



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:41 PM UTC

PDB ID : 3A6J / pdb_00003a6j
Title : E122Q mutant creatininase complexed with creatine
Authors : Nakajima, Y.; Yamashita, K.; Ito, K.; Yoshimoto, T.
Deposited on : 2009-09-02
Resolution : 2.00 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 : 4-5-2 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

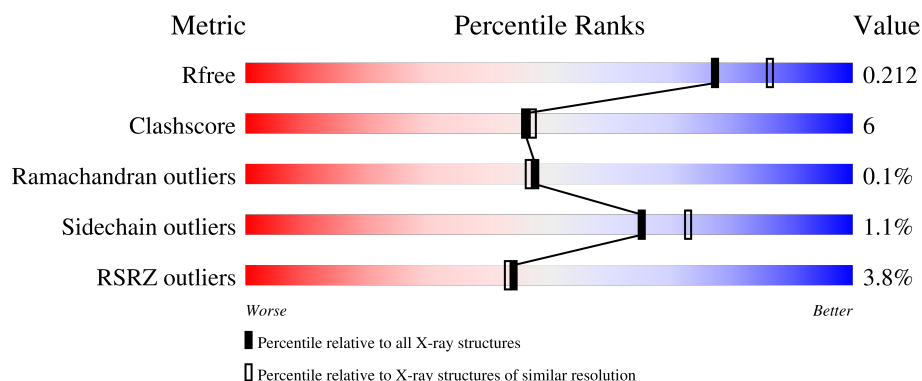
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	3% 85% 13% .
1	B	260	2% 85% 12% ..
1	C	260	2% 85% 13% .
1	D	260	5% 81% 17% ..
1	E	260	6% 79% 17% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	260	4% 87% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CRN	A	303	-	-	X	-
3	CRN	E	306	-	-	X	-
4	SO4	B	416	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12836 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
1	A	257	Total	C	N	O	S	0	0	0
			1981	1269	337	364	11			
1	B	254	Total	C	N	O	S	0	0	0
			1971	1264	335	361	11			
1	C	255	Total	C	N	O	S	0	0	0
			1975	1266	336	362	11			
1	D	256	Total	C	N	O	S	0	0	0
			1980	1269	337	363	11			
1	E	255	Total	C	N	O	S	0	0	0
			1976	1267	336	362	11			
1	F	255	Total	C	N	O	S	0	0	0
			1971	1263	335	362	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	GLN	GLU	engineered mutation	UNP P83772
B	122	GLN	GLU	engineered mutation	UNP P83772
C	122	GLN	GLU	engineered mutation	UNP P83772
D	122	GLN	GLU	engineered mutation	UNP P83772
E	122	GLN	GLU	engineered mutation	UNP P83772
F	122	GLN	GLU	engineered mutation	UNP P83772

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

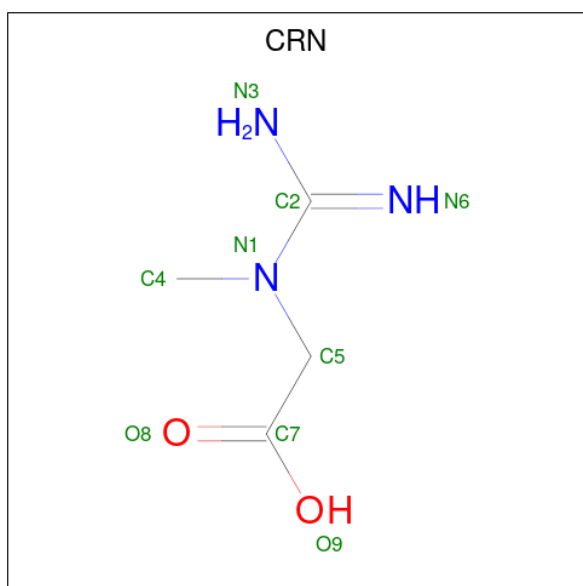
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is N-[(E)-AMINO(IMINO)METHYL]-N-METHYLGLYCINE (CCD ID: CRN) (formula: C₄H₉N₃O₂).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

