



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 06:09 AM EST

PDB ID : 1V7Z
Title : creatininase-product complex
Authors : Yoshimoto, T.; Tanaka, N.; Kanada, N.; Inoue, T.; Nakajima, Y.; Haratake, M.; Nakamura, K.T.; Xu, Y.; Ito, K.
Deposited on : 2003-12-26
Resolution : 1.60 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

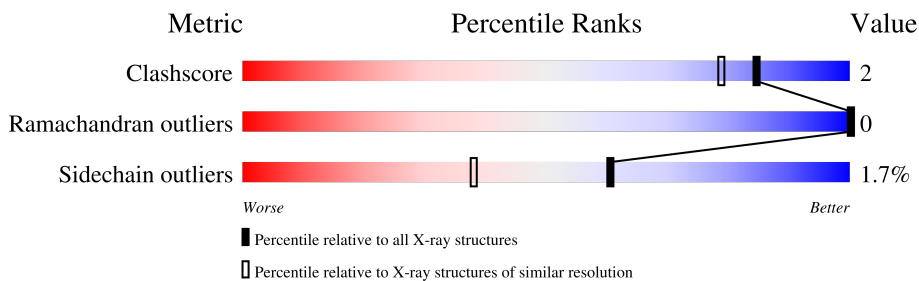
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (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 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	92% 7% .
1	B	260	92% 6% ..
1	C	260	91% 7% .
1	D	260	91% 7% ..
1	E	260	90% 8% ..
1	F	260	93% 5% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13919 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	257	1988	1273	337	367	11	0	0	0
1	B	257	1988	1273	337	367	11	0	0	0
1	C	257	1988	1273	337	367	11	0	0	0
1	D	257	1988	1273	337	367	11	0	0	0
1	E	257	1988	1273	337	367	11	0	0	0
1	F	257	1988	1273	337	367	11	0	0	0

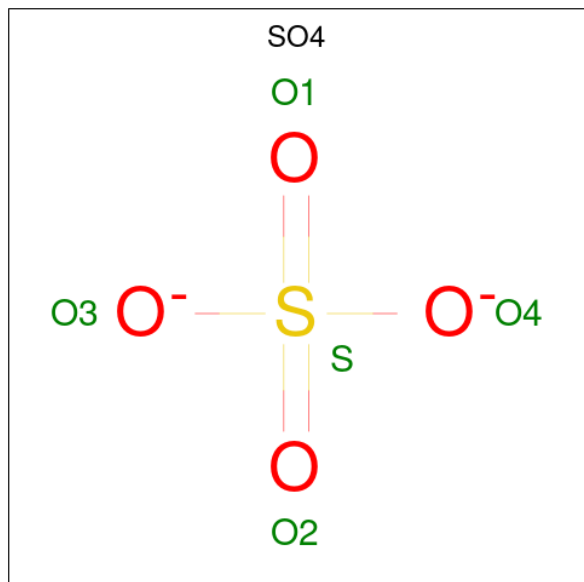
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: 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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



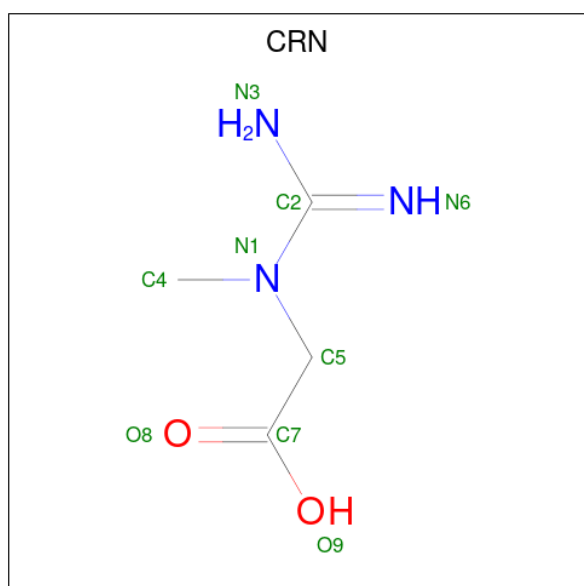
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	C	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	E	1	5	4	1	0	0
4	E	1	5	4	1	0	0
4	E	1	5	4	1	0	0
4	F	1	5	4	1	0	0
4	F	1	5	4	1	0	0
4	F	1	5	4	1	0	0

