Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 01:07 PM EDT

PDB ID	:	2PI2
Title	:	Full-length Replication protein A subunits RPA14 and RPA32
Authors	:	Deng, X.; Borgstahl, G.E.
Deposited on	:	2007-04-12
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

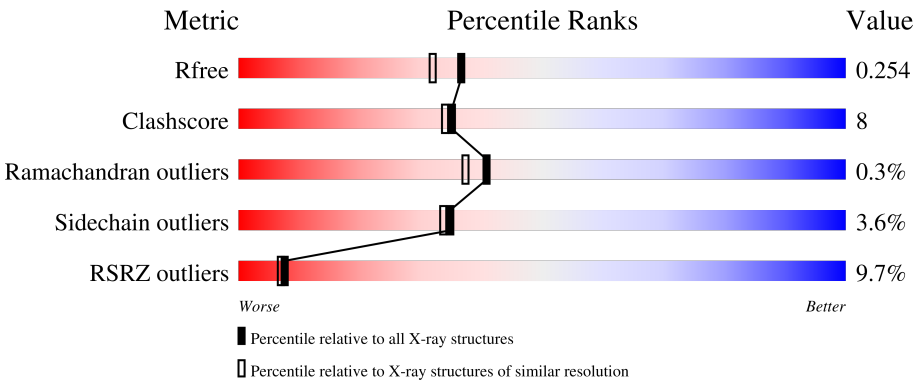
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	270	5% 40% 7% • 52%
1	B	270	% 37% 8% • 54%
1	C	270	10% 36% 10% 54%
1	D	270	8% 37% 7% • 54%
2	E	142	4% 76% 6% • 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	142	6% 66% 14% • 16%
2	G	142	5% 74% 7% • 17%
2	H	142	5% 73% 8% •• 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7880 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 Replication protein A 32 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1010	643	175	186	6	0	0	0
1	B	124	973	622	168	177	6	0	0	0
1	C	125	979	625	167	181	6	0	0	0
1	D	123	962	616	164	176	6	0	0	0

- Molecule 2 is a protein called Replication protein A 14 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	117	915	590	148	170	7	0	0	0
2	F	119	934	601	153	173	7	0	0	0
2	G	118	924	595	150	172	7	0	0	0
2	H	117	915	590	148	170	7	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	MET	-	expression tag	UNP P35244
E	-19	GLY	-	expression tag	UNP P35244
E	-18	HIS	-	expression tag	UNP P35244
E	-17	HIS	-	expression tag	UNP P35244
E	-16	HIS	-	expression tag	UNP P35244
E	-15	HIS	-	expression tag	UNP P35244
E	-14	HIS	-	expression tag	UNP P35244
E	-13	HIS	-	expression tag	UNP P35244

Continued on next page...

Continued from previous page...

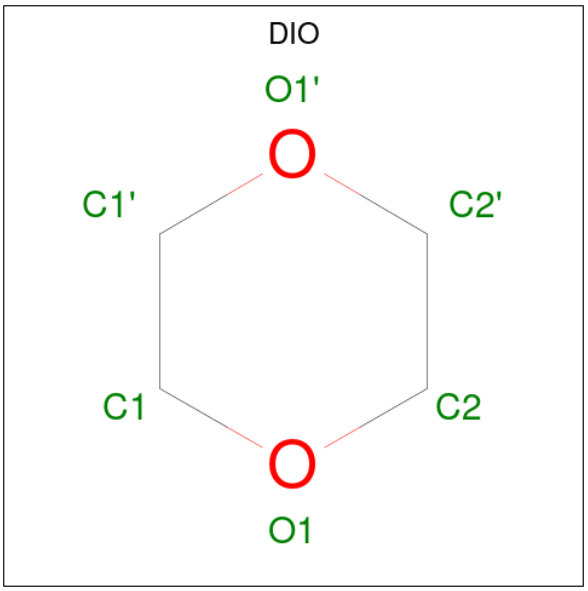
Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP P35244
E	-11	HIS	-	expression tag	UNP P35244
E	-10	HIS	-	expression tag	UNP P35244
E	-9	HIS	-	expression tag	UNP P35244
E	-8	SER	-	expression tag	UNP P35244
E	-7	SER	-	expression tag	UNP P35244
E	-6	GLY	-	expression tag	UNP P35244
E	-5	HIS	-	expression tag	UNP P35244
E	-4	ILE	-	expression tag	UNP P35244
E	-3	GLU	-	expression tag	UNP P35244
E	-2	GLY	-	expression tag	UNP P35244
E	-1	ARG	-	expression tag	UNP P35244
E	0	HIS	-	expression tag	UNP P35244
F	-20	MET	-	expression tag	UNP P35244
F	-19	GLY	-	expression tag	UNP P35244
F	-18	HIS	-	expression tag	UNP P35244
F	-17	HIS	-	expression tag	UNP P35244
F	-16	HIS	-	expression tag	UNP P35244
F	-15	HIS	-	expression tag	UNP P35244
F	-14	HIS	-	expression tag	UNP P35244
F	-13	HIS	-	expression tag	UNP P35244
F	-12	HIS	-	expression tag	UNP P35244
F	-11	HIS	-	expression tag	UNP P35244
F	-10	HIS	-	expression tag	UNP P35244
F	-9	HIS	-	expression tag	UNP P35244
F	-8	SER	-	expression tag	UNP P35244
F	-7	SER	-	expression tag	UNP P35244
F	-6	GLY	-	expression tag	UNP P35244
F	-5	HIS	-	expression tag	UNP P35244
F	-4	ILE	-	expression tag	UNP P35244
F	-3	GLU	-	expression tag	UNP P35244
F	-2	GLY	-	expression tag	UNP P35244
F	-1	ARG	-	expression tag	UNP P35244
F	0	HIS	-	expression tag	UNP P35244
G	-20	MET	-	expression tag	UNP P35244
G	-19	GLY	-	expression tag	UNP P35244
G	-18	HIS	-	expression tag	UNP P35244
G	-17	HIS	-	expression tag	UNP P35244
G	-16	HIS	-	expression tag	UNP P35244
G	-15	HIS	-	expression tag	UNP P35244
G	-14	HIS	-	expression tag	UNP P35244
G	-13	HIS	-	expression tag	UNP P35244

