



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:15 AM BST

PDB ID : 6DXD
Title : Crystal structure of chalcone synthase from Arabidopsis thaliana - C347S mutant
Authors : Liou, G.; Chiang, Y.C.; Wang, Y.; Weng, J.K.
Deposited on : 2018-06-28
Resolution : 1.59 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

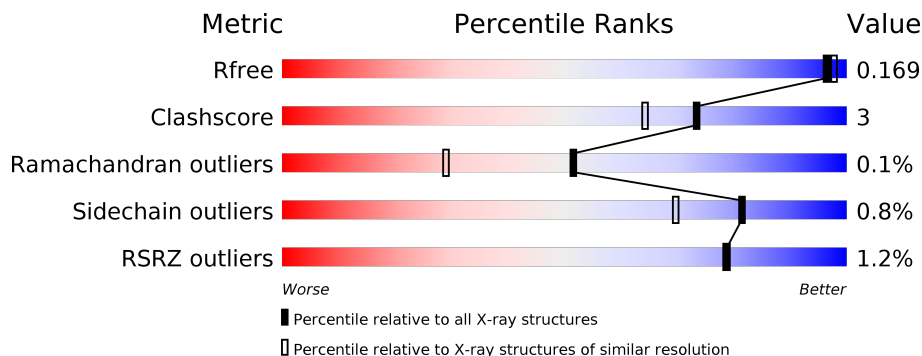
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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	395	 93% 5% ••
1	B	395	 91% 7% ••
1	C	395	 92% 7% •
1	D	395	 93% 5% •

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25972 atoms, of which 12119 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 Chalcone synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	389	6042	1902	3033	519	570	18	0	3	0
1	B	389	6024	1897	3023	518	569	17	0	2	0
1	C	389	6040	1902	3031	519	570	18	0	3	0
1	D	389	6041	1902	3032	519	570	18	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	SER	CYS	engineered mutation	UNP P13114
B	347	SER	CYS	engineered mutation	UNP P13114
C	347	SER	CYS	engineered mutation	UNP P13114
D	347	SER	CYS	engineered mutation	UNP P13114

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	463	Total	O	0	0
			463	463		
2	B	451	Total	O	0	0
			451	451		
2	C	441	Total	O	0	0
			441	441		
2	D	470	Total	O	0	0
			470	470		

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.

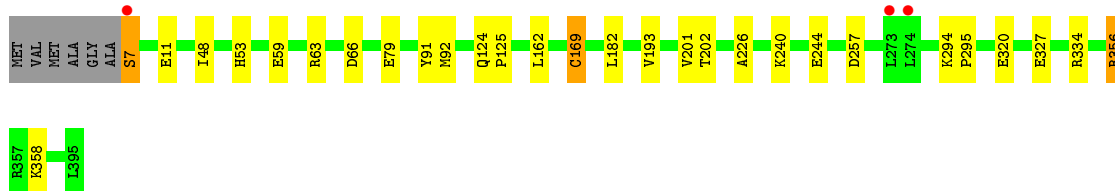
- Molecule 1: Chalcone synthase

Chain A: 




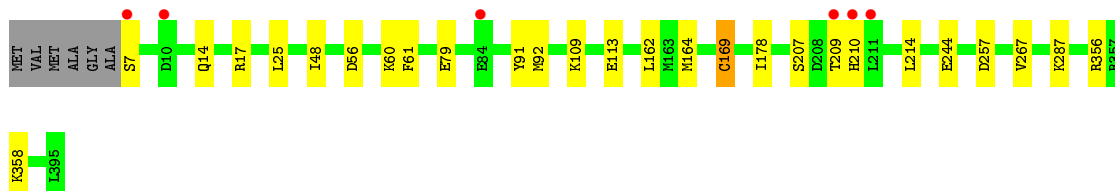
- Molecule 1: Chalcone synthase

Chain B: 