- Molecule 5 is N-[(E)-AMINO(IMINO)METHYL]-N-METHYLGLYCINE (three-letter code: CRN) (formula: C₄H₉N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	4	3	2		
5	B	1	Total	C	N	O	0	0
			9	4	3	2		
5	C	1	Total	C	N	O	0	0
			9	4	3	2		
5	D	1	Total	C	N	O	0	0
			9	4	3	2		
5	E	1	Total	C	N	O	0	0
			9	4	3	2		
5	F	1	Total	C	N	O	0	0
			9	4	3	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	327	Total	O	0	0
			327	327		
6	B	298	Total	O	0	0
			298	298		
6	C	308	Total	O	0	0
			308	308		
6	D	271	Total	O	0	0
			271	271		
6	E	305	Total	O	0	0
			305	305		
6	F	326	Total	O	0	0
			326	326		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: creatinine amidohydrolase

Chain A:  92% 7%




- Molecule 1: creatinine amidohydrolase

Chain B:  92% 6% ..



- Molecule 1: creatinine amidohydrolase

Chain C:  91% 7%




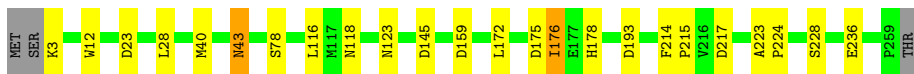
- Molecule 1: creatinine amidohydrolase

Chain D:  91% 7% ..

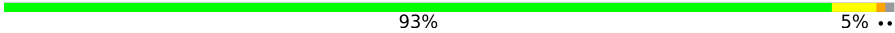


- Molecule 1: creatinine amidohydrolase

Chain E:  90% 8% ..



- Molecule 1: creatinine amidohydrolase

Chain F:  93% 5% ..



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.19Å 152.21Å 167.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60	Depositor
% Data completeness (in resolution range)	97.8 (40.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.182 , 0.198	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13919	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: ZN, CRN, MN, SO4

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	0.35	0/2037	0.68	5/2772 (0.2%)
1	B	0.33	0/2037	0.68	6/2772 (0.2%)
1	C	0.33	0/2037	0.68	5/2772 (0.2%)
1	D	0.33	0/2037	0.69	5/2772 (0.2%)
1	E	0.33	0/2037	0.70	6/2772 (0.2%)
1	F	0.33	0/2037	0.69	4/2772 (0.1%)
All	All	0.33	0/12222	0.69	31/16632 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	ASP	CB-CG-OD2	6.68	124.31	118.30
1	E	23	ASP	CB-CG-OD2	6.49	124.14	118.30
1	E	175	ASP	CB-CG-OD2	6.46	124.11	118.30
1	D	175	ASP	CB-CG-OD2	6.42	124.08	118.30
1	F	175	ASP	CB-CG-OD2	6.18	123.86	118.30
1	F	23	ASP	CB-CG-OD2	6.17	123.86	118.30
1	D	193	ASP	CB-CG-OD2	6.06	123.75	118.30
1	C	23	ASP	CB-CG-OD2	5.96	123.66	118.30
1	E	217	ASP	CB-CG-OD2	5.94	123.65	118.30
1	E	145	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	145	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	145	ASP	CB-CG-OD2	5.89	123.61	118.30
1	B	193	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	193	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	23	ASP	CB-CG-OD2	5.80	123.53	118.30
1	F	193	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	23	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	23	ASP	CB-CG-OD2	5.71	123.44	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	193	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	217	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	145	ASP	CB-CG-OD2	5.55	123.29	118.30
1	E	193	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	217	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	217	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	145	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	175	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	159	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	175	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	217	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	159	ASP	CB-CG-OD2	5.03	122.83	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	1988	0	1969	9	0
1	B	1988	0	1969	7	0
1	C	1988	0	1969	8	0
1	D	1988	0	1969	9	0
1	E	1988	0	1969	12	0
1	F	1988	0	1969	7	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
4	E	15	0	0	0	0
4	F	15	0	0	0	0
5	A	9	0	7	2	0
5	B	9	0	7	3	0
5	C	9	0	7	0	0
5	D	9	0	7	2	0
5	E	9	0	7	2	0
5	F	9	0	7	2	0
6	A	327	0	0	1	0
6	B	298	0	0	2	0
6	C	308	0	0	1	0
6	D	271	0	0	2	0
6	E	305	0	0	1	0
6	F	326	0	0	1	0
All	All	13919	0	11856	56	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 2.