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-12	HIS	-	expression tag	UNP P35244
G	-11	HIS	-	expression tag	UNP P35244
G	-10	HIS	-	expression tag	UNP P35244
G	-9	HIS	-	expression tag	UNP P35244
G	-8	SER	-	expression tag	UNP P35244
G	-7	SER	-	expression tag	UNP P35244
G	-6	GLY	-	expression tag	UNP P35244
G	-5	HIS	-	expression tag	UNP P35244
G	-4	ILE	-	expression tag	UNP P35244
G	-3	GLU	-	expression tag	UNP P35244
G	-2	GLY	-	expression tag	UNP P35244
G	-1	ARG	-	expression tag	UNP P35244
G	0	HIS	-	expression tag	UNP P35244
H	-20	MET	-	expression tag	UNP P35244
H	-19	GLY	-	expression tag	UNP P35244
H	-18	HIS	-	expression tag	UNP P35244
H	-17	HIS	-	expression tag	UNP P35244
H	-16	HIS	-	expression tag	UNP P35244
H	-15	HIS	-	expression tag	UNP P35244
H	-14	HIS	-	expression tag	UNP P35244
H	-13	HIS	-	expression tag	UNP P35244
H	-12	HIS	-	expression tag	UNP P35244
H	-11	HIS	-	expression tag	UNP P35244
H	-10	HIS	-	expression tag	UNP P35244
H	-9	HIS	-	expression tag	UNP P35244
H	-8	SER	-	expression tag	UNP P35244
H	-7	SER	-	expression tag	UNP P35244
H	-6	GLY	-	expression tag	UNP P35244
H	-5	HIS	-	expression tag	UNP P35244
H	-4	ILE	-	expression tag	UNP P35244
H	-3	GLU	-	expression tag	UNP P35244
H	-2	GLY	-	expression tag	UNP P35244
H	-1	ARG	-	expression tag	UNP P35244
H	0	HIS	-	expression tag	UNP P35244

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	4	2	0	0
3	B	1	6	4	2	0	0
3	C	1	6	4	2	0	0
3	D	1	6	4	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	25	25	25	0	0
4	B	26	26	26	0	0
4	C	7	7	7	0	0
4	D	5	5	5	0	0
4	E	56	56	56	0	0
4	F	41	41	41	0	0
4	G	47	47	47	0	0
4	H	37	37	37	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: Replication protein A 32 kDa subunit

Chain A: 5% 40% 7% • 52%

MET TRP ASN SER GLY PHE GLU SER TYR GLY SER SER SER TYR GLY GLY ALA GLY GLY TYR THR GLN SER PRO GLY GLY PHE GLY SER PRO ALA PRO SER GLN ALA GLU LYS LYS SER ARG A41 Q44 H45 I46 R65 T75 I79 K85 A86 P87 T88 N89 I94

