Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 06:22 pm GMT

PDB ID	:	4Z11
Title	:	Latent aurone synthase (polyphenol oxidase) from natural source
Authors	:	Molitor, C.; Mauracher, S.G.; Rompel, A.
Deposited on	:	2015-03-26
Resolution	:	2.50 Å(reported)

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

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

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

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

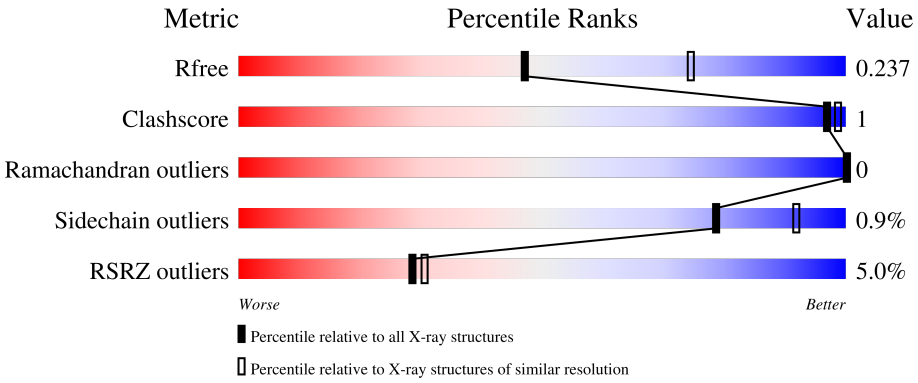
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	517	3% 97%
1	B	517	4% 91% 5%
1	C	517	5% 96%
1	D	517	7% 94%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30898 atoms, of which 14632 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 Aurone synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	H	N	O	S	0	1	0
			7707	2546	3708	691	747	15			
1	B	489	Total	C	H	N	O	S	0	0	0
			7416	2453	3578	663	709	13			
1	C	510	Total	C	H	N	O	S	0	0	0
			7720	2543	3726	689	747	15			
1	D	501	Total	C	H	N	O	S	0	0	0
			7527	2495	3620	672	725	15			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is water.

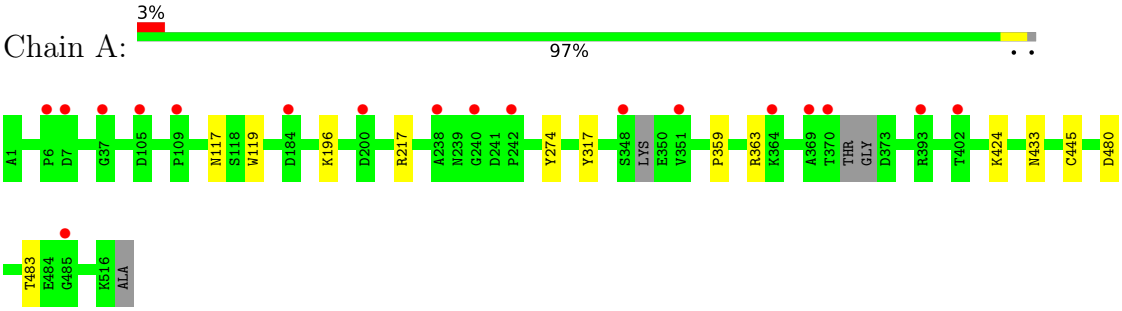
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		
3	B	110	Total	O	0	0
			110	110		
3	C	133	Total	O	0	0
			133	133		
3	D	127	Total	O	0	0
			127	127		

3 Residue-property plots

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.

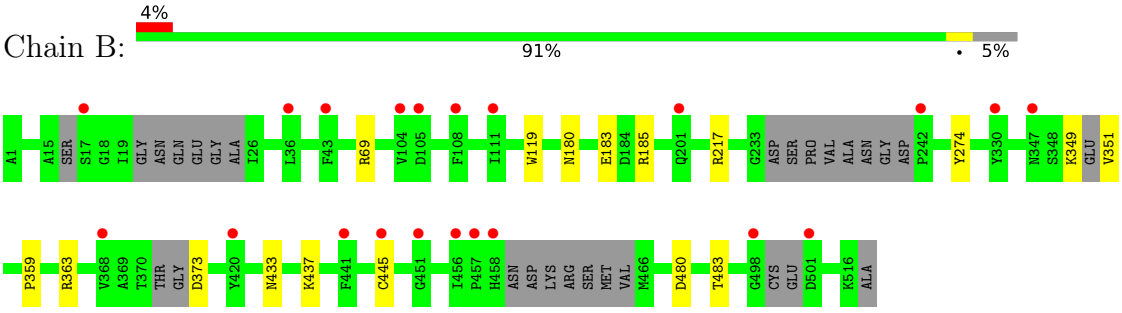
- Molecule 1: Aurone synthase

Chain A:



