



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:40 PM UTC

PDB ID : 3A6F / pdb_00003a6f
Title : W174F mutant creatininase, Type II
Authors : Nakajima, Y.; Yamashita, K.; Ito, K.; Yoshimoto, T.
Deposited on : 2009-08-31
Resolution : 1.78 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

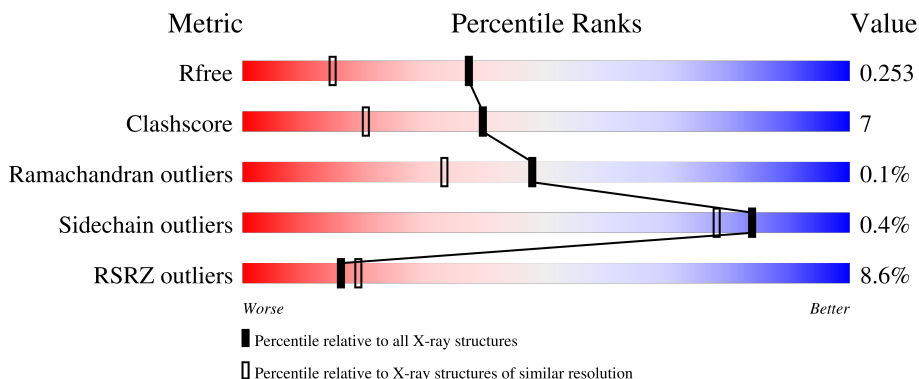
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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.



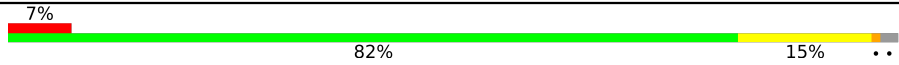
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	260	 11% 80% 18% ..
1	B	260	 9% 82% 16% ..
1	C	260	 9% 82% 16% ..
1	D	260	 8% 82% 16% .
1	E	260	 7% 85% 13% ..

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Mol	Chain	Length	Quality of chain
1	F	260	 <p>7% 82% 15% ..</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12656 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 Creatinine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	1984	1271	337	365	11	0	0	0
1	B	257	1981	1269	336	365	11	0	0	0
1	C	257	1977	1267	335	364	11	0	0	0
1	D	257	1977	1266	335	365	11	0	0	0
1	E	257	1970	1263	334	362	11	0	0	0
1	F	256	1961	1257	332	361	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	PHE	TRP	engineered mutation	UNP P83772
B	174	PHE	TRP	engineered mutation	UNP P83772
C	174	PHE	TRP	engineered mutation	UNP P83772
D	174	PHE	TRP	engineered mutation	UNP P83772
E	174	PHE	TRP	engineered mutation	UNP P83772
F	174	PHE	TRP	engineered mutation	UNP P83772

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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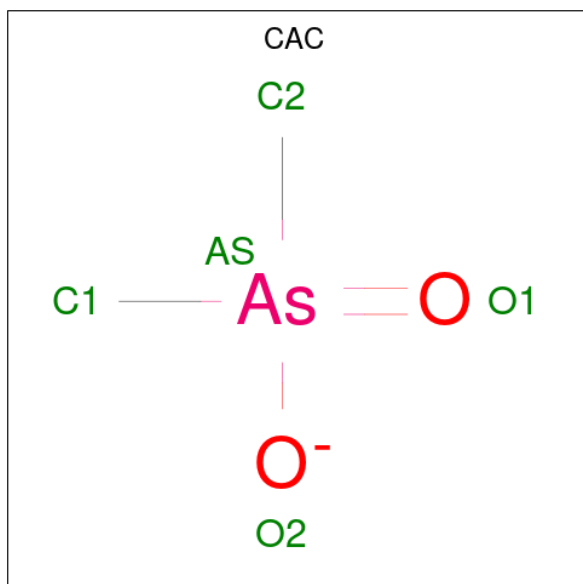
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	C	1	Total	As	C	O	0	0
			5	1	2	2		
4	D	1	Total	As	C	O	0	0
			5	1	2	2		
4	E	1	Total	As	C	O	0	0
			5	1	2	2		
4	F	1	Total	As	C	O	0	0
			5	1	2	2		