P101 V104 W107 V108 D109 THR ASP ASP THR SER SER GLU N117 T118 E123 F155 H158 V162 N173 S174 Q175 P176 SER ALA GLY ARG ALA PRO ILE SER ASN PRO GLY MET SER GLU ALA GLY ASN PHE GLY GLY ASN SER PHE MET PRO ALA ASN GLY LEU THR VAL

ALA GLN ASN GLN VAL LEU ASN LEU ILE LYS ALA CYS PRO ARG PRO GLU GLY LEU ASN PHE GLN ASP LEU LYS ASN GLN LEU LYS HIS MET SER VAL SER SER ILE LYS GLN ALA VAL ASP PHE LEU SER ASN GLU GLY HIS ILE TYR SER THR VAL ASP ASP ASP HIS PHE LYS SER THR

ASP ALA GLU

• Molecule 1: Replication protein A 32 kDa subunit

Chain B: % 37% 8% • 54%

MET TRP ASN SER GLY PHE GLU SER TYR GLY SER SER SER TYR GLY GLY ALA GLY GLY TYR THR GLN SER PRO GLY GLY PHE GLY SER PRO ALA PRO SER GLN ALA GLU LYS LYS SER ARG ALA R42 S56 A57 T58 L59 V60 D61 E62 V63 F64 R65 I66 I71 T75 I79

N89 I90 V91 I94 A100 P101 V104 R105 V108 ASP THR ASP ASP THR SER SER GLU ASN T118 V128 N137 M147 F155 N173 S174 GLN PRO SER ALA GLY ARG ALA PRO ILE SER ASN PRO GLY MET SER GLU ALA GLY ASN PHE GLY GLY ASN SER PHE

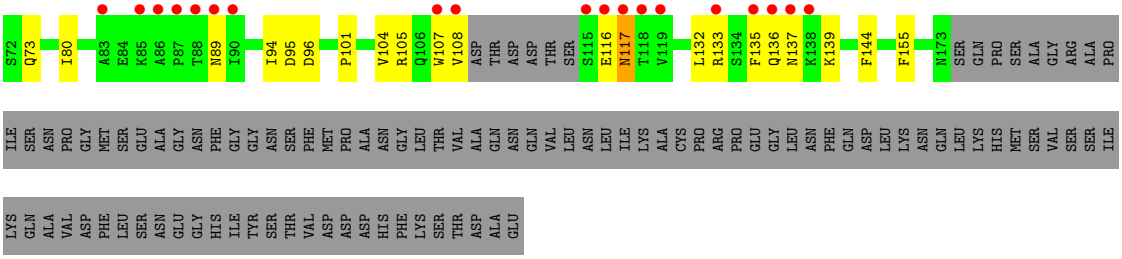
MET PRO ALA ASN GLY LEU THR VAL ALA GLN ASN GLN VAL LEU ASN LEU ILE LYS ALA CYS PRO ARG PRO GLU GLY LEU ASN PHE GLN ASP LEU LYS ASN GLN LEU LYS HIS MET SER VAL SER SER ILE LYS GLN ALA VAL ASP PHE LEU SER ASN GLU GLY HIS ILE TYR SER THR VAL

ASP ASP ASP HIS PHE LYS SER THR ASP ALA GLU

• Molecule 1: Replication protein A 32 kDa subunit

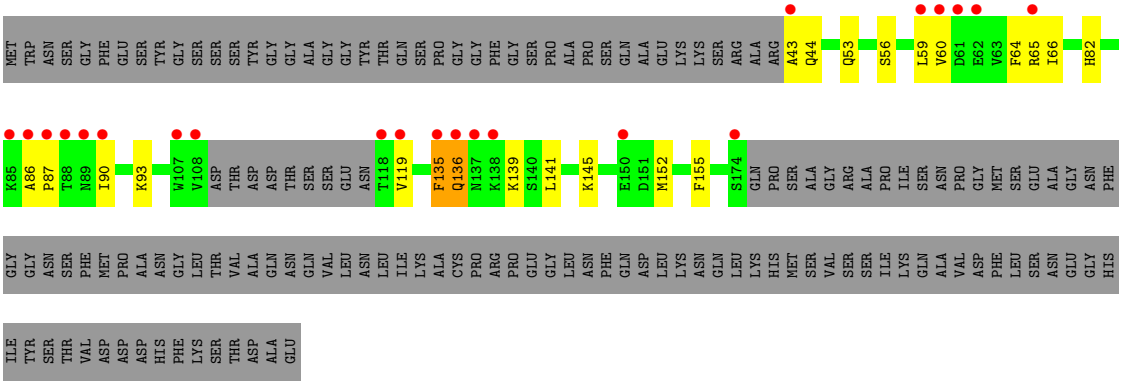
Chain C: 10% 36% 10% 54%

MET TRP ASN SER GLY PHE GLU SER TYR GLY SER SER SER TYR GLY GLY ALA GLY GLY TYR THR GLN SER PRO GLY GLY PHE GLY SER PRO ALA PRO SER GLN ALA GLU LYS LYS SER ARG ALA ARG A43 Q44 H45 Q53 A57 T58 L59 V60 D61 E62 V63 F64 R65 I66 I71