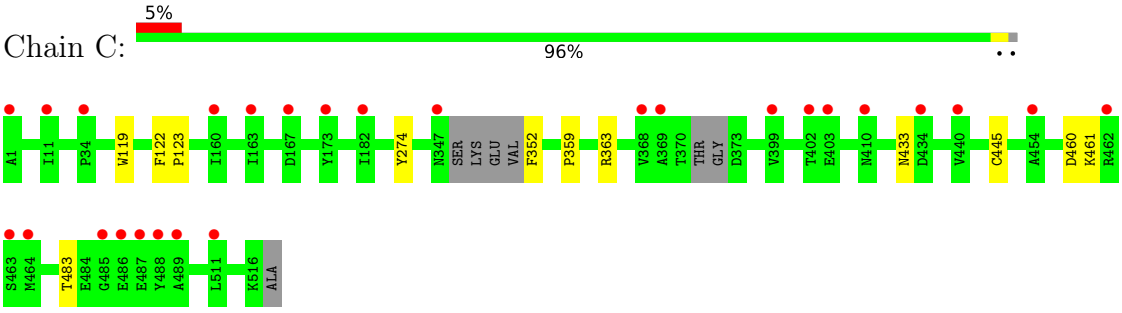
- Molecule 1: Aurone synthase

Chain B:



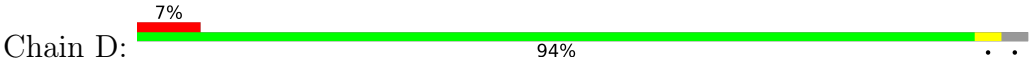
- Molecule 1: Aurone synthase

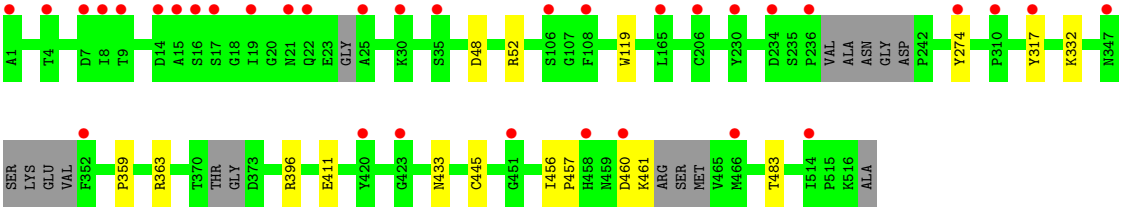
Chain C:



- Molecule 1: Aurone synthase

Chain D:




A1
T4
D7
I8
T9
D14
A15
S16
S17
G18
I19
G20
N21
Q22
E23
GLY
A25
K30
S35
D48
R52
S106
G107
F108
W119
L165
C206
Y230
D234
S235
P236
VAL
ALA
ASN
GLY
ASP
P242
Y274
P310
Y317
K332
N347
SER
LYS
GLU
VAL
F352
P359
R363
T370
THR
GLY
D373
R396
E411
Y420
G423
N433
C445
G451
I456
P457
H458
N459
D460
K461
ARG
SER
MET
V465
M466
T483
I514
P515
K516
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.57Å 174.10Å 102.54Å 90.00° 105.27° 90.00°	Depositor
Resolution (Å)	46.38 – 2.50 48.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.38-2.50) 97.8 (48.77-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.183 , 0.234 0.188 , 0.237	Depositor DCC
R_{free} test set	3569 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	47.5	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30898	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: CU

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	0.22	0/4109	0.37	0/5603
1	B	0.22	0/3941	0.37	0/5363
1	C	0.22	0/4104	0.37	0/5594
1	D	0.22	0/4014	0.37	0/5471
All	All	0.22	0/16168	0.37	0/22031

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3999	3708	3711	6	0
1	B	3838	3578	3579	10	0
1	C	3994	3726	3727	6	0
1	D	3907	3620	3621	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	150	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	110	0	0	4	0
3	C	133	0	0	1	0
3	D	127	0	0	2	0
All	All	16266	14632	14638	27	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 1.