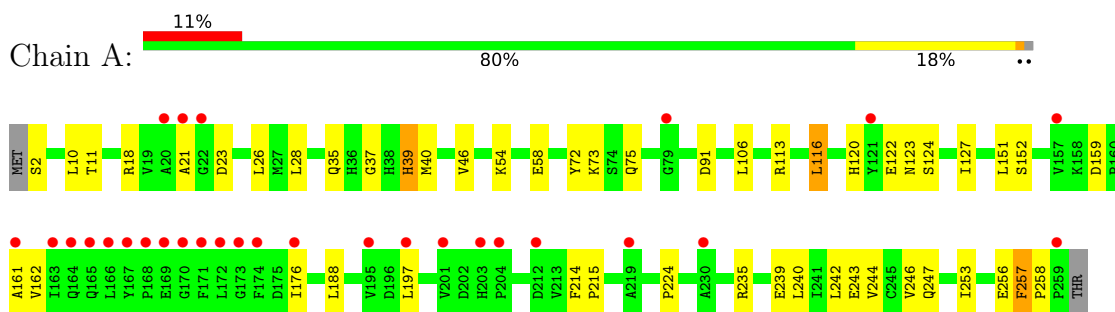
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	124	Total	O	0	0
			124	124		
5	C	126	Total	O	0	0
			126	126		
5	D	128	Total	O	0	0
			128	128		
5	E	125	Total	O	0	0
			125	125		
5	F	150	Total	O	0	0
			150	150		

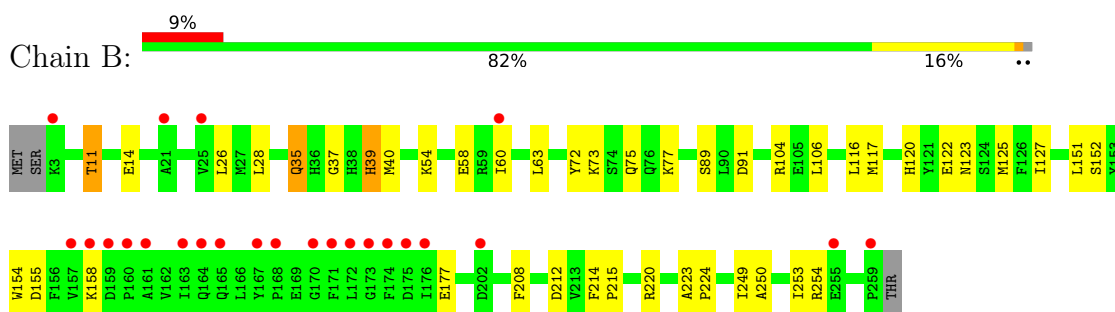
3 Residue-property plots [i](#)

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.

