CE	1:A:247:CYS:HB2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:GLU:CB	2:B:236:ASP:HA	2.38	0.50
1:A:194:LYS:NZ	1:A:247:CYS:SG	2.82	0.50
2:B:25:ASP:CG	2:B:28:SER:HB3	2.32	0.50
2:B:212:PRO:CB	2:B:215:CYS:HB3	2.41	0.50
2:B:197:MET:HE2	2:B:200:VAL:HG21	1.94	0.50
2:B:272:LEU:HD12	2:B:276:LEU:HG	1.93	0.49
1:A:259:LEU:C	1:A:259:LEU:HD22	2.33	0.49
2:B:121:MET:SD	2:B:207:MET:HE1	2.52	0.49
2:B:193:THR:N	2:B:194:PRO:CD	2.76	0.49
1:A:95:LYS:H	1:A:95:LYS:HZ1	1.58	0.48
1:A:157:PRO:HG2	1:A:186:VAL:HG13	1.94	0.48
1:A:209:VAL:HG23	1:A:233:LEU:HD12	1.95	0.48
2:B:128:LEU:HD13	2:B:128:LEU:C	2.33	0.48
2:B:175:VAL:C	2:B:176:VAL:HG23	2.33	0.48
2:B:178:LEU:CD2	2:B:181:ARG:HB2	2.43	0.48
2:B:198:TRP:HB2	2:B:283:ARG:NH1	2.28	0.48
2:B:74:LEU:HD21	2:B:77:VAL:CG2	2.43	0.48
2:B:213:LEU:HD13	2:B:214:PHE:CD1	2.49	0.48
1:A:226:TYR:CG	1:A:227:TYR:N	2.81	0.48
2:B:122:ARG:O	2:B:126:ARG:HG3	2.13	0.48
1:A:38:CYS:O	1:A:87:ARG:HD2	2.13	0.48
1:A:95:LYS:HZ3	1:A:98:ARG:HH11	1.62	0.48
2:B:197:MET:O	2:B:200:VAL:HB	2.13	0.48
1:A:157:PRO:HG2	1:A:186:VAL:CG1	2.43	0.48
2:B:96:VAL:CG1	2:B:97:ASP:N	2.76	0.48
2:B:167:TYR:HB3	3:B:2006:HOH:O	2.13	0.48
1:A:142:LEU:HD21	2:B:49:LEU:HD21	1.95	0.47
2:B:15:GLY:O	2:B:17:TYR:N	2.46	0.47
2:B:244:LEU:N	2:B:245:PRO:HD3	2.28	0.47
2:B:4:SER:O	2:B:6:TYR:N	2.38	0.47
2:B:149:THR:HG23	2:B:150:SER:N	2.29	0.47
2:B:209:ARG:O	2:B:209:ARG:HG3	2.14	0.47
2:B:232:LEU:HD12	2:B:250:PRO:O	2.14	0.47
2:B:258:GLN:HA	2:B:261:VAL:HG23	1.96	0.47
2:B:70:ASN:HD22	2:B:127:GLY:CA	2.27	0.47
2:B:134:ASN:O	2:B:135:CYS:HB2	2.15	0.47
2:B:2:ALA:HB1	2:B:3:THR:CA	2.43	0.47
2:B:68:HIS:ND1	2:B:69:PRO:CD	2.77	0.47
2:B:194:PRO:O	2:B:197:MET:N	2.44	0.47
2:B:79:ALA:CB	2:B:87:ILE:HD11	2.44	0.47
2:B:124:PHE:HD1	2:B:156:LEU:HD21	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:PRO:CB	2:B:174:VAL:CA	2.93	0.47
2:B:213:LEU:CD1	2:B:214:PHE:CD1	2.98	0.47
2:B:13:GLY:O	2:B:20:VAL:HG22	2.15	0.47
1:A:101:LEU:HG	1:A:140:MET:HG3	1.96	0.47
2:B:257:VAL:O	2:B:261:VAL:HG22	2.14	0.47
1:A:95:LYS:HB3	3:A:2042:HOH:O	2.14	0.46
1:A:230:THR:O	1:A:234:SER:OG	2.29	0.46
1:A:236:VAL:O	1:A:238:LYS:HD2	2.15	0.46
2:B:50:PRO:O	2:B:54:VAL:HG13	2.16	0.46
2:B:71:VAL:HG21	2:B:131:LEU:CD1	2.46	0.46
2:B:70:ASN:ND2	2:B:127:GLY:CA	2.79	0.46
2:B:267:SER:O	2:B:270:GLN:N	2.48	0.46
1:A:145:VAL:CG1	1:A:150:TRP:CE2	2.98	0.46
2:B:201:GLY:HA2	2:B:204:PHE:HB3	1.97	0.46
2:B:289:ALA:C	2:B:291:GLN:H	2.19	0.46
2:B:150:SER:C	2:B:152:GLY:H	2.20	0.46