All (27) 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:52:ARG:NH1	3:D:813:HOH:O	2.24	0.71
1:B:373:ASP:N	3:B:809:HOH:O	2.27	0.67
1:C:352:PHE:N	3:C:810:HOH:O	2.31	0.62
1:D:48:ASP:OD2	1:D:52:ARG:NH1	2.37	0.58
1:A:363:ARG:NH2	1:B:359:PRO:O	2.37	0.58
1:B:349:LYS:O	1:B:351:VAL:N	2.38	0.56
1:C:359:PRO:O	1:D:363:ARG:NH2	2.40	0.54
1:D:460:ASP:OD1	1:D:461:LYS:N	2.41	0.54
1:B:69:ARG:NH2	3:B:813:HOH:O	2.40	0.54
1:B:180:ASN:O	1:B:185:ARG:NE	2.40	0.54
1:B:433:ASN:ND2	1:B:483:THR:OG1	2.45	0.50
1:C:363:ARG:NH2	1:D:359:PRO:O	2.43	0.50
1:A:117:ASN:ND2	3:A:822:HOH:O	2.44	0.50
1:B:437:LYS:NZ	3:B:817:HOH:O	2.45	0.50
1:C:433:ASN:ND2	1:C:483:THR:OG1	2.47	0.47
1:D:433:ASN:ND2	1:D:483:THR:OG1	2.48	0.46
1:B:217:ARG:NH2	1:B:480:ASP:OD2	2.44	0.45
1:B:183:GLU:N	3:B:811:HOH:O	2.50	0.45
1:C:460:ASP:OD2	1:C:461:LYS:N	2.49	0.45
1:A:196:LYS:NZ	3:A:813:HOH:O	2.46	0.44
1:D:396:ARG:NE	1:D:411:GLU:OE2	2.47	0.43
1:A:359:PRO:O	1:B:363:ARG:NH2	2.53	0.42
1:A:433:ASN:ND2	1:A:483:THR:OG1	2.52	0.42
1:D:332:LYS:NZ	3:D:825:HOH:O	2.49	0.42
1:C:122:PHE:N	1:C:123:PRO:HD2	2.35	0.41
1:D:456:ILE:HG23	1:D:457:PRO:HD2	2.02	0.41
1:A:217:ARG:NH2	1:A:480:ASP:OD2	2.47	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	508/517 (98%)	495 (97%)	13 (3%)	0	100	100
1	B	473/517 (92%)	463 (98%)	10 (2%)	0	100	100
1	C	504/517 (98%)	492 (98%)	12 (2%)	0	100	100
1	D	489/517 (95%)	479 (98%)	10 (2%)	0	100	100
All	All	1974/2068 (96%)	1929 (98%)	45 (2%)	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	409/454 (90%)	404 (99%)	5 (1%)	71	88
1	B	393/454 (87%)	390 (99%)	3 (1%)	81	93
1	C	412/454 (91%)	409 (99%)	3 (1%)	84	94
1	D	397/454 (87%)	393 (99%)	4 (1%)	76	90
All	All	1611/1816 (89%)	1596 (99%)	15 (1%)	78	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	TRP
1	A	274	TYR

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Mol	Chain	Res	Type
1	A	317	TYR
1	A	424	LYS
1	A	445	CYS
1	B	119	TRP
1	B	274	TYR
1	B	445	CYS
1	C	119	TRP
1	C	274	TYR
1	C	445	CYS
1	D	119	TRP
1	D	274	TYR
1	D	317	TYR
1	D	445	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	347	ASN
1	B	433	ASN
1	B	455	GLN
1	C	455	GLN
1	D	433	ASN
1	D	458	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