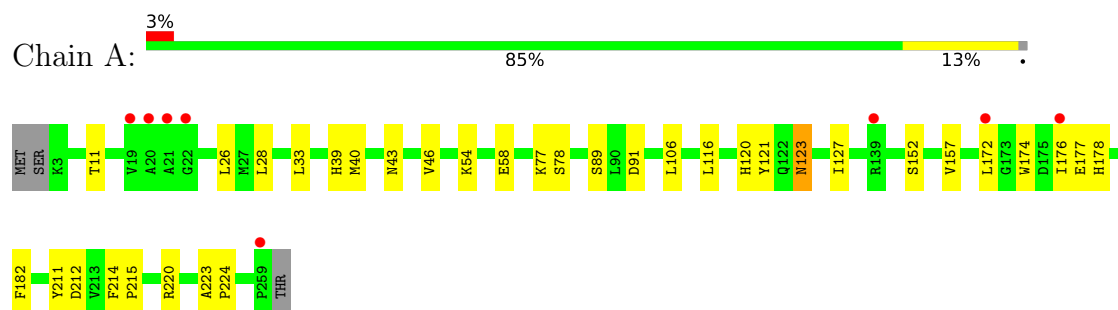
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total 154	O 154	0	0
5	B	147	Total 147	O 147	0	0
5	C	137	Total 137	O 137	0	0
5	D	141	Total 141	O 141	0	0
5	E	129	Total 129	O 129	0	0
5	F	158	Total 158	O 158	0	0

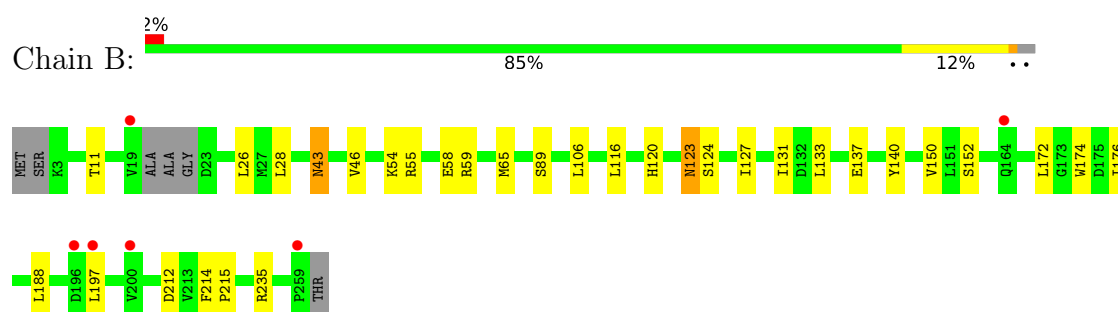
3 Residue-property plots [i](#)

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.