All (56) 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:216:VAL:HG11	6:B:2263:HOH:O	1.80	0.80
5:B:3401:CRN:C7	5:B:3401:CRN:HN31	1.98	0.75
1:A:39:HIS:CD2	1:A:40:MET:HG3	2.24	0.72
5:A:401:CRN:HN31	5:A:401:CRN:C7	2.04	0.70
5:F:7401:CRN:C7	5:F:7401:CRN:HN31	2.15	0.60
1:F:216:VAL:HG11	6:F:2089:HOH:O	2.03	0.59
5:F:7401:CRN:C7	5:F:7401:CRN:N3	2.68	0.56
1:D:162:VAL:HG12	6:D:2513:HOH:O	2.04	0.56
5:B:3401:CRN:C7	5:B:3401:CRN:N3	2.62	0.56
1:F:39:HIS:CD2	1:F:40:MET:HB2	2.41	0.54
1:B:214:PHE:HA	1:B:215:PRO:C	2.28	0.53
5:A:401:CRN:C7	5:A:401:CRN:N3	2.67	0.53
1:E:28:LEU:HD23	1:E:116:LEU:CD2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD23	1:A:116:LEU:HD21	1.90	0.53
5:B:3401:CRN:H42	6:B:2653:HOH:O	2.08	0.53
1:A:28:LEU:HD23	1:A:116:LEU:CD2	2.39	0.52
1:C:39:HIS:CD2	1:C:40:MET:HB2	2.44	0.52
1:E:28:LEU:HD23	1:E:116:LEU:HD21	1.92	0.51
1:E:178:HIS:HB2	5:E:6401:CRN:N3	2.26	0.51
1:D:214:PHE:HA	1:D:215:PRO:C	2.31	0.50
1:D:166:LEU:HD11	6:D:2513:HOH:O	2.12	0.49
1:E:78:SER:O	5:E:6401:CRN:N3	2.35	0.49
1:C:43:ASN:C	1:C:43:ASN:HD22	2.16	0.49
1:E:214:PHE:HA	1:E:215:PRO:C	2.33	0.49
1:C:214:PHE:HA	1:C:215:PRO:C	2.34	0.47
1:F:214:PHE:HA	1:F:215:PRO:C	2.34	0.47
1:E:172:LEU:HB3	1:E:176:ILE:HD11	1.97	0.47
1:A:43:ASN:HD22	1:A:43:ASN:C	2.18	0.46
1:D:78:SER:O	5:D:5401:CRN:N3	2.38	0.46
1:A:214:PHE:HA	1:A:215:PRO:C	2.35	0.45
1:F:43:ASN:C	1:F:43:ASN:HD22	2.19	0.45
1:D:178:HIS:HB2	5:D:5401:CRN:N3	2.32	0.45
1:B:43:ASN:C	1:B:43:ASN:HD22	2.20	0.44
1:E:176:ILE:HD12	1:E:228:SER:HB3	2.00	0.44
1:C:26:LEU:CD1	1:C:106:LEU:HD22	2.48	0.43
1:D:43:ASN:C	1:D:43:ASN:HD22	2.22	0.43