Of 8 ligands modelled in this entry, 8 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	513/517 (99%)	0.60	18 (3%)	44	47	37, 53, 80, 104	0
1	B	489/517 (94%)	0.59	21 (4%)	35	38	31, 51, 87, 108	0
1	C	510/517 (98%)	0.66	27 (5%)	26	28	39, 53, 78, 123	0
1	D	501/517 (96%)	0.78	34 (6%)	17	17	35, 54, 87, 113	0
All	All	2013/2068 (97%)	0.66	100 (4%)	28	30	31, 53, 84, 123	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	466	MET	6.2
1	D	423	GLY	6.1
1	D	16	SER	5.6
1	D	15	ALA	4.6
1	B	458	HIS	4.4
1	B	498	GLY	4.4
1	C	182	ILE	4.3
1	B	501	ASP	4.2
1	A	351	VAL	4.1
1	D	7	ASP	3.9
1	C	368	VAL	3.8
1	D	420	TYR	3.8
1	D	17	SER	3.7
1	D	352	PHE	3.6
1	B	420	TYR	3.6
1	C	34	PRO	3.5
1	C	511	LEU	3.5
1	D	14	ASP	3.5
1	A	109	PRO	3.3
1	C	369	ALA	3.3
1	C	402	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	393	ARG	3.3
1	D	21	ASN	3.3
1	D	9	THR	3.3
1	D	25	ALA	3.3
1	C	1	ALA	3.2
1	D	310	PRO	3.2
1	D	234	ASP	3.1
1	A	369	ALA	3.1
1	B	441	PHE	3.1
1	A	238	ALA	3.0
1	C	487	GLU	3.0
1	A	105	ASP	2.9
1	B	111	ILE	2.9
1	C	486	GLU	2.9
1	C	167	ASP	2.9
1	C	489	ALA	2.9
1	D	19	ILE	2.9
1	C	462	ARG	2.9
1	D	458	HIS	2.8
1	C	399	VAL	2.8
1	D	4	THR	2.8
1	D	274	TYR	2.8
1	A	485	GLY	2.8
1	A	370	THR	2.8
1	D	35	SER	2.8
1	B	330	TYR	2.7
1	A	402	THR	2.7
1	B	108	PHE	2.7
1	B	457	PRO	2.6
1	A	6	PRO	2.6
1	D	236	PRO	2.5
1	C	463	SER	2.5
1	B	104	VAL	2.5
1	B	105	ASP	2.5
1	D	106	SER	2.5
1	B	201	GLN	2.5
1	C	347	ASN	2.5
1	B	445	CYS	2.5
1	C	454	ALA	2.5
1	D	347	ASN	2.4
1	B	17	SER	2.4
1	C	410	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	2.4
1	C	485	GLY	2.4
1	D	8	ILE	2.4
1	D	206	CYS	2.4
1	C	173	TYR	2.3
1	D	460	ASP	2.3
1	A	240	GLY	2.3
1	C	160	ILE	2.3
1	D	230	TYR	2.3
1	D	451	GLY	2.2
1	D	514	ILE	2.2
1	D	30	LYS	2.2
1	B	242	PRO	2.2
1	C	434	ASP	2.2
1	C	488	TYR	2.2
1	C	464	MET	2.2
1	A	200	ASP	2.2
1	B	451	GLY	2.1
1	A	242	PRO	2.1
1	A	37	GLY	2.1
1	C	11	ILE	2.1
1	A	184	ASP	2.1
1	B	368	VAL	2.1
1	B	347	ASN	2.1
1	A	348	SER	2.1
1	A	364	LYS	2.1
1	B	456	ILE	2.1
1	C	440	VAL	2.0
1	B	36	LEU	2.0
1	B	43	PHE	2.0
1	D	22	GLN	2.0
1	D	108	PHE	2.0
1	C	403	GLU	2.0
1	D	165	LEU	2.0
1	D	317	TYR	2.0
1	A	7	ASP	2.0
1	C	163	ILE	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	C	701	1/1	0.98	0.16	57,57,57,57	0
2	CU	D	701	1/1	0.98	0.15	49,49,49,49	0
2	CU	B	700	1/1	0.99	0.14	46,46,46,46	0
2	CU	B	701	1/1	0.99	0.17	47,47,47,47	0
2	CU	C	700	1/1	0.99	0.18	48,48,48,48	0
2	CU	A	700	1/1	0.99	0.16	46,46,46,46	0
2	CU	D	700	1/1	0.99	0.11	47,47,47,47	0
2	CU	A	701	1/1	0.99	0.15	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.