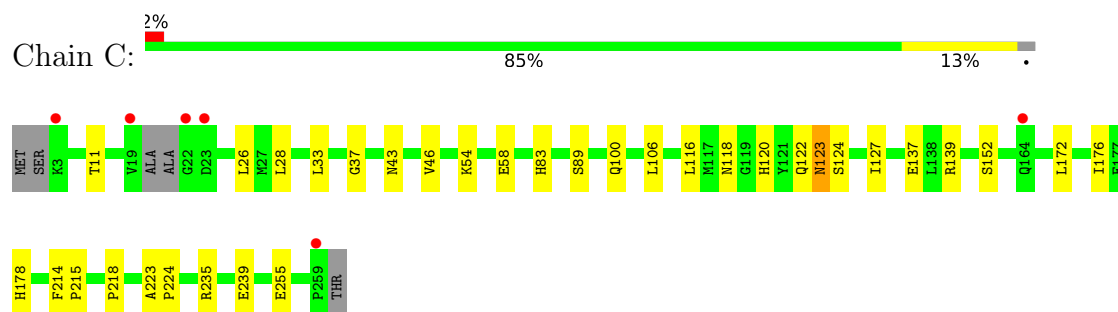
- Molecule 1: Creatinine amidohydrolase



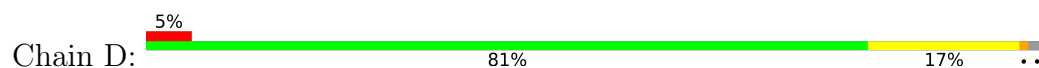
- Molecule 1: Creatinine amidohydrolase

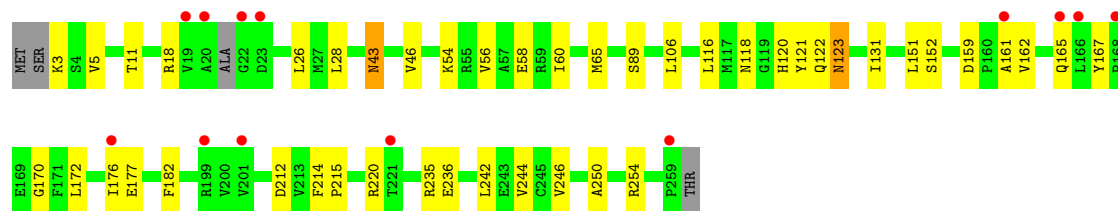


- Molecule 1: Creatinine amidohydrolase

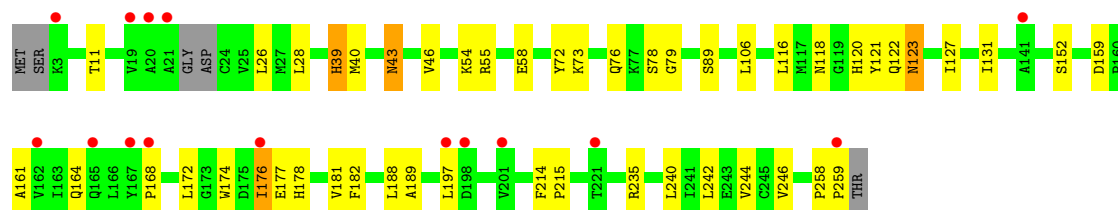
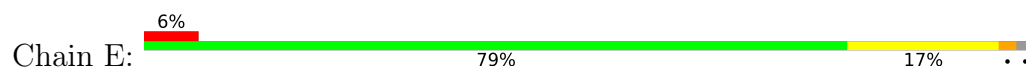


- Molecule 1: Creatinine amidohydrolase

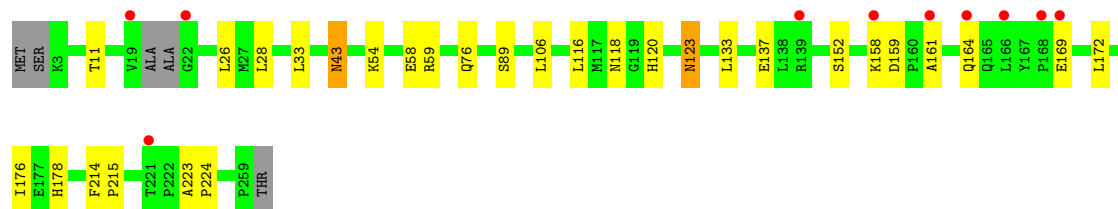
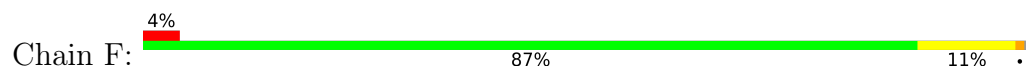




● Molecule 1: Creatinine amidohydrolase



● Molecule 1: Creatinine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.20Å 152.70Å 166.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.00) 99.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.58 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.212 0.195 , 0.212	Depositor DCC
R_{free} test set	8787 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12836	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, CRN