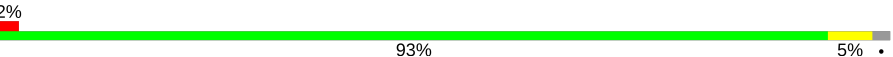


- Molecule 1: Chalcone synthase

Chain C: 



- Molecule 1: Chalcone synthase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.86Å 138.22Å 108.90Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	32.92 – 1.59 34.14 – 1.59	Depositor EDS
% Data completeness (in resolution range)	93.3 (32.92-1.59) 93.3 (34.14-1.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.59Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.145 , 0.169 0.145 , 0.169	Depositor DCC
R_{free} test set	1855 reflections (0.92%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25972	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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](#)

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

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	0.46	0/3060	0.65	1/4138 (0.0%)
1	B	0.47	0/3052	0.66	1/4128 (0.0%)
1	C	0.47	0/3060	0.66	0/4138
1	D	0.44	0/3060	0.65	1/4138 (0.0%)
All	All	0.46	0/12232	0.66	3/16542 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	MET	CG-SD-CE	-6.04	90.53	100.20
1	B	356	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	181	ASP	CB-CG-OD1	5.39	123.15	118.30

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	3009	3033	3029	20	0
1	B	3001	3023	3021	22	0
1	C	3009	3031	3029	25	0
1	D	3009	3032	3029	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	463	0	0	12	0
2	B	451	0	0	12	0
2	C	441	0	0	15	0
2	D	470	0	0	7	1
All	All	13853	12119	12108	80	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (80) 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:50:ASN:ND2	2:A:401:HOH:O	1.91	1.03
1:A:361:LYS:NZ	2:A:402:HOH:O	2.01	0.93
1:C:14:GLN:OE1	2:C:401:HOH:O	1.87	0.92
1:B:66:ASP:OD1	2:B:401:HOH:O	1.90	0.88
1:D:274:LEU:O	2:D:401:HOH:O	1.94	0.85
1:D:7:SER:N	2:D:403:HOH:O	2.10	0.84
1:C:17:ARG:NH1	2:C:401:HOH:O	2.09	0.84
1:B:244:GLU:OE1	2:B:402:HOH:O	1.97	0.81
1:C:91:TYR:OH	1:C:210:HIS:CG	2.34	0.81
1:A:372:GLU:HG3	2:A:695:HOH:O	1.81	0.80
1:A:66:ASP:OD1	2:A:403:HOH:O	2.05	0.74
1:B:169:CSD:OD2	2:B:403:HOH:O	2.05	0.73
1:D:255:ASP:OD2	2:D:402:HOH:O	2.04	0.73
1:B:53:HIS:ND1	2:B:406:HOH:O	2.22	0.71
1:B:7:SER:N	2:B:405:HOH:O	2.22	0.71
1:C:244:GLU:OE1	2:C:402:HOH:O	2.09	0.70
1:C:113:GLU:OE2	2:C:403:HOH:O	2.10	0.69
1:C:257:ASP:OD1	2:C:405:HOH:O	2.13	0.66
1:C:56:ASP:OD2	2:C:404:HOH:O	2.13	0.66
1:B:63:ARG:NH1	2:B:408:HOH:O	2.29	0.65
1:C:17:ARG:HD3	2:C:401:HOH:O	1.97	0.64
1:A:169:CSD:OD2	2:A:404:HOH:O	2.13	0.64
1:D:79:GLU:OE2	1:D:83:LYS:NZ	2.31	0.64