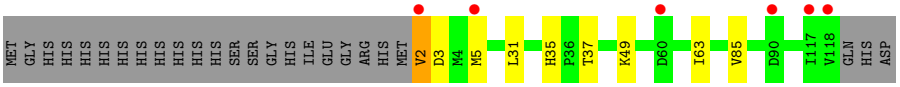
- Molecule 1: Replication protein A 32 kDa subunit

Chain D:



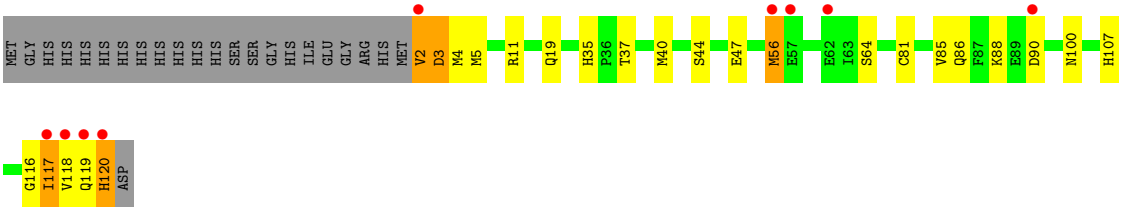
- Molecule 2: Replication protein A 14 kDa subunit

Chain E:



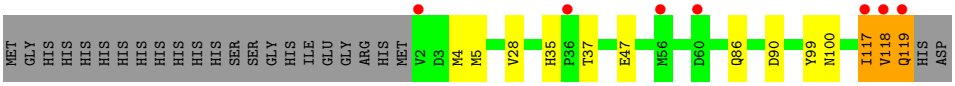
- Molecule 2: Replication protein A 14 kDa subunit

Chain F:



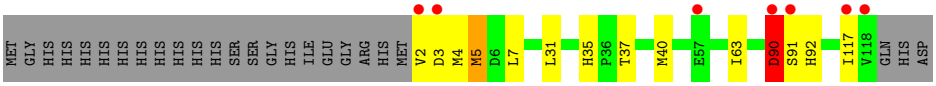
- Molecule 2: Replication protein A 14 kDa subunit

Chain G:



• Molecule 2: Replication protein A 14 kDa subunit

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.48Å 139.83Å 171.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 40.97 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.00) 97.8 (40.97-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.232 , 0.255 0.234 , 0.254	Depositor DCC
R_{free} test set	8172 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7880	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 (i)

5.1 Standard geometry (i)

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

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	0.51	0/1028	0.62	0/1398
1	B	0.58	0/990	0.67	0/1345
1	C	0.59	0/996	0.62	0/1354
1	D	0.53	0/979	0.71	3/1331 (0.2%)
2	E	0.61	0/934	0.65	0/1262
2	F	0.63	0/954	0.66	0/1289
2	G	0.58	0/943	0.61	0/1274
2	H	0.55	0/934	0.63	0/1262
All	All	0.57	0/7758	0.65	3/10515 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	1	0
2	E	0	1
2	F	0	1
2	G	0	2
2	H	0	1
All	All	1	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	135	PHE	N-CA-C	9.33	136.19	111.00
1	D	135	PHE	CB-CA-C	-6.98	96.45	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	136	GLN	N-CA-C	-5.49	96.17	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	136	GLN	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	TRP	Peptide
2	E	2	VAL	Peptide
2	F	117	ILE	Peptide
2	G	117	ILE	Peptide
2	G	118	VAL	Peptide
2	H	90	ASP	Peptide

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	1010	0	1034	22	0
1	B	973	0	1004	23	0
1	C	979	0	1003	17	0
1	D	962	0	991	16	0
2	E	915	0	921	8	0
2	F	934	0	936	19	0
2	G	924	0	929	14	0
2	H	915	0	921	18	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
3	D	6	0	8	1	0
4	A	25	0	0	1	0
4	B	26	0	0	1	0
4	C	7	0	0	0	0
4	D	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	56	0	0	1	0
4	F	41	0	0	0	0
4	G	47	0	0	1	0
4	H	37	0	0	0	0
All	All	7880	0	7771	127	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 8.