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	0.38	0/2030	0.92	9/2764 (0.3%)
1	B	0.36	0/2019	0.90	7/2746 (0.3%)
1	C	0.35	0/2023	0.88	8/2751 (0.3%)
1	D	0.36	0/2028	0.89	6/2758 (0.2%)
1	E	0.37	0/2024	0.89	9/2753 (0.3%)
1	F	0.36	0/2019	0.89	6/2747 (0.2%)
All	All	0.36	0/12143	0.89	45/16519 (0.3%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ASN	N-CA-C	7.70	119.75	111.36
1	B	123	ASN	N-CA-C	7.51	120.54	111.82
1	C	123	ASN	N-CA-C	7.40	119.43	111.36
1	B	11	THR	N-CA-C	-6.96	101.56	110.53
1	F	123	ASN	N-CA-C	6.93	119.86	111.82
1	D	11	THR	N-CA-C	-6.49	102.16	110.53
1	E	123	ASN	N-CA-C	6.33	119.16	111.82
1	E	46	VAL	N-CA-C	-6.06	105.91	111.67
1	E	152	SER	N-CA-C	-5.97	98.79	108.52
1	A	127	ILE	N-CA-C	-5.84	105.04	110.53
1	D	123	ASN	N-CA-C	5.76	118.50	111.82
1	B	152	SER	N-CA-C	-5.71	99.43	108.73
1	E	76	GLN	N-CA-C	5.68	117.93	111.11
1	F	33	LEU	N-CA-C	-5.67	98.11	108.02
1	C	152	SER	N-CA-C	-5.63	99.55	108.73
1	A	11	THR	N-CA-C	-5.63	102.19	110.52
1	F	89	SER	N-CA-C	5.59	118.84	109.95
1	C	11	THR	N-CA-C	-5.58	102.26	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	SER	N-CA-C	5.56	118.79	109.95
1	E	11	THR	N-CA-C	-5.55	102.30	110.52
1	A	152	SER	N-CA-C	-5.55	99.48	108.52
1	B	127	ILE	N-CA-C	-5.50	105.16	110.72
1	E	127	ILE	N-CA-C	-5.49	105.17	110.72
1	C	33	LEU	N-CA-C	-5.47	98.44	108.02
1	D	121	TYR	N-CA-C	5.44	117.92	111.33
1	F	152	SER	N-CA-C	-5.43	99.87	108.73
1	C	46	VAL	N-CA-C	-5.41	106.53	111.67
1	A	33	LEU	N-CA-C	-5.38	98.60	108.02
1	D	152	SER	N-CA-C	-5.35	99.80	108.52
1	E	39	HIS	N-CA-C	5.34	119.94	113.38
1	A	121	TYR	N-CA-C	5.32	117.76	111.33
1	F	11	THR	N-CA-C	-5.29	102.69	110.52
1	F	76	GLN	N-CA-C	5.27	117.43	111.11
1	B	89	SER	N-CA-C	5.22	118.25	109.95
1	D	46	VAL	N-CA-C	-5.22	106.71	111.67
1	C	89	SER	N-CA-C	5.19	118.21	109.95
1	E	121	TYR	N-CA-C	5.19	117.61	111.33
1	C	124	SER	N-CA-C	5.18	121.83	110.80
1	A	46	VAL	N-CA-C	-5.14	106.79	111.67
1	E	181	VAL	N-CA-C	5.13	115.35	110.42
1	B	124	SER	N-CA-C	5.11	121.69	110.80
1	C	127	ILE	N-CA-C	-5.08	105.59	110.72
1	D	89	SER	N-CA-C	5.08	118.02	109.95
1	A	91	ASP	N-CA-C	-5.07	103.70	110.55
1	B	46	VAL	N-CA-C	-5.03	106.89	111.67

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	1981	0	1958	20	0
1	B	1971	0	1955	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1975	0	1958	17	0
1	D	1980	0	1963	29	0
1	E	1976	0	1963	31	0
1	F	1971	0	1947	16	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	9	0	7	5	0
3	B	9	0	7	3	0
3	C	9	0	7	2	0
3	E	9	0	7	4	0
3	F	9	0	7	1	0
4	A	15	0	0	0	0
4	B	10	0	0	2	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	1	0
5	A	154	0	0	2	0
5	B	147	0	0	0	0
5	C	137	0	0	0	0
5	D	141	0	0	2	0
5	E	129	0	0	0	0
5	F	158	0	0	0	0
All	All	12836	0	11779	137	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 6.