1:E:3:LYS:N	6:E:2654:HOH:O	2.50	0.43
1:A:13:LYS:NZ	6:A:2621:HOH:O	2.52	0.42
1:F:116:LEU:HD13	1:F:131:ILE:HD11	2.01	0.42
1:C:24:CYS:HB3	6:C:2607:HOH:O	2.19	0.42
1:C:74:SER:H	1:C:82:ASN:HD22	1.67	0.42
1:B:28:LEU:HD23	1:B:116:LEU:CD2	2.49	0.42
1:B:28:LEU:HD23	1:B:116:LEU:HD21	2.01	0.42
1:E:43:ASN:C	1:E:43:ASN:HD22	2.22	0.42
1:F:72:TYR:CG	1:F:73:LYS:N	2.88	0.42
1:D:26:LEU:CD1	1:D:106:LEU:HD22	2.51	0.41
1:E:223:ALA:N	1:E:224:PRO:CD	2.83	0.41
1:A:37:GLY:HA2	1:A:224:PRO:O	2.21	0.41
1:A:35:GLN:HB2	1:F:12:TRP:CD1	2.56	0.41
1:A:39:HIS:NE2	1:A:40:MET:HG3	2.36	0.41
1:B:35:GLN:HB2	1:C:12:TRP:CD1	2.56	0.41
1:B:223:ALA:N	1:B:224:PRO:CD	2.84	0.41
1:D:223:ALA:N	1:D:224:PRO:CD	2.84	0.41
1:D:35:GLN:HB2	1:E:12:TRP:CD1	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ALA:N	1:C:224:PRO:CD	2.84	0.40
1:E:118:ASN:ND2	1:E:123:ASN:HB2	2.37	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	255/260 (98%)	252 (99%)	3 (1%)	0	100	100
1	B	255/260 (98%)	251 (98%)	4 (2%)	0	100	100
1	C	255/260 (98%)	252 (99%)	3 (1%)	0	100	100
1	D	255/260 (98%)	253 (99%)	2 (1%)	0	100	100
1	E	255/260 (98%)	253 (99%)	2 (1%)	0	100	100
1	F	255/260 (98%)	252 (99%)	3 (1%)	0	100	100
All	All	1530/1560 (98%)	1513 (99%)	17 (1%)	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	212/215 (99%)	209 (99%)	3 (1%)	67	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	212/215 (99%)	208 (98%)	4 (2%)	57	34
1	C	212/215 (99%)	209 (99%)	3 (1%)	67	47
1	D	212/215 (99%)	207 (98%)	5 (2%)	49	24
1	E	212/215 (99%)	208 (98%)	4 (2%)	57	34
1	F	212/215 (99%)	209 (99%)	3 (1%)	67	47
All	All	1272/1290 (99%)	1250 (98%)	22 (2%)	60	38