2:B:9:VAL:N	2:B:22:LYS:O	2.38	0.45
1:A:228:ARG:CG	1:A:231:ARG:HG3	2.46	0.45
1:A:60:VAL:HG21	1:A:99:LEU:CG	2.47	0.45
2:B:108:PRO:HG2	2:B:109:PRO:HD3	1.98	0.45
2:B:149:THR:CG2	2:B:150:SER:N	2.79	0.45
1:A:213:GLN:O	1:A:217:LEU:HD13	2.16	0.45
2:B:51:ILE:CG2	2:B:55:ARG:NH2	2.79	0.45
2:B:71:VAL:CG1	2:B:159:PHE:HE2	2.29	0.45
1:A:260:ARG:O	1:A:264:GLN:HG3	2.17	0.45
2:B:240:ARG:CB	2:B:241:ASP:CB	2.95	0.45
2:B:24:ARG:O	2:B:26:PRO:HD3	2.17	0.45
1:A:228:ARG:HD3	1:A:231:ARG:NE	2.33	0.44
2:B:108:PRO:CG	2:B:109:PRO:HD3	2.47	0.44
2:B:112:LEU:CB	2:B:113:PRO:HA	2.30	0.44
2:B:227:PHE:CE2	2:B:233:PRO:HD2	2.52	0.44
2:B:249:PHE:HB2	2:B:250:PRO:HD3	1.99	0.44
2:B:183:PRO:HB2	2:B:278:PHE:CE1	2.52	0.44
2:B:280:PRO:HA	2:B:283:ARG:HD3	1.99	0.44
2:B:68:HIS:CD2	2:B:130:PHE:CG	3.06	0.44
2:B:240:ARG:CB	2:B:241:ASP:CA	2.95	0.44
2:B:264:MET:HE3	2:B:268:GLY:HA3	1.98	0.44
1:A:185:PHE:CD2	1:A:251:ILE:CG2	3.00	0.44
2:B:172:ALA:N	2:B:173:PRO:CD	2.74	0.44
2:B:171:LEU:HD22	2:B:173:PRO:HB3	1.99	0.44
2:B:197:MET:CE	2:B:200:VAL:HG21	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:HZ2	2:B:79:ALA:HB2	1.82	0.44
2:B:232:LEU:C	2:B:232:LEU:HD23	2.37	0.44
2:B:242:VAL:O	2:B:243:SER:HB2	2.18	0.44
2:B:259:SER:OG	2:B:260:VAL:N	2.51	0.44
1:A:228:ARG:NE	1:A:228:ARG:CA	2.78	0.44
2:B:62:ARG:O	2:B:62:ARG:HG2	2.16	0.44
2:B:192:ALA:CB	2:B:194:PRO:HD2	2.48	0.44
2:B:240:ARG:CB	2:B:241:ASP:HB2	2.40	0.44
1:A:88:PHE:HE1	1:A:147:LYS:HG3	1.77	0.44
2:B:35:LYS:HB2	2:B:35:LYS:NZ	2.32	0.44
1:A:170:GLU:O	1:A:175:LYS:HE3	2.18	0.43
2:B:21:TYR:CD1	2:B:34:LEU:HB2	2.52	0.43
2:B:71:VAL:HG11	2:B:131:LEU:HD11	2.00	0.43
2:B:4:SER:C	2:B:6:TYR:H	2.18	0.43
2:B:212:PRO:HB2	2:B:215:CYS:CB	2.48	0.43
1:A:51:GLU:OE1	1:A:96:LYS:HG2	2.18	0.43
1:A:121:ALA:N	2:B:44:GLU:OE2	2.29	0.43
2:B:51:ILE:HG22	2:B:55:ARG:CZ	2.48	0.43
2:B:123:GLN:O	2:B:126:ARG:HB2	2.18	0.43
2:B:142:LYS:O	2:B:146:ILE:HG13	2.19	0.43
2:B:71:VAL:CG1	2:B:131:LEU:HD11	2.47	0.43
2:B:139:ARG:NH2	2:B:162:ALA:HB1	2.32	0.43
2:B:116:THR:O	2:B:116:THR:HG22	2.18	0.43
1:A:194:LYS:CE	1:A:247:CYS:SG	3.07	0.43
1:A:177:ILE:O	1:A:181:HIS:ND1	2.52	0.43
2:B:137:VAL:HG13	2:B:196:ASP:HB2	1.99	0.43
2:B:149:THR:HG23	2:B:150:SER:OG	2.18	0.43
2:B:260:VAL:O	2:B:260:VAL:HG22	2.17	0.43
1:A:28:LEU:HD12	1:A:28:LEU:O	2.18	0.43
2:B:71:VAL:CG1	2:B:159:PHE:CE2	3.02	0.43
2:B:101:ARG:HH12	2:B:144:GLU:HG3	1.84	0.43
1:A:120:THR:HG23	3:B:2011:HOH:O	2.19	0.42
2:B:122:ARG:HG3	2:B:290:LEU:HD23	2.01	0.42
2:B:183:PRO:HB2	2:B:278:PHE:HE1	1.84	0.42
