Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 06:03 AM EDT

PDB ID	:	1I89
Title	:	Chalcone synthase (G256L)
Authors	:	Jez, J.M.; Bowman, M.E.; Noel, J.P.
Deposited on	:	2001-03-12
Resolution	:	1.86 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 following versions of software and data (see references (i)) were used in the production of this report:

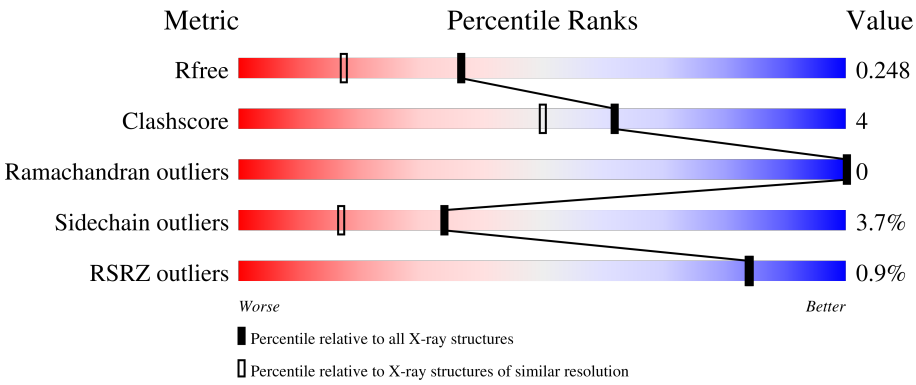
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

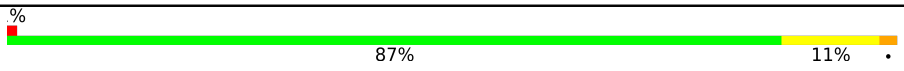
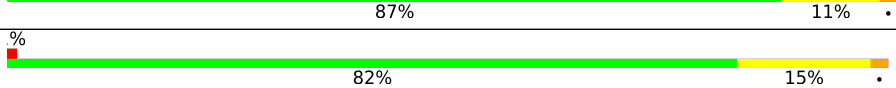
The reported resolution of this entry is 1.86 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	389	
1	B	389	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6433 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 CHALCONE SYNTHASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	2993	1904	504	566	19	0	0	0
1	B	388	2993	1904	504	566	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	LEU	GLY	engineered mutation	UNP P30074
B	256	LEU	GLY	engineered mutation	UNP P30074

- Molecule 2 is water.

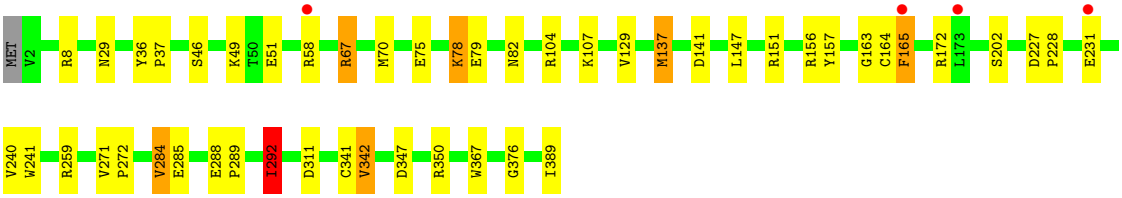
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	225	225	225	0	0
2	B	222	222	222	0	0

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.

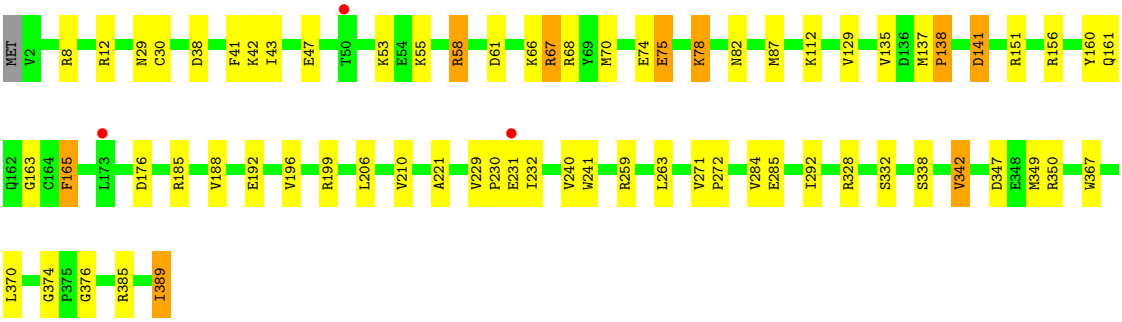
• Molecule 1: CHALCONE SYNTHASE 2

Chain A:



• Molecule 1: CHALCONE SYNTHASE 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	98.10Å 98.10Å 131.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.20 – 1.86 31.19 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.3 (31.20-1.86) 97.7 (31.19-1.86)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 1.87Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.259 0.200 , 0.248	Depositor DCC
R_{free} test set	3050 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6433	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 94.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1326e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 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	0.74	2/3042 (0.1%)	1.38	27/4118 (0.7%)
1	B	0.68	0/3042	1.40	30/4118 (0.7%)
All	All	0.71	2/6084 (0.0%)	1.39	57/8236 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	PHE	N-CA	-12.18	1.22	1.46
1	A	164	CSD	C-N	-10.21	1.10	1.34

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	259	ARG	NE-CZ-NH2	12.88	126.74	120.30
1	B	8	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	164	CSD	O-C-N	10.10	138.87	122.70
1	B	58	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	B	376	GLY	O-C-N	-9.84	106.95	122.70
1	B	376	GLY	CA-C-N	9.45	137.99	117.20
1	A	67	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	A	342	VAL	CG1-CB-CG2	9.32	125.81	110.90
1	A	376	GLY	O-C-N	-8.80	108.62	122.70
1	B	259	ARG	NH1-CZ-NH2	-8.57	109.97	119.40
1	B	347	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	A	376	GLY	CA-C-N	8.40	135.69	117.20
1	A	347	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	141	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	151	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	8	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	B	58	ARG	NE-CZ-NH2	-8.04	116.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	156	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	165	PHE	CB-CA-C	-7.49	95.42	110.40
1	A	104	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	164	CSD	C-N-CA	-7.48	103.00	121.70
1	B	185	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	A	342	VAL	N-CA-CB	-6.93	96.25	111.50
1	B	347	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	259	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	151	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	165	PHE	N-CA-CB	6.69	122.64	110.60
1	A	347	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	61	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	A	67	ARG	CD-NE-CZ	6.47	132.66	123.60
1	B	328	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	A	8	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	67	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	176	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	68	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	A	58	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	156	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	259	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	164	CSD	CA-C-N	-5.84	104.34	117.20
1	B	138	PRO	N-CA-CB	5.81	110.27	103.30
1	B	67	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	311	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	12	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	292	ILE	CA-CB-CG2	5.56	122.02	110.90
1	A	137	MET	CA-C-O	-5.54	108.47	120.10
1	A	157	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	B	385	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	104	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	B	385	ARG	CD-NE-CZ	5.47	131.26	123.60
1	B	199	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	87	MET	CA-CB-CG	5.26	122.25	113.30
1	B	349	MET	CG-SD-CE	5.17	108.46	100.20
1	B	385	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	231	GLU	CA-CB-CG	5.09	124.59	113.40
1	B	8	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	172	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	376	GLY	N-CA-C	-5.01	100.57	113.10

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	2993	0	3038	19	1
1	B	2993	0	3039	34	0
2	A	225	0	0	3	0
2	B	222	0	0	6	1
All	All	6433	0	6077	53	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 4.