All (127) 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:135:PHE:O	1:D:136:GLN:HG2	1.11	1.22
1:B:66:ILE:HD12	1:B:71:ILE:HD13	1.23	1.11
1:D:135:PHE:O	1:D:136:GLN:CG	1.99	1.10
1:C:44:GLN:HB2	1:C:45:HIS:HA	1.37	1.06
2:H:90:ASP:HB2	2:H:91:SER:HB2	1.43	0.98
2:G:117:ILE:HD12	2:G:119:GLN:NE2	1.79	0.96
1:B:89:ASN:ND2	1:B:105:ARG:HH21	1.72	0.88
2:H:3:ASP:HB3	2:H:4:MET:HA	1.57	0.86
1:A:175:GLN:HB3	1:A:176:PRO:HD2	1.59	0.85
1:A:175:GLN:HB3	1:A:176:PRO:CD	2.08	0.84
1:B:94:ILE:HD12	1:B:104:VAL:HG21	1.64	0.79
1:B:173:ASN:O	1:B:174:SER:HB2	1.80	0.79
2:G:117:ILE:CD1	2:G:119:GLN:HE22	1.97	0.78
2:G:117:ILE:CD1	2:G:119:GLN:NE2	2.46	0.78
1:B:66:ILE:CD1	1:B:71:ILE:HD13	2.11	0.76
2:H:91:SER:OG	2:H:92:HIS:CD2	2.39	0.75
1:A:44:GLN:NE2	1:A:44:GLN:HA	2.01	0.75
2:H:90:ASP:HB2	2:H:91:SER:CB	2.16	0.74
2:F:11:ARG:O	2:F:107:HIS:HE1	1.71	0.74
2:G:117:ILE:HD12	2:G:119:GLN:HE22	1.52	0.74
1:C:95:ASP:OD1	1:C:96:ASP:O	2.07	0.73
1:A:94:ILE:HD12	1:A:104:VAL:HG21	1.71	0.72
1:C:44:GLN:CB	1:C:45:HIS:HA	2.19	0.70
1:C:57:ALA:O	1:C:139:LYS:NZ	2.22	0.70
1:B:89:ASN:ND2	1:B:105:ARG:NH2	2.40	0.69
2:H:3:ASP:HB3	2:H:4:MET:CA	2.24	0.67
1:B:61:ASP:N	1:B:62:GLU:HA	2.10	0.67
1:C:44:GLN:HB2	1:C:45:HIS:CA	2.18	0.67
1:B:61:ASP:H	1:B:63:VAL:H	1.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:SER:OG	2:H:92:HIS:HD2	1.78	0.66
2:H:35:HIS:CD2	2:H:37:THR:H	2.14	0.64
2:F:35:HIS:HB2	2:F:40:MET:HB3	1.80	0.64
1:C:66:ILE:HD11	1:C:71:ILE:HD13	1.81	0.62
1:D:53:GLN:HB3	1:D:66:ILE:HD13	1.82	0.62
1:A:79:ILE:HD13	2:E:85:VAL:HG21	1.82	0.61
1:C:53:GLN:HB3	1:C:66:ILE:HD13	1.83	0.60
2:G:117:ILE:HD12	2:G:119:GLN:HE21	1.65	0.59
2:E:2:VAL:HA	2:E:3:ASP:HB3	1.85	0.58
1:B:59:LEU:HD11	1:B:62:GLU:HB2	1.86	0.58
2:H:31:LEU:HD22	2:H:63:ILE:O	2.02	0.58
2:F:117:ILE:HG13	2:F:118:VAL:N	2.18	0.58
1:A:79:ILE:HD11	1:A:123:GLU:HA	1.85	0.58
1:A:94:ILE:HD12	1:A:104:VAL:CG2	2.35	0.57
1:B:66:ILE:HD12	1:B:71:ILE:CD1	2.16	0.56
2:E:49:LYS:HE2	4:E:135:HOH:O	2.05	0.55
2:F:116:GLY:HA3	2:F:118:VAL:O	2.06	0.55
2:E:35:HIS:HD2	2:E:37:THR:OG1	1.90	0.54
1:B:79:ILE:CD1	2:F:85:VAL:HG21	2.37	0.54
1:B:56:SER:HB2	4:B:323:HOH:O	2.06	0.54
1:A:174:SER:HA	1:A:175:GLN:HB2	1.89	0.54
1:D:60:VAL:HB	1:D:65:ARG:HH21	1.72	0.54
1:C:80:ILE:HD13	1:C:94:ILE:HG12	1.89	0.54
1:D:135:PHE:O	1:D:136:GLN:CB	2.54	0.53
1:B:94:ILE:HD13	1:B:128:VAL:HG21	1.91	0.53
2:G:35:HIS:HD2	2:G:37:THR:OG1	1.92	0.52
1:B:173:ASN:O	1:B:174:SER:CB	2.55	0.52
1:A:173:ASN:O	1:A:175:GLN:HB2	2.10	0.52
1:B:100:ALA:H	2:F:120:HIS:HB3	1.74	0.52
1:B:94:ILE:HD12	1:B:104:VAL:CG2	2.36	0.52
1:C:132:LEU:HD11	1:C:139:LYS:HG2	1.91	0.52
1:D:90:ILE:HD11	1:D:119:VAL:HG23	1.91	0.51
1:B:101:PRO:HD3	2:F:5:MET:O	2.10	0.51
2:F:119:GLN:O	2:F:120:HIS:HB2	2.09	0.51
2:F:35:HIS:CB	2:F:40:MET:HB3	2.39	0.51
1:D:56:SER:HA	2:H:117:ILE:HD11	1.93	0.51
2:H:3:ASP:CB	2:H:4:MET:HA	2.35	0.51
2:G:117:ILE:CG1	2:G:119:GLN:NE2	2.74	0.51
2:F:117:ILE:HG13	2:F:119:GLN:H	1.76	0.50
1:D:135:PHE:C	1:D:135:PHE:CD1	2.85	0.49