1:D:120:LYS:NZ	2:D:404:HOH:O	2.12	0.61
1:B:7:SER:CA	2:B:405:HOH:O	2.48	0.61
1:B:7:SER:HA	2:B:405:HOH:O	2.01	0.61
1:A:164[B]:MET:SD	1:A:178:ILE:CD1	2.91	0.58
1:D:59:GLU:HG2	2:D:782:HOH:O	2.04	0.57
1:A:240:LYS:HD3	2:A:777:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164[B]:MET:SD	1:C:178:ILE:CD1	2.95	0.55
1:D:164[B]:MET:SD	1:D:178:ILE:CD1	2.95	0.55
1:C:48:ILE:HD13	1:C:79:GLU:HG3	1.90	0.54
1:A:48:ILE:HD13	1:A:79:GLU:HG3	1.90	0.53
1:B:7:SER:N	1:B:11:GLU:OE1	2.42	0.52
1:C:25:LEU:HD21	2:C:514:HOH:O	2.10	0.51
1:C:60:LYS:NZ	2:C:414:HOH:O	2.44	0.51
1:C:164[B]:MET:SD	1:C:178:ILE:HD12	2.52	0.49
1:C:91:TYR:OH	1:C:210:HIS:ND1	2.45	0.49
1:A:137:THR:HG22	1:A:137:THR:O	2.12	0.49
1:A:59:GLU:HG2	2:A:840:HOH:O	2.11	0.49
1:A:112:LYS:NZ	2:A:413:HOH:O	2.46	0.48
1:C:92:MET:SD	1:C:267:VAL:HG21	2.54	0.47
1:A:372:GLU:CG	2:A:695:HOH:O	2.53	0.47
1:B:201:VAL:HG23	1:B:202:THR:HG23	1.95	0.47
1:A:160:LYS:NZ	2:A:408:HOH:O	2.36	0.46
1:A:164[B]:MET:SD	1:A:178:ILE:HD12	2.55	0.46
1:B:320:GLU:OE1	1:B:334:ARG:NH1	2.47	0.46
1:D:91:TYR:CD2	1:D:92:MET:HG2	2.50	0.46
1:C:17:ARG:CD	2:C:401:HOH:O	2.60	0.46
1:C:358:LYS:NZ	2:C:422:HOH:O	2.49	0.46
1:D:120:LYS:CE	2:D:404:HOH:O	2.58	0.45
1:B:162:LEU:HG	2:B:523:HOH:O	2.16	0.45
1:B:327:GLU:H	1:B:327:GLU:CD	2.18	0.45
1:A:59:GLU:HG2	2:A:773:HOH:O	2.16	0.45
1:B:48:ILE:HD13	1:B:79:GLU:HG3	1.99	0.44
1:A:326:LYS:HE3	2:A:757:HOH:O	2.16	0.44
1:A:91:TYR:CE2	1:A:92:MET:HG3	2.53	0.44
1:B:257:ASP:OD2	2:B:404:HOH:O	2.21	0.44
1:D:240:LYS:HD3	2:D:743:HOH:O	2.17	0.43
1:A:61:PHE:CD1	1:A:214:LEU:HG	2.54	0.43
1:C:91:TYR:CD2	1:C:92:MET:HG2	2.55	0.42
1:C:109:LYS:HG2	2:C:403:HOH:O	2.20	0.42
1:A:91:TYR:CD2	1:A:92:MET:HG2	2.54	0.42
1:B:193:VAL:O	1:B:226:ALA:HA	2.19	0.42
1:D:193:VAL:O	1:D:226:ALA:HA	2.20	0.42
1:D:137:THR:O	1:D:137:THR:HG22	2.20	0.42
1:C:287:LYS:HG3	2:C:611:HOH:O	2.21	0.41
1:C:169:CSD:OD2	2:C:406:HOH:O	2.21	0.41
1:C:61:PHE:CD1	1:C:214:LEU:HG	2.55	0.41
1:C:17:ARG:CZ	2:C:401:HOH:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:N	1:B:295:PRO:CD	2.84	0.41
1:D:212:ASP:OD1	1:D:212:ASP:N	2.54	0.41
1:D:77:LEU:HD11	1:D:200:ALA:HA	2.03	0.41
1:B:59:GLU:HG2	2:B:790:HOH:O	2.21	0.40
1:B:91:TYR:CD2	1:B:92:MET:HG2	2.56	0.40
1:A:178:ILE:HD11	1:C:162:LEU:HD22	2.03	0.40
1:C:207:SER:OG	1:C:209:THR:OG1	2.38	0.40
1:B:182:LEU:HD23	1:D:181:ASP:OD2	2.22	0.40
1:B:63:ARG:NH1	2:B:407:HOH:O	2.22	0.40
1:B:124:GLN:HB3	1:B:125:PRO:HD2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:593:HOH:O	2:D:611:HOH:O[1_455]	2.17	0.03