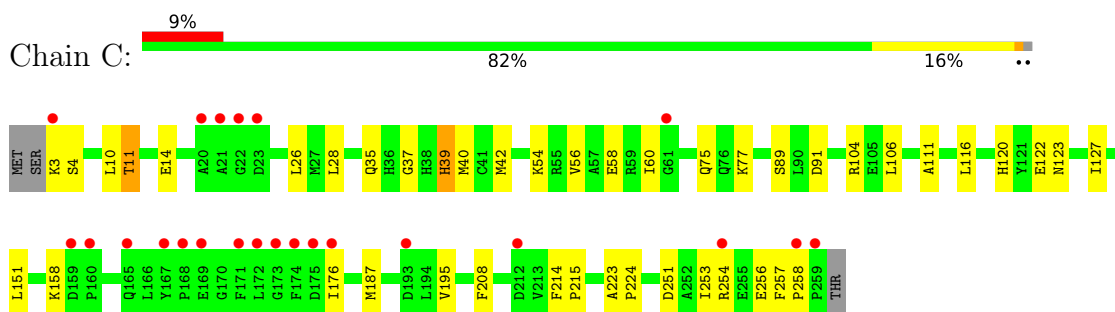
- Molecule 1: Creatinine amidohydrolase



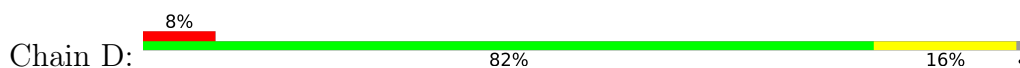
- Molecule 1: Creatinine amidohydrolase

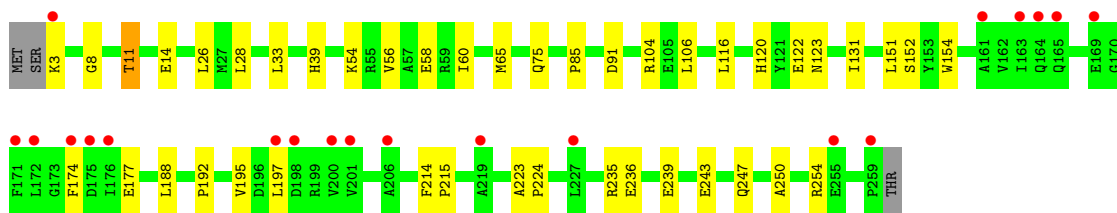


- Molecule 1: Creatinine amidohydrolase

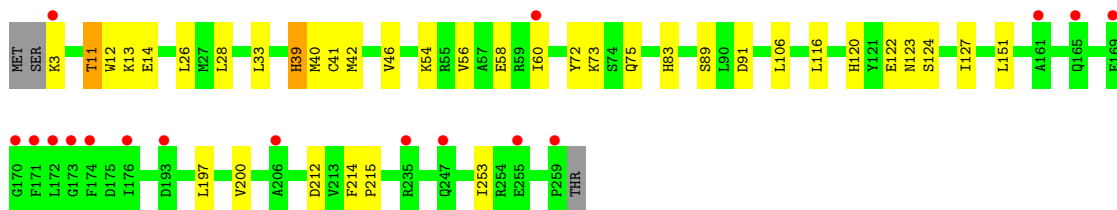
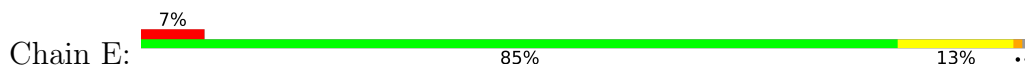


- Molecule 1: Creatinine amidohydrolase

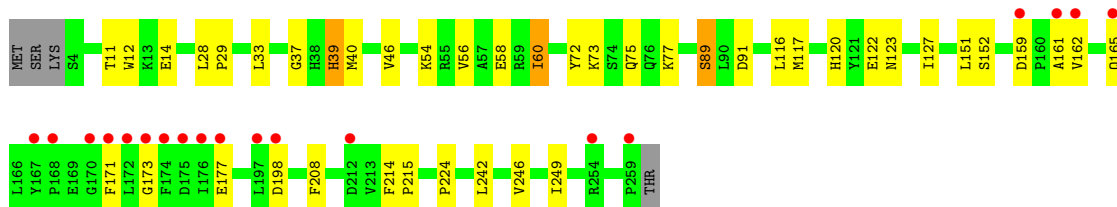
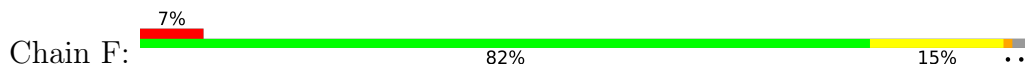




● Molecule 1: Creatinine amidohydrolase



● Molecule 1: Creatinine amidohydrolase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.30Å 164.30Å 163.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.78 20.00 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.78) 99.7 (20.00-1.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.78Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.257 0.233 , 0.253	Depositor DCC
R_{free} test set	12157 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12656	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: MN, CAC, ZN

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	0.39	0/2032	0.90	9/2764 (0.3%)
1	B	0.39	0/2029	0.88	6/2760 (0.2%)
1	C	0.39	0/2025	0.89	5/2755 (0.2%)
1	D	0.39	0/2025	0.89	4/2756 (0.1%)
1	E	0.41	0/2018	0.90	7/2747 (0.3%)
1	F	0.40	0/2009	0.91	9/2736 (0.3%)
All	All	0.39	0/12138	0.89	40/16518 (0.2%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	11	THR	N-CA-C	-7.90	100.33	110.53
1	E	11	THR	N-CA-C	-6.08	101.53	110.52
1	B	11	THR	N-CA-C	-6.03	102.41	110.55
1	C	91	ASP	N-CA-C	-5.98	102.64	110.53
1	B	39	HIS	N-CA-C	5.97	120.72	113.38

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	1984	0	1967	29	0
1	B	1981	0	1964	28	0
1	C	1977	0	1958	28	0
1	D	1977	0	1953	31	0
1	E	1970	0	1945	23	0
1	F	1961	0	1932	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
5	A	111	0	0	1	0
5	B	124	0	0	3	0
5	C	126	0	0	3	0
5	D	128	0	0	4	0
5	E	125	0	0	2	0
5	F	150	0	0	1	0
All	All	12656	0	11719	159	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 7.