All (137) 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:172:LEU:HB3	1:D:176:ILE:HD11	1.55	0.89
1:E:172:LEU:HB3	1:E:176:ILE:HD11	1.57	0.86
1:B:172:LEU:HB3	1:B:176:ILE:HD11	1.62	0.79
1:E:178:HIS:HB2	3:E:306:CRN:N3	2.06	0.71
3:B:304:CRN:HN31	3:B:304:CRN:C7	2.06	0.69
1:D:54:LYS:O	1:D:58:GLU:HG3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HB3	1:C:176:ILE:HD11	1.79	0.65
1:E:172:LEU:HB3	1:E:176:ILE:CD1	2.27	0.64
1:E:26:LEU:HD13	1:E:106:LEU:HD22	1.78	0.64
1:E:78:SER:O	3:E:306:CRN:N3	2.30	0.64
1:A:178:HIS:HB2	3:A:303:CRN:N3	2.14	0.63
1:B:188:LEU:HD21	1:B:197:LEU:HD11	1.79	0.63
1:D:250:ALA:O	1:D:254:ARG:HG3	2.00	0.62
1:C:120:HIS:HB3	1:C:123:ASN:ND2	2.14	0.62
1:F:26:LEU:HD13	1:F:106:LEU:HD22	1.81	0.62
1:E:189:ALA:HA	1:E:235:ARG:HG3	1.83	0.60
1:D:3:LYS:NZ	1:D:18:ARG:HH11	1.99	0.60
1:C:26:LEU:HD13	1:C:106:LEU:HD22	1.82	0.60
1:F:54:LYS:O	1:F:58:GLU:HG3	2.01	0.59
1:C:139:ARG:HH11	1:C:139:ARG:HG2	1.68	0.59
1:E:54:LYS:O	1:E:58:GLU:HG3	2.02	0.59
1:E:164:GLN:NE2	1:E:168:PRO:HA	2.18	0.57
1:B:54:LYS:O	1:B:58:GLU:HG3	2.04	0.57
1:C:28:LEU:HD23	1:C:116:LEU:HD21	1.87	0.57
1:C:178:HIS:HB2	3:C:305:CRN:N3	2.19	0.56
1:E:188:LEU:HD21	1:E:197:LEU:CD1	2.36	0.56
1:E:188:LEU:HD21	1:E:197:LEU:HD11	1.88	0.56
1:D:214:PHE:HA	1:D:215:PRO:C	2.32	0.55
1:F:120:HIS:HB3	1:F:123:ASN:ND2	2.21	0.55
1:B:235:ARG:HB2	1:B:235:ARG:HH21	1.72	0.55
1:B:28:LEU:HD23	1:B:116:LEU:HD21	1.89	0.55
1:F:172:LEU:HB3	1:F:176:ILE:HD11	1.88	0.55
1:F:59:ARG:HD3	4:F:402:SO4:O3	2.07	0.54
1:D:220:ARG:HD3	5:D:1587:HOH:O	2.08	0.54
1:E:174:TRP:O	3:E:306:CRN:N6	2.41	0.54
1:B:188:LEU:HD21	1:B:197:LEU:CD1	2.37	0.53
1:B:214:PHE:HA	1:B:215:PRO:C	2.33	0.53
1:F:26:LEU:CD1	1:F:106:LEU:HD22	2.38	0.53
1:C:54:LYS:O	1:C:58:GLU:HG3	2.07	0.53
1:E:235:ARG:HB3	1:E:235:ARG:NH2	2.23	0.53
1:E:214:PHE:HA	1:E:215:PRO:C	2.32	0.53
1:A:172:LEU:HB2	1:A:176:ILE:HD11	1.91	0.52
1:F:178:HIS:HB2	3:F:307:CRN:N3	2.24	0.52
1:E:28:LEU:HD23	1:E:116:LEU:CD2	2.39	0.52
1:A:26:LEU:HD13	1:A:106:LEU:HD22	1.92	0.51
1:F:214:PHE:HA	1:F:215:PRO:C	2.35	0.51
1:B:188:LEU:HD11	1:B:197:LEU:HD11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:LEU:HD11	1:E:197:LEU:HD11	1.91	0.51
1:E:177:GLU:CD	1:E:182:PHE:HB3	2.36	0.51
1:A:157:VAL:HG21	1:A:182:PHE:HE2	1.76	0.51
1:C:214:PHE:HA	1:C:215:PRO:C	2.35	0.50
1:D:177:GLU:CD	1:D:182:PHE:HB3	2.36	0.50
1:B:235:ARG:HB2	1:B:235:ARG:NH2	2.27	0.50
1:E:39:HIS:CD2	1:E:40:MET:HG3	2.46	0.50
1:D:5:VAL:HG22	5:D:1648:HOH:O	2.09	0.50
1:E:26:LEU:CD1	1:E:106:LEU:HD22	2.41	0.50
1:E:28:LEU:HD23	1:E:116:LEU:HD21	1.94	0.50
1:A:214:PHE:HA	1:A:215:PRO:C	2.35	0.50
1:D:28:LEU:HD23	1:D:116:LEU:HD21	1.94	0.50
1:D:56:VAL:O	1:D:60:ILE:HG12	2.12	0.50
1:A:178:HIS:HB2	3:A:303:CRN:HN32	1.75	0.49
1:A:78:SER:O	3:A:303:CRN:N3	2.38	0.49
1:D:161:ALA:O	1:D:165:GLN:HG3	2.11	0.49
1:B:59:ARG:HD3	4:B:416:SO4:S	2.51	0.49
1:A:54:LYS:O	1:A:58:GLU:HG3	2.13	0.49
3:A:303:CRN:C7	3:A:303:CRN:HN31	2.25	0.49
1:D:235:ARG:HH21	1:D:235:ARG:HG2	1.76	0.49
1:C:26:LEU:CD1	1:C:106:LEU:HD22	2.42	0.48
1:F:169:GLU:HG2	1:F:169:GLU:O	2.12	0.48
1:C:178:HIS:HB2	3:C:305:CRN:HN32	1.78	0.48
1:A:220:ARG:HD3	5:A:1863:HOH:O	2.13	0.48
1:E:120:HIS:HB3	1:E:123:ASN:ND2	2.29	0.48
1:A:28:LEU:HD23	1:A:116:LEU:HD21	1.95	0.48