2:B:223:LEU:HD23	2:B:223:LEU:O	2.19	0.42
2:B:258:GLN:CD	2:B:258:GLN:H	2.22	0.42
1:A:107:MET:HE3	1:A:124:LEU:CD2	2.49	0.42
2:B:60:LEU:CB	2:B:74:LEU:HD12	2.49	0.42
2:B:108:PRO:N	2:B:109:PRO:HD2	2.34	0.42
2:B:11:GLU:HA	2:B:21:TYR:HA	2.01	0.42
2:B:96:VAL:HG13	2:B:97:ASP:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ARG:C	2:B:103:TYR:N	2.73	0.42
2:B:218:SER:HB3	2:B:221:ASP:HB3	2.02	0.42
2:B:104:LEU:HD22	2:B:209:ARG:NH2	2.34	0.42
2:B:272:LEU:CD1	2:B:276:LEU:HG	2.50	0.42
1:A:95:LYS:NZ	1:A:95:LYS:N	2.57	0.42
2:B:37:VAL:HG23	2:B:165:TYR:CD2	2.54	0.42
2:B:41:ASN:HB3	2:B:85:ARG:H	1.84	0.42
2:B:60:LEU:HB2	2:B:74:LEU:HD12	2.02	0.42
2:B:139:ARG:HB2	2:B:139:ARG:NH1	2.34	0.42
2:B:177:THR:O	2:B:179:TRP:N	2.45	0.42
2:B:22:LYS:HD2	2:B:95:HIS:NE2	2.35	0.41
2:B:78:CYS:HB3	2:B:90:THR:HG23	2.01	0.41
2:B:188:GLN:NE2	2:B:190:THR:CG2	2.83	0.41
2:B:88:LYS:NZ	3:B:2017:HOH:O	2.52	0.41
2:B:123:GLN:HG2	2:B:154:VAL:HG22	2.02	0.41
2:B:63:LEU:CD2	2:B:134:ASN:ND2	2.79	0.41
1:A:78:PHE:N	1:A:79:PRO:HD2	2.36	0.41
1:A:175:LYS:O	1:A:179:ARG:HB2	2.21	0.41
2:B:124:PHE:CE2	2:B:200:VAL:HG22	2.55	0.41
1:A:44:TYR:CE2	1:A:89:LEU:HB3	2.56	0.41
1:A:95:LYS:H	1:A:95:LYS:HZ2	1.60	0.41
1:A:228:ARG:HG3	1:A:231:ARG:HB2	2.03	0.41
1:A:237:ILE:HG22	1:A:237:ILE:O	2.21	0.41
2:B:150:SER:C	2:B:152:GLY:N	2.73	0.41
2:B:265:GLU:HG2	2:B:266:GLU:HG2	2.03	0.41
1:A:120:THR:HG22	1:A:122:GLU:N	2.35	0.41
2:B:22:LYS:HD2	2:B:95:HIS:CE1	2.56	0.41
2:B:37:VAL:HB	2:B:165:TYR:CE2	2.56	0.41
1:A:123:LYS:HB2	1:A:123:LYS:HE3	1.84	0.40
2:B:37:VAL:HG23	2:B:165:TYR:CE2	2.56	0.40
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.95	0.40
1:A:241:PRO:HG2	3:A:2096:HOH:O	2.20	0.40
2:B:56:GLU:HA	2:B:56:GLU:OE2	2.20	0.40
2:B:271:LEU:HD22	2:B:292:HIS:ND1	2.37	0.40
2:B:62:ARG:NH1	3:B:2014:HOH:O	2.44	0.40
2:B:210:ARG:NE	2:B:211:LYS:O	2.54	0.40
2:B:231:GLY:O	2:B:233:PRO:HD3	2.22	0.40
1:A:178:ILE:CD1	1:A:212:VAL:HG22	2.52	0.40
2:B:32:VAL:HG11	2:B:92:VAL:CG1	2.37	0.40
2:B:221:ASP:O	2:B:225:LYS:HB2	2.22	0.40
2:B:222:GLN:HA	2:B:225:LYS:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:PHE:HD1	2:B:249:PHE:HA	1.70	0.40
1:A:139:GLN:HG3	2:B:82:ARG:NH1	2.36	0.40
2:B:54:VAL:CG2	2:B:55:ARG:N	2.84	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	244/271 (90%)	228 (93%)	15 (6%)	1 (0%)	34	66
2	B	289/306 (94%)	211 (73%)	52 (18%)	26 (9%)	1	1
All	All	533/577 (92%)	439 (82%)	67 (13%)	27 (5%)	2	6

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	ALA