All (53) 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:B:165:PHE:C	1:B:165:PHE:CD1	2.62	0.71
1:B:75:GLU:O	1:B:78:LYS:HD3	1.92	0.70
1:A:75:GLU:O	1:A:78:LYS:HG3	1.94	0.68
1:B:342:VAL:HG13	1:B:370:LEU:HD11	1.77	0.66
1:B:30:CYS:SG	2:B:590:HOH:O	2.53	0.66
1:A:241:TRP:CH2	1:A:285:GLU:HG2	2.37	0.59
1:B:241:TRP:HH2	1:B:285:GLU:HG2	1.66	0.59
1:B:165:PHE:C	1:B:165:PHE:HD1	2.06	0.59
1:B:241:TRP:CH2	1:B:285:GLU:HG2	2.39	0.57
1:B:229:VAL:HG12	1:B:232:ILE:HD13	1.88	0.56
1:A:271:VAL:HB	1:A:272:PRO:HD3	1.88	0.54
1:B:163:GLY:CA	2:B:602:HOH:O	2.55	0.54
1:A:49:LYS:HG2	2:A:566:HOH:O	2.07	0.54
1:A:163:GLY:CA	2:A:609:HOH:O	2.56	0.53
1:B:66:LYS:HG3	1:B:332:SER:OG	2.10	0.51
1:B:129:VAL:HG21	1:B:141:ASP:HA	1.92	0.51
1:B:43:ILE:HD13	1:B:74:GLU:HG3	1.93	0.50
1:A:165:PHE:CD1	1:A:165:PHE:C	2.84	0.50
1:B:271:VAL:HB	1:B:272:PRO:HD3	1.94	0.50
1:A:75:GLU:O	1:A:79:GLU:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:O	1:B:221:ALA:HA	2.12	0.48
1:A:107:LYS:HD2	1:A:147:LEU:HB3	1.96	0.47
1:B:389:ILE:HD13	2:B:523:HOH:O	2.15	0.46
1:B:165:PHE:HD1	1:B:165:PHE:O	1.98	0.46
1:A:129:VAL:HG21	1:A:141:ASP:HA	1.97	0.46
1:B:42:LYS:HG3	1:B:47:GLU:HG2	1.98	0.46
1:A:163:GLY:HA3	2:A:609:HOH:O	2.15	0.46
1:B:137:MET:HA	1:B:138:PRO:C	2.37	0.45
1:B:342:VAL:HB	2:B:392:HOH:O	2.17	0.44
1:A:29:ASN:HB3	1:A:70:MET:O	2.16	0.44
1:B:240:VAL:HG21	1:B:367:TRP:HZ3	1.83	0.44
1:A:36:TYR:N	1:A:37:PRO:CD	2.82	0.43
1:B:389:ILE:HD12	1:B:389:ILE:HA	1.66	0.43
1:B:196:VAL:HB	2:B:462:HOH:O	2.18	0.43
1:B:230:PRO:O	1:B:232:ILE:HD12	2.18	0.43
1:A:240:VAL:HG21	1:A:367:TRP:CZ3	2.54	0.43
1:A:227:ASP:N	1:A:228:PRO:HD3	2.34	0.42
1:A:284:VAL:HB	1:A:288:GLU:OE1	2.20	0.42
1:B:42:LYS:HG3	1:B:47:GLU:CG	2.49	0.42
1:B:161:GLN:HE22	1:B:263:LEU:HD13	1.85	0.42
1:B:192:GLU:HG3	1:B:338:SER:HB3	2.02	0.42
1:B:29:ASN:HB3	1:B:70:MET:O	2.20	0.42
1:B:161:GLN:NE2	1:B:263:LEU:HD13	2.35	0.42
1:B:38:ASP:OD1	1:B:53:LYS:NZ	2.44	0.41
1:A:288:GLU:N	1:A:289:PRO:CD	2.84	0.41
1:B:112:LYS:NZ	2:B:518:HOH:O	2.52	0.41
1:B:135:VAL:HA	1:B:160:TYR:CE1	2.56	0.41
1:B:165:PHE:HB3	1:B:374:GLY:HA3	2.03	0.40
1:B:41:PHE:CD2	1:B:53:LYS:HB2	2.57	0.40
1:A:240:VAL:HG21	1:A:367:TRP:HZ3	1.85	0.40
1:B:206:LEU:O	1:B:210:VAL:HG23	2.21	0.40
1:A:46:SER:HB3	1:A:49:LYS:HD2	2.04	0.40
1:A:292:ILE:O	1:A:292:ILE:HG13	2.19	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)
1:A:137:MET:CE	2:B:602:HOH:O[3_554]	0.62	1.58

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	385/389 (99%)	376 (98%)	9 (2%)	0	100	100
1	B	385/389 (99%)	375 (97%)	10 (3%)	0	100	100
All	All	770/778 (99%)	751 (98%)	19 (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	324/325 (100%)	312 (96%)	12 (4%)	34	17
1	B	324/325 (100%)	312 (96%)	12 (4%)	34	17
All	All	648/650 (100%)	624 (96%)	24 (4%)	34	17

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	67	ARG
1	A	78	LYS
1	A	82	ASN
1	A	202	SER
1	A	231	GLU
1	A	284	VAL
1	A	292	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	341	CYS
1	A	342	VAL
1	A	350	ARG
1	A	389	ILE
1	B	55	LYS
1	B	58	ARG
1	B	67	ARG
1	B	75	GLU
1	B	78	LYS
1	B	82	ASN
1	B	165	PHE
1	B	284	VAL
1	B	292	ILE
1	B	342	VAL
1	B	350	ARG
1	B	389	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	312	GLN
1	A	356	ASN
1	B	82	ASN
1	B	312	GLN
1	B	356	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	164	1	3,7,8	0.80	0	1,8,10	1.51	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	164	1	-	0/2/6/8	-

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.

5.5 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	164:CSD	C	165:PHE	N	1.10

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	387/389 (99%)	-0.22	4 (1%)	82	82	12, 20, 33, 49	0
1	B	387/389 (99%)	-0.21	3 (0%)	86	86	11, 20, 36, 68	0
All	All	774/778 (99%)	-0.21	7 (0%)	84	84	11, 20, 35, 68	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	GLU	3.5
1	A	231	GLU	3.3
1	A	173	LEU	3.2
1	B	50	THR	2.7
1	B	173	LEU	2.6
1	A	165	PHE	2.2
1	A	58	ARG	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(Å^2)	Q<0.9
1	CSD	A	164	8/9	0.77	0.19	16,22,26,28	0
1	CSD	B	164	8/9	0.78	0.19	16,25,31,32	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.