1:B:28:LEU:HD23	1:B:116:LEU:CD2	2.44	0.47
1:E:159:ASP:OD2	1:E:161:ALA:HB3	2.14	0.47
1:A:174:TRP:O	3:A:303:CRN:N6	2.47	0.47
1:D:120:HIS:HB3	1:D:123:ASN:ND2	2.28	0.47
1:B:59:ARG:HD3	4:B:416:SO4:O1	2.14	0.47
1:A:212:ASP:HB3	1:B:150:VAL:CG1	2.45	0.47
1:B:120:HIS:HB3	1:B:123:ASN:ND2	2.30	0.47
1:C:28:LEU:HD23	1:C:116:LEU:CD2	2.44	0.47
1:F:28:LEU:HD23	1:F:116:LEU:CD2	2.44	0.47
1:B:174:TRP:O	3:B:304:CRN:N6	2.48	0.46
1:D:26:LEU:HD13	1:D:106:LEU:HD22	1.96	0.46
1:D:159:ASP:OD2	1:D:161:ALA:HB3	2.16	0.46
1:D:28:LEU:HD23	1:D:116:LEU:CD2	2.45	0.46
1:A:39:HIS:CD2	1:A:40:MET:HG3	2.50	0.46
1:D:172:LEU:HB3	1:D:176:ILE:CD1	2.37	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ARG:HH11	1:E:55:ARG:HG3	1.80	0.46
1:D:3:LYS:HZ3	1:D:18:ARG:HH11	1.62	0.46
1:A:28:LEU:HD23	1:A:116:LEU:CD2	2.45	0.46
1:C:100:GLN:NE2	1:C:137:GLU:OE2	2.45	0.46
3:B:304:CRN:C7	3:B:304:CRN:N3	2.75	0.45
1:A:77:LYS:HE3	1:A:211:TYR:O	2.17	0.45
1:A:176:ILE:C	1:A:176:ILE:HD12	2.42	0.45
1:D:167:TYR:HB3	1:D:170:GLY:O	2.16	0.45
1:B:116:LEU:HD12	1:B:131:ILE:HD11	1.98	0.45
1:B:133:LEU:O	1:B:137:GLU:HG3	2.17	0.45
1:A:177:GLU:HG3	5:A:1189:HOH:O	2.16	0.44
1:A:26:LEU:CD1	1:A:106:LEU:HD22	2.48	0.44
1:B:26:LEU:HD13	1:B:106:LEU:HD22	1.98	0.44
1:E:116:LEU:HD12	1:E:131:ILE:HD11	1.99	0.44
1:D:26:LEU:CD1	1:D:106:LEU:HD22	2.48	0.44
1:D:242:LEU:O	1:D:246:VAL:HG23	2.17	0.44
1:C:223:ALA:N	1:C:224:PRO:HD2	2.34	0.43
1:E:43:ASN:HD22	1:E:43:ASN:C	2.26	0.43
1:E:118:ASN:ND2	1:E:123:ASN:HB2	2.32	0.43
1:D:118:ASN:ND2	1:D:123:ASN:HB2	2.34	0.43
1:D:65:MET:HE2	1:D:106:LEU:HD21	2.00	0.43
1:F:118:ASN:ND2	1:F:123:ASN:HB2	2.34	0.43
1:C:83:HIS:CD2	1:C:218:PRO:HB3	2.54	0.43
1:E:242:LEU:O	1:E:246:VAL:HG23	2.19	0.43
1:F:133:LEU:O	1:F:137:GLU:HG3	2.18	0.43
1:C:37:GLY:HA2	1:C:224:PRO:O	2.19	0.42
1:B:65:MET:HE2	1:B:106:LEU:HD21	2.00	0.42
1:B:137:GLU:HA	1:B:140:TYR:CD2	2.55	0.42
1:C:118:ASN:ND2	1:C:123:ASN:HB2	2.34	0.42
1:E:178:HIS:HB2	3:E:306:CRN:HN32	1.80	0.42
1:E:258:PRO:HA	1:E:259:PRO:HD3	1.88	0.42
1:A:120:HIS:HB3	1:A:123:ASN:ND2	2.35	0.42
1:D:162:VAL:HG21	1:D:244:VAL:HG21	2.01	0.42
1:D:151:LEU:HD12	1:D:151:LEU:C	2.45	0.42
1:B:55:ARG:HH11	1:B:55:ARG:HG3	1.83	0.42
1:F:158:LYS:HG2	1:F:158:LYS:O	2.19	0.42
1:D:235:ARG:NH1	1:D:236:GLU:OE1	2.53	0.42
1:E:240:LEU:O	1:E:244:VAL:HG23	2.19	0.42
1:E:72:TYR:CG	1:E:73:LYS:N	2.88	0.41
1:E:73:LYS:HA	1:E:89:SER:CB	2.51	0.41
1:F:43:ASN:C	1:F:43:ASN:HD22	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ALA:HB3	1:F:224:PRO:HD3	2.03	0.41
1:D:43:ASN:C	1:D:43:ASN:HD22	2.29	0.40
1:D:116:LEU:HD12	1:D:131:ILE:HD11	2.02	0.40
1:B:43:ASN:C	1:B:43:ASN:HD22	2.29	0.40
1:D:235:ARG:HG2	1:D:235:ARG:NH2	2.35	0.40
1:F:159:ASP:OD2	1:F:161:ALA:HB3	2.21	0.40
1:A:223:ALA:HB3	1:A:224:PRO:HD3	2.02	0.40
1:C:235:ARG:O	1:C:239:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	249 (98%)	6 (2%)	0	100	100
1	B	250/260 (96%)	243 (97%)	7 (3%)	0	100	100
1	C	251/260 (96%)	244 (97%)	7 (3%)	0	100	100
1	D	252/260 (97%)	245 (97%)	7 (3%)	0	100	100
1	E	251/260 (96%)	244 (97%)	6 (2%)	1 (0%)	30	27
1	F	251/260 (96%)	245 (98%)	6 (2%)	0	100	100
All	All	1510/1560 (97%)	1470 (97%)	39 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	79	GLY