2:F:35:HIS:HD2	2:F:37:THR:OG1	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ALA:HB1	1:A:87:PRO:HD2	1.94	0.49
1:D:56:SER:OG	2:H:117:ILE:HD12	2.12	0.49
1:A:175:GLN:CB	1:A:176:PRO:CD	2.85	0.49
1:B:91:VAL:HG22	1:B:105:ARG:HG3	1.93	0.49
2:H:4:MET:HB2	2:H:7:LEU:HD12	1.94	0.48
2:H:90:ASP:CB	2:H:91:SER:HB2	2.29	0.48
1:D:152:MET:SD	3:D:304:DIO:H21	2.54	0.48
1:D:86:ALA:HB1	1:D:87:PRO:HD2	1.96	0.47
1:D:43:ALA:N	1:D:44:GLN:HA	2.28	0.47
1:C:44:GLN:CB	1:C:45:HIS:CA	2.84	0.47
1:D:59:LEU:HB2	1:D:64:PHE:CE2	2.50	0.47
2:H:35:HIS:HD2	2:H:37:THR:H	1.61	0.47
1:A:46:ILE:HG22	1:A:75:THR:HG23	1.98	0.46
1:A:174:SER:CA	1:A:175:GLN:HB2	2.46	0.46
1:A:101:PRO:HD3	2:E:5:MET:O	2.15	0.46
1:B:58:THR:O	1:B:64:PHE:HA	2.16	0.46
1:C:73:GLN:HE21	1:C:144:PHE:HZ	1.62	0.46
2:G:47:GLU:HG3	2:G:100:ASN:ND2	2.30	0.46
1:D:56:SER:HA	2:H:117:ILE:CD1	2.46	0.46
1:B:100:ALA:HB3	2:F:120:HIS:ND1	2.31	0.45
1:A:88:THR:HG23	1:A:89:ASN:OD1	2.17	0.45
2:G:117:ILE:H	2:G:119:GLN:HB3	1.82	0.45
1:A:44:GLN:HG3	4:A:317:HOH:O	2.17	0.45
2:H:3:ASP:HB3	2:H:5:MET:H	1.81	0.45
1:A:108:VAL:HG12	1:A:109:ASP:N	2.30	0.45
2:E:31:LEU:HD13	2:E:63:ILE:HG13	1.98	0.45
1:D:82:HIS:HB3	1:D:93:LYS:HG3	1.99	0.45
1:A:44:GLN:HA	1:A:44:GLN:HE21	1.78	0.45
1:A:175:GLN:CB	1:A:176:PRO:HD2	2.40	0.45
1:C:133:ARG:HB3	1:C:135:PHE:CD2	2.52	0.44
1:C:94:ILE:HD12	1:C:104:VAL:HG21	2.00	0.44
2:F:2:VAL:HA	2:F:3:ASP:HA	1.73	0.44
2:H:2:VAL:HA	2:H:3:ASP:HA	1.67	0.44
1:C:89:ASN:ND2	1:C:105:ARG:HH21	2.16	0.43
1:B:75:THR:HA	1:B:128:VAL:O	2.18	0.43
1:B:89:ASN:HD21	1:B:105:ARG:NH2	2.12	0.43
3:B:302:DIO:H1'2	2:F:88:LYS:HB3	2.01	0.43
1:C:101:PRO:HD3	2:G:5:MET:O	2.18	0.43
2:G:117:ILE:HG13	2:G:119:GLN:NE2	2.34	0.43
2:E:35:HIS:CD2	2:E:37:THR:OG1	2.71	0.43
2:F:47:GLU:HG3	2:F:100:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:HIS:O	1:A:162:VAL:HG23	2.18	0.43
2:F:56:MET:SD	2:F:81:CYS:O	2.77	0.42
1:C:135:PHE:HA	1:C:136:GLN:HA	1.56	0.42
2:F:117:ILE:HG13	2:F:119:GLN:N	2.35	0.42
1:D:141:LEU:HA	1:D:141:LEU:HD12	1.82	0.42
1:A:44:GLN:NE2	1:A:44:GLN:CA	2.76	0.41
2:E:35:HIS:CD2	2:E:37:THR:H	2.38	0.41
2:F:116:GLY:HA3	2:F:119:GLN:HA	2.03	0.41
2:H:90:ASP:CB	2:H:91:SER:CB	2.94	0.41
1:A:173:ASN:C	1:A:175:GLN:HB2	2.40	0.41
2:F:64:SER:H	2:F:86:GLN:NE2	2.18	0.41
2:G:86:GLN:HB3	4:G:147:HOH:O	2.21	0.41
1:C:135:PHE:CD2	1:C:135:PHE:N	2.89	0.40
1:B:94:ILE:CD1	1:B:128:VAL:HG21	2.51	0.40
2:G:28:VAL:HB	2:G:99:TYR:CE2	2.56	0.40
2:G:35:HIS:CD2	2:G:37:THR:H	2.39	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	125/270 (46%)	119 (95%)	5 (4%)	1 (1%)	19	13
1	B	120/270 (44%)	116 (97%)	4 (3%)	0	100	100
1	C	121/270 (45%)	116 (96%)	4 (3%)	1 (1%)	19	13
1	D	119/270 (44%)	112 (94%)	7 (6%)	0	100	100
2	E	115/142 (81%)	115 (100%)	0	0	100	100
2	F	117/142 (82%)	115 (98%)	2 (2%)	0	100	100
2	G	116/142 (82%)	112 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	115/142 (81%)	110 (96%)	4 (4%)	1 (1%)	17	11
All	All	948/1648 (58%)	915 (96%)	30 (3%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
2	H	90	ASP
1	C	117	ASN