The worst 5 of 159 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:E:120:HIS:HB3	1:E:123:ASN:ND2	1.94	0.81
1:A:120:HIS:HB3	1:A:123:ASN:ND2	2.00	0.76
1:C:28:LEU:HD23	1:C:116:LEU:HD21	1.69	0.75
1:A:54:LYS:O	1:A:58:GLU:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:LEU:O	1:D:192:PRO:HG3	1.91	0.70

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	256/260 (98%)	247 (96%)	9 (4%)	0	100	100
1	B	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
1	C	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
1	D	255/260 (98%)	248 (97%)	7 (3%)	0	100	100
1	E	255/260 (98%)	248 (97%)	6 (2%)	1 (0%)	30	16
1	F	254/260 (98%)	248 (98%)	6 (2%)	0	100	100
All	All	1530/1560 (98%)	1488 (97%)	41 (3%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	124	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	211/215 (98%)	210 (100%)	1 (0%)	81	73
1	B	211/215 (98%)	209 (99%)	2 (1%)	70	59
1	C	210/215 (98%)	209 (100%)	1 (0%)	81	73
1	D	210/215 (98%)	210 (100%)	0	100	100
1	E	208/215 (97%)	207 (100%)	1 (0%)	81	73
1	F	207/215 (96%)	207 (100%)	0	100	100
All	All	1257/1290 (97%)	1252 (100%)	5 (0%)	84	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	B	35	GLN
1	B	212	ASP
1	C	158	LYS
1	E	212	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	247	GLN
1	F	120	HIS
1	C	76	GLN
1	F	247	GLN
1	E	76	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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
4	CAC	D	303	2,3	2,4,4	2.55	2 (100%)	4,6,6	0.34	0
4	CAC	C	303	2,3	2,4,4	2.60	2 (100%)	4,6,6	0.36	0
4	CAC	F	303	2,3	2,4,4	2.56	2 (100%)	4,6,6	0.41	0
4	CAC	A	303	2,3	2,4,4	2.71	2 (100%)	4,6,6	0.53	0
4	CAC	B	303	2,3	2,4,4	2.54	2 (100%)	4,6,6	0.26	0
4	CAC	E	303	2,3	2,4,4	2.66	2 (100%)	4,6,6	0.31	0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	CAC	AS-C2	2.88	1.97	1.90
4	F	303	CAC	AS-C2	2.73	1.96	1.90
4	E	303	CAC	AS-C2	2.71	1.96	1.90
4	C	303	CAC	AS-C2	2.69	1.96	1.90
4	D	303	CAC	AS-C2	2.63	1.96	1.90

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	CAC	1	0
4	A	303	CAC	1	0
4	B	303	CAC	1	0
4	E	303	CAC	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	258/260 (99%)	0.69	29 (11%) 10 11	12, 24, 47, 59	0
1	B	257/260 (98%)	0.61	24 (9%) 14 16	14, 22, 43, 56	0
1	C	257/260 (98%)	0.61	23 (8%) 15 17	13, 23, 44, 54	0
1	D	257/260 (98%)	0.56	20 (7%) 19 22	12, 23, 43, 53	0
1	E	257/260 (98%)	0.52	17 (6%) 24 29	11, 21, 41, 56	0
1	F	256/260 (98%)	0.44	19 (7%) 20 24	12, 20, 41, 58	0
All	All	1542/1560 (98%)	0.57	132 (8%) 16 19	11, 22, 44, 59	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	172	LEU	6.7
1	A	172	LEU	6.4
1	F	171	PHE	5.9
1	D	176	ILE	5.7
1	D	174	PHE	5.0

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 oligosaccharides 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
4	CAC	A	303	5/5	0.94	0.20	38,38,40,40	0
2	MN	F	300	1/1	0.95	0.16	36,36,36,36	0
2	MN	B	300	1/1	0.96	0.13	39,39,39,39	0
2	MN	D	300	1/1	0.96	0.15	40,40,40,40	0
4	CAC	C	303	5/5	0.96	0.16	35,37,38,39	0
4	CAC	D	303	5/5	0.96	0.14	32,33,35,36	0
4	CAC	E	303	5/5	0.96	0.15	34,34,36,37	0
4	CAC	B	303	5/5	0.97	0.16	30,30,35,35	0
4	CAC	F	303	5/5	0.98	0.13	26,30,32,34	0
3	ZN	E	301	1/1	0.99	0.04	25,25,25,25	0
2	MN	A	300	1/1	0.99	0.09	34,34,34,34	0
2	MN	E	300	1/1	0.99	0.11	33,33,33,33	0
2	MN	C	300	1/1	0.99	0.10	31,31,31,31	0
3	ZN	A	301	1/1	0.99	0.03	27,27,27,27	0
3	ZN	B	301	1/1	0.99	0.02	26,26,26,26	0
3	ZN	D	301	1/1	0.99	0.02	26,26,26,26	0
3	ZN	C	301	1/1	1.00	0.01	25,25,25,25	0
3	ZN	F	301	1/1	1.00	0.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.