5.3.2 Protein sidechains ⓘ

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	210/215 (98%)	209 (100%)	1 (0%)	81	87
1	B	211/215 (98%)	209 (99%)	2 (1%)	70	78
1	C	211/215 (98%)	208 (99%)	3 (1%)	59	66
1	D	211/215 (98%)	208 (99%)	3 (1%)	59	66
1	E	211/215 (98%)	208 (99%)	3 (1%)	59	66
1	F	210/215 (98%)	208 (99%)	2 (1%)	68	75
All	All	1264/1290 (98%)	1250 (99%)	14 (1%)	65	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	B	43	ASN
1	B	212	ASP
1	C	43	ASN
1	C	122	GLN
1	C	255	GLU
1	D	43	ASN
1	D	122	GLN
1	D	212	ASP
1	E	43	ASN
1	E	122	GLN
1	E	176	ILE
1	F	43	ASN
1	F	164	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	118	ASN
1	A	122	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	165	GLN
1	B	43	ASN
1	B	118	ASN
1	B	122	GLN
1	C	43	ASN
1	C	118	ASN
1	C	122	GLN
1	D	43	ASN
1	D	118	ASN
1	D	122	GLN
1	D	144	GLN
1	D	165	GLN
1	E	43	ASN
1	E	76	GLN
1	E	118	ASN
1	E	122	GLN
1	E	144	GLN
1	E	164	GLN
1	E	165	GLN
1	F	43	ASN
1	F	118	ASN
1	F	122	GLN
1	F	144	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\# Z > 2$
3	CRN	A	303	2	7,8,8	1.15	0	8,10,10	1.69	2 (25%)
3	CRN	C	305	2	7,8,8	1.21	0	8,10,10	1.38	1 (12%)
3	CRN	F	307	2	7,8,8	1.23	0	8,10,10	1.44	1 (12%)
4	SO4	E	413	-	4,4,4	0.36	0	6,6,6	0.12	0
4	SO4	E	401	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	F	414	-	4,4,4	0.37	0	6,6,6	0.05	0
4	SO4	B	410	-	4,4,4	0.37	0	6,6,6	0.11	0
4	SO4	A	409	-	4,4,4	0.38	0	6,6,6	0.13	0
4	SO4	D	400	-	4,4,4	0.37	0	6,6,6	0.07	0
4	SO4	B	416	-	4,4,4	0.38	0	6,6,6	0.07	0
4	SO4	C	411	-	4,4,4	0.37	0	6,6,6	0.07	0
4	SO4	C	417	-	4,4,4	0.37	0	6,6,6	0.06	0
4	SO4	A	403	-	4,4,4	0.38	0	6,6,6	0.06	0
4	SO4	D	412	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	F	402	-	4,4,4	0.38	0	6,6,6	0.12	0
3	CRN	B	304	2	7,8,8	1.47	2 (28%)	8,10,10	2.12	3 (37%)
4	SO4	A	415	-	4,4,4	0.37	0	6,6,6	0.09	0
3	CRN	E	306	2	7,8,8	1.19	0	8,10,10	1.54	1 (12%)