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	115/228 (50%)	112 (97%)	3 (3%)	46	48
1	B	111/228 (49%)	106 (96%)	5 (4%)	27	24
1	C	112/228 (49%)	106 (95%)	6 (5%)	22	18
1	D	110/228 (48%)	107 (97%)	3 (3%)	44	46
2	E	102/124 (82%)	102 (100%)	0	100	100
2	F	104/124 (84%)	96 (92%)	8 (8%)	13	8
2	G	103/124 (83%)	99 (96%)	4 (4%)	32	30
2	H	102/124 (82%)	100 (98%)	2 (2%)	55	58
All	All	859/1408 (61%)	828 (96%)	31 (4%)	35	34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	79	ILE
1	A	155	PHE
1	B	42	ARG
1	B	71	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	147	MET
1	B	155	PHE
1	B	174	SER
1	C	63	VAL
1	C	108	VAL
1	C	116	GLU
1	C	117	ASN
1	C	137	ASN
1	C	155	PHE
1	D	139	LYS
1	D	145	LYS
1	D	155	PHE
2	F	2	VAL
2	F	3	ASP
2	F	4	MET
2	F	19	GLN
2	F	44	SER
2	F	56	MET
2	F	90	ASP
2	F	120	HIS
2	G	4	MET
2	G	90	ASP
2	G	118	VAL
2	G	119	GLN
2	H	5	MET
2	H	40	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	175	GLN
1	B	89	ASN
1	B	173	ASN
1	C	89	ASN
1	D	158	HIS
2	E	35	HIS
2	F	19	GLN
2	F	35	HIS
2	F	86	GLN
2	F	92	HIS
2	F	107	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	35	HIS
2	G	86	GLN
2	G	119	GLN
2	H	35	HIS
2	H	92	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DIO	C	303	-	6,6,6	0.54	0	6,6,6	0.74	0
3	DIO	D	304	-	6,6,6	0.56	0	6,6,6	0.70	0
3	DIO	B	302	-	6,6,6	0.59	0	6,6,6	0.74	0
3	DIO	A	301	-	6,6,6	0.49	0	6,6,6	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	C	303	-	-	-	0/1/1/1
3	DIO	D	304	-	-	-	0/1/1/1
3	DIO	B	302	-	-	-	0/1/1/1
3	DIO	A	301	-	-	-	0/1/1/1