2	B	16	ALA
2	B	161	LEU
2	B	177	THR
2	B	283	ARG
2	B	9	VAL
2	B	84	ASP
2	B	151	GLY
2	B	217	ASN
2	B	5	ARG
2	B	259	SER
2	B	290	LEU
2	B	262	PRO
1	A	224	LEU
2	B	63	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	102	THR
2	B	169	MET
2	B	173	PRO
2	B	189	SER
2	B	178	LEU
2	B	249	PHE
2	B	152	GLY
2	B	154	VAL
2	B	160	GLY
2	B	176	VAL
2	B	112	LEU
2	B	239	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	222/243 (91%)	204 (92%)	18 (8%)	11	33
2	B	250/264 (95%)	224 (90%)	26 (10%)	7	21
All	All	472/507 (93%)	428 (91%)	44 (9%)	9	26

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

Mol	Chain	Res	Type
1	A	24	ASN
1	A	50	LYS
1	A	60	VAL
1	A	65	LEU
1	A	89	LEU
1	A	95	LYS
1	A	98	ARG
1	A	116	THR
1	A	140	MET
1	A	143	LEU
1	A	165	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	GLU
1	A	235	ARG
1	A	252	GLU
1	A	256	GLU
1	A	259	LEU
1	A	260	ARG
1	A	264	GLN
2	B	21	TYR
2	B	27	HIS
2	B	35	LYS
2	B	52	SER
2	B	54	VAL
2	B	70	ASN
2	B	74	LEU
2	B	83	THR
2	B	87	ILE
2	B	90	THR
2	B	112	LEU
2	B	119	ASP
2	B	139	ARG
2	B	147	LEU
2	B	148	VAL
2	B	153	THR
2	B	159	PHE
2	B	174	VAL
2	B	179	TRP
2	B	181	ARG
2	B	197	MET
2	B	210	ARG
2	B	249	PHE
2	B	270	GLN
2	B	283	ARG
2	B	290	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	71	GLN
1	A	139	GLN
1	A	158	HIS
1	A	176	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	GLN
1	A	198	ASN
1	A	261	GLN
2	B	41	ASN
2	B	70	ASN
2	B	98	GLN
2	B	123	GLN
2	B	134	ASN
2	B	258	GLN
2	B	270	GLN
2	B	291	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	246/271 (90%)	0.10	3 (1%) 79 73	32, 51, 108, 157	0
2	B	291/306 (95%)	0.68	38 (13%) 3 2	59, 112, 151, 171	0
All	All	537/577 (93%)	0.42	41 (7%) 13 7	32, 87, 143, 171	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	232	LEU	5.2
2	B	238	TRP	4.4
2	B	125	LEU	4.0
2	B	264	MET	3.8
2	B	242	VAL	3.7
2	B	249	PHE	3.5
2	B	12	ILE	3.4
2	B	235	GLU	3.2
2	B	128	LEU	3.2
2	B	197	MET	3.2
2	B	2	ALA	3.1
2	B	8	PRO	2.9
2	B	9	VAL	2.9
2	B	6	TYR	2.8
2	B	117	ILE	2.8
2	B	185	VAL	2.8
2	B	195	VAL	2.8
2	B	234	PRO	2.8
2	B	122	ARG	2.7
2	B	207	MET	2.6
1	A	261	GLN	2.6
1	A	267	ASP	2.6
2	B	252	ARG	2.6
2	B	278	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	233	PRO	2.5
2	B	187	LEU	2.5
2	B	7	GLU	2.5
2	B	191	TYR	2.5
2	B	236	ASP	2.4
2	B	154	VAL	2.4
2	B	5	ARG	2.3
2	B	139	ARG	2.3
2	B	189	SER	2.3
2	B	214	PHE	2.3
2	B	205	ALA	2.2
1	A	262	ALA	2.2
2	B	103	TYR	2.2
2	B	237	ASP	2.2
2	B	241	ASP	2.2
2	B	21	TYR	2.1
2	B	65	ALA	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.