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	389/395 (98%)	381 (98%)	8 (2%)	0	100	100
1	B	388/395 (98%)	380 (98%)	8 (2%)	0	100	100
1	C	389/395 (98%)	381 (98%)	8 (2%)	0	100	100
1	D	389/395 (98%)	381 (98%)	7 (2%)	1 (0%)	41	21
All	All	1555/1580 (98%)	1523 (98%)	31 (2%)	1 (0%)	51	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	95	SER

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	327/327 (100%)	323 (99%)	4 (1%)	71	54
1	B	326/327 (100%)	322 (99%)	4 (1%)	71	54
1	C	327/327 (100%)	325 (99%)	2 (1%)	86	77
1	D	327/327 (100%)	326 (100%)	1 (0%)	92	87
All	All	1307/1308 (100%)	1296 (99%)	11 (1%)	81	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	240	LYS
1	A	257	ASP
1	A	356	ARG
1	B	7	SER
1	B	240	LYS
1	B	356	ARG
1	B	358	LYS
1	C	7	SER
1	C	356	ARG
1	D	356	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	CSD	A	169	1	3,7,8	0.91	0	1,8,10	2.07	1 (100%)
1	CSD	B	169	1	3,7,8	1.08	0	1,8,10	2.68	1 (100%)
1	CSD	C	169	1	3,7,8	1.30	1 (33%)	1,8,10	1.38	0
1	CSD	D	169	1	3,7,8	1.02	0	1,8,10	1.31	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
1	CSD	A	169	1	-	1/2/6/8	-
1	CSD	B	169	1	-	1/2/6/8	-
1	CSD	C	169	1	-	1/2/6/8	-
1	CSD	D	169	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	CSD	CA-N	-2.12	1.41	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	CSD	OD1-SG-CB	-2.68	100.43	105.54
1	A	169	CSD	OD1-SG-CB	-2.07	101.59	105.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	169	CSD	CA-CB-SG-OD1
1	B	169	CSD	CA-CB-SG-OD1
1	C	169	CSD	CA-CB-SG-OD1
1	D	169	CSD	CA-CB-SG-OD1
1	D	169	CSD	N-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	169	CSD	1	0
1	B	169	CSD	1	0
1	C	169	CSD	1	0

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	388/395 (98%)	-0.32	1 (0%) 94 93	9, 14, 40, 67	0
1	B	388/395 (98%)	-0.32	3 (0%) 86 86	8, 16, 39, 60	0
1	C	388/395 (98%)	-0.26	6 (1%) 73 73	9, 16, 42, 74	0
1	D	388/395 (98%)	-0.24	8 (2%) 63 62	9, 15, 43, 62	0
All	All	1552/1580 (98%)	-0.29	18 (1%) 79 78	8, 15, 42, 74	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	210	HIS	4.6
1	A	7	SER	4.3
1	D	55	THR	4.0
1	B	7	SER	3.4
1	C	211	LEU	3.2
1	B	274	LEU	3.0
1	C	7	SER	2.8
1	D	56	ASP	2.7
1	C	10	ASP	2.3
1	D	53	HIS	2.2
1	D	210	HIS	2.2
1	B	273	LEU	2.2
1	D	57	LEU	2.2
1	D	54	MET	2.2
1	C	84	GLU	2.2
1	D	59	GLU	2.2
1	D	7	SER	2.1
1	C	209	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	CSD	A	169	8/9	0.96	0.09	12,17,32,39	0
1	CSD	B	169	8/9	0.96	0.09	14,18,30,36	0
1	CSD	D	169	8/9	0.97	0.08	11,15,33,40	0
1	CSD	C	169	8/9	0.98	0.08	13,16,26,31	0

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.