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	139	ARG
1	A	212	ASP
1	B	3	LYS
1	B	43	ASN
1	B	172	LEU
1	B	175	ASP
1	C	43	ASN
1	C	116	LEU
1	C	169	GLU
1	D	3	LYS
1	D	40	MET
1	D	43	ASN
1	D	166	LEU
1	D	169	GLU
1	E	40	MET
1	E	43	ASN
1	E	176	ILE
1	E	236	GLU
1	F	3	LYS
1	F	43	ASN
1	F	116	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	82	ASN
1	A	118	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	ASN
1	B	82	ASN
1	B	118	ASN
1	C	43	ASN
1	C	75	GLN
1	C	82	ASN
1	C	118	ASN
1	D	43	ASN
1	D	82	ASN
1	D	118	ASN
1	D	165	GLN
1	E	43	ASN
1	E	82	ASN
1	E	118	ASN
1	F	43	ASN
1	F	82	ASN
1	F	118	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](#)

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](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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
5	CRN	C	4401	2,3	8,8,8	0.96	0	7,10,10	1.98	2 (28%)
4	SO4	B	3502	-	4,4,4	0.14	0	6,6,6	0.06	0
5	CRN	A	401	2,3	8,8,8	0.89	0	7,10,10	1.16	1 (14%)
4	SO4	C	4502	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	F	7503	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.29	0
4	SO4	E	6502	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	F	7501	-	4,4,4	0.16	0	6,6,6	0.15	0
5	CRN	E	6401	2,3	8,8,8	0.92	0	7,10,10	0.92	0
4	SO4	C	4501	-	4,4,4	0.14	0	6,6,6	0.19	0
4	SO4	F	7502	-	4,4,4	0.14	0	6,6,6	0.12	0
5	CRN	B	3401	2,3	8,8,8	0.95	0	7,10,10	1.21	1 (14%)
5	CRN	F	7401	2,3	8,8,8	0.96	0	7,10,10	1.26	1 (14%)
4	SO4	B	3503	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	D	5502	-	4,4,4	0.13	0	6,6,6	0.09	0
4	SO4	C	4503	-	4,4,4	0.12	0	6,6,6	0.08	0
4	SO4	E	6501	-	4,4,4	0.15	0	6,6,6	0.18	0
4	SO4	B	3501	-	4,4,4	0.17	0	6,6,6	0.13	0
4	SO4	D	5503	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SO4	E	6503	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	D	5501	-	4,4,4	0.14	0	6,6,6	0.14	0
5	CRN	D	5401	2,3	8,8,8	0.95	0	7,10,10	0.95	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
5	CRN	C	4401	2,3	-	4/8/8/8	-
5	CRN	A	401	2,3	-	4/8/8/8	-
5	CRN	B	3401	2,3	-	4/8/8/8	-
5	CRN	F	7401	2,3	-	4/8/8/8	-
5	CRN	E	6401	2,3	-	3/8/8/8	-
5	CRN	D	5401	2,3	-	4/8/8/8	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4401	CRN	N3-C2-N1	4.19	123.55	118.53
5	B	3401	CRN	N3-C2-N1	2.76	121.84	118.53
5	F	7401	CRN	N3-C2-N1	2.57	121.62	118.53
5	A	401	CRN	N3-C2-N1	2.28	121.27	118.53
5	C	4401	CRN	C4-N1-C5	-2.19	113.76	116.97

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	CRN	C7-C5-N1-C4
5	A	401	CRN	C7-C5-N1-C2
5	B	3401	CRN	C7-C5-N1-C4
5	B	3401	CRN	C7-C5-N1-C2
5	C	4401	CRN	C7-C5-N1-C4
5	C	4401	CRN	C7-C5-N1-C2
5	D	5401	CRN	N1-C5-C7-O9
5	D	5401	CRN	C7-C5-N1-C4
5	D	5401	CRN	C7-C5-N1-C2
5	F	7401	CRN	N1-C5-C7-O9
5	F	7401	CRN	C7-C5-N1-C4
5	F	7401	CRN	C7-C5-N1-C2
5	A	401	CRN	N1-C5-C7-O9
5	A	401	CRN	N1-C5-C7-O8
5	B	3401	CRN	N1-C5-C7-O9
5	B	3401	CRN	N1-C5-C7-O8
5	D	5401	CRN	N1-C5-C7-O8
5	E	6401	CRN	N1-C5-C7-O8
5	F	7401	CRN	N1-C5-C7-O8
5	C	4401	CRN	N1-C5-C7-O8
5	C	4401	CRN	N1-C5-C7-O9
5	E	6401	CRN	N1-C5-C7-O9
5	E	6401	CRN	C7-C5-N1-C4

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	CRN	2	0
5	E	6401	CRN	2	0
5	B	3401	CRN	3	0
5	F	7401	CRN	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5401	CRN	2	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.