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	304	DIO	1	0
3	B	302	DIO	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	129/270 (47%)	0.67	13 (10%)	7	6	22, 37, 59, 67	0
1	B	124/270 (45%)	0.31	4 (3%)	47	46	23, 35, 53, 61	0
1	C	125/270 (46%)	1.15	26 (20%)	1	0	24, 50, 69, 82	0
1	D	123/270 (45%)	1.15	22 (17%)	1	1	20, 53, 70, 77	0
2	E	117/142 (82%)	0.01	6 (5%)	28	27	23, 30, 48, 57	0
2	F	119/142 (83%)	0.29	9 (7%)	13	13	22, 32, 54, 69	0
2	G	118/142 (83%)	0.12	7 (5%)	22	21	24, 37, 54, 62	0
2	H	117/142 (82%)	-0.01	7 (5%)	21	20	27, 38, 55, 60	0
All	All	972/1648 (58%)	0.47	94 (9%)	7	7	20, 38, 65, 82	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	120	HIS	10.3
2	F	118	VAL	9.4
1	C	115	SER	9.1
1	A	176	PRO	7.6
2	G	119	GLN	6.9
1	C	135	PHE	6.9
1	A	41	ALA	6.7
1	C	116	GLU	6.4
1	A	117	ASN	6.3
1	A	175	GLN	6.2
1	D	60	VAL	6.0
1	D	118	THR	6.0
1	B	61	ASP	5.9
1	C	61	ASP	5.9
1	C	117	ASN	5.8
1	D	135	PHE	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	118	VAL	5.6
1	D	108	VAL	5.4
1	A	109	ASP	5.4
1	D	87	PRO	5.4
1	C	108	VAL	5.3
1	C	44	GLN	5.3
1	D	136	GLN	5.2
1	C	118	THR	5.2
1	C	60	VAL	5.0
1	D	43	ALA	4.9
1	D	61	ASP	4.9
1	D	90	ILE	4.7
2	F	2	VAL	4.7
1	D	88	THR	4.6
2	G	2	VAL	4.5
1	D	86	ALA	4.5
1	C	87	PRO	4.5
1	D	89	ASN	4.1
1	D	107	TRP	4.1
1	D	85	LYS	4.1
1	C	107	TRP	4.1
1	C	89	ASN	4.1
1	C	137	ASN	4.1
1	D	137	ASN	4.0
2	H	117	ILE	3.8
1	C	138	LYS	3.8
1	C	88	THR	3.7
1	A	108	VAL	3.5
1	D	62	GLU	3.5
2	H	2	VAL	3.5
2	H	118	VAL	3.4
1	A	87	PRO	3.4
1	A	118	THR	3.3
1	C	86	ALA	3.3
1	D	59	LEU	3.3
2	H	57	GLU	3.3
1	B	60	VAL	3.2
1	C	85	LYS	3.1
1	A	174	SER	3.0
1	D	174	SER	2.9
1	C	62	GLU	2.9
2	F	119	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	90	ASP	2.7
2	E	90	ASP	2.6
1	B	62	GLU	2.6
1	A	107	TRP	2.6
2	E	2	VAL	2.6
2	H	3	ASP	2.6
1	C	59	LEU	2.6
1	C	133	ARG	2.6
2	G	117	ILE	2.5
2	E	118	VAL	2.5
2	E	60	ASP	2.5
1	B	137	ASN	2.4
1	C	119	VAL	2.4
1	A	85	LYS	2.4
2	F	57	GLU	2.4
1	C	136	GLN	2.4
1	C	43	ALA	2.3
2	F	90	ASP	2.2
1	D	119	VAL	2.2
1	C	83	ALA	2.2
1	A	65	ARG	2.2
1	C	65	ARG	2.2
2	H	91	SER	2.2
1	D	65	ARG	2.2
2	F	56	MET	2.1
2	E	117	ILE	2.1
1	A	86	ALA	2.1
2	E	5	MET	2.1
2	F	62	GLU	2.1
1	C	90	ILE	2.1
2	G	56	MET	2.1
1	D	138	LYS	2.0
2	G	36	PRO	2.0
2	F	117	ILE	2.0
1	D	150	GLU	2.0
2	G	60	ASP	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DIO	B	302	6/6	0.96	0.10	31,33,34,35	0
3	DIO	C	303	6/6	0.96	0.10	43,44,45,45	0
3	DIO	D	304	6/6	0.96	0.07	53,53,54,54	0
3	DIO	A	301	6/6	0.98	0.11	42,43,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.