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
3	CRN	A	303	2	-	4/8/8/8	-
3	CRN	C	305	2	-	4/8/8/8	-
3	CRN	F	307	2	-	2/8/8/8	-
3	CRN	B	304	2	-	4/8/8/8	-
3	CRN	E	306	2	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	304	CRN	C5-N1	2.49	1.50	1.46
3	B	304	CRN	C2-N1	2.09	1.39	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	304	CRN	N3-C2-N1	4.05	123.08	118.64
3	A	303	CRN	N3-C2-N1	3.05	121.98	118.64
3	C	305	CRN	N3-C2-N1	2.82	121.73	118.64
3	E	306	CRN	N3-C2-N1	2.76	121.67	118.64
3	B	304	CRN	C4-N1-C5	-2.73	112.87	116.89
3	F	307	CRN	N3-C2-N1	2.57	121.46	118.64
3	B	304	CRN	C7-C5-N1	2.48	117.72	113.16
3	A	303	CRN	C4-N1-C5	-2.00	113.94	116.89

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	CRN	N1-C5-C7-O9
3	A	303	CRN	N1-C5-C7-O8
3	A	303	CRN	C7-C5-N1-C4
3	A	303	CRN	C7-C5-N1-C2
3	B	304	CRN	N1-C5-C7-O8
3	B	304	CRN	C7-C5-N1-C2
3	C	305	CRN	N1-C5-C7-O9
3	E	306	CRN	C7-C5-N1-C4
3	E	306	CRN	C7-C5-N1-C2
3	B	304	CRN	N1-C5-C7-O9
3	C	305	CRN	N1-C5-C7-O8
3	E	306	CRN	N1-C5-C7-O9
3	E	306	CRN	N1-C5-C7-O8
3	B	304	CRN	C7-C5-N1-C4
3	C	305	CRN	C7-C5-N1-C4
3	F	307	CRN	N1-C5-C7-O8
3	F	307	CRN	C7-C5-N1-C4
3	C	305	CRN	C7-C5-N1-C2

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	CRN	5	0
3	C	305	CRN	2	0
3	F	307	CRN	1	0
4	B	416	SO4	2	0
4	F	402	SO4	1	0
3	B	304	CRN	3	0
3	E	306	CRN	4	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

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	257/260 (98%)	-0.18	8 (3%) 51 50	14, 21, 35, 48	0
1	B	254/260 (97%)	-0.14	6 (2%) 59 59	14, 23, 39, 45	0
1	C	255/260 (98%)	-0.14	6 (2%) 59 59	15, 24, 38, 45	0
1	D	256/260 (98%)	0.08	13 (5%) 33 32	15, 25, 39, 43	0
1	E	255/260 (98%)	0.08	15 (5%) 28 27	15, 25, 39, 49	0
1	F	255/260 (98%)	-0.16	10 (3%) 43 42	14, 22, 38, 47	0
All	All	1532/1560 (98%)	-0.08	58 (3%) 44 43	14, 24, 38, 49	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	20	ALA	7.1
1	A	22	GLY	6.9
1	A	21	ALA	5.6
1	D	20	ALA	4.5
1	C	19	VAL	4.3
1	D	22	GLY	4.2
1	D	19	VAL	4.2
1	E	19	VAL	4.2
1	A	20	ALA	4.1
1	C	22	GLY	4.1
1	E	21	ALA	4.0
1	C	259	PRO	3.9
1	F	19	VAL	3.7
1	B	259	PRO	3.6
1	D	259	PRO	3.5
1	F	169	GLU	3.4
1	A	19	VAL	3.3
1	E	176	ILE	3.2
1	D	23	ASP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	23	ASP	3.2
1	F	158	LYS	3.1
1	F	164	GLN	3.1
1	D	165	GLN	3.1
1	B	197	LEU	3.0
1	A	259	PRO	2.9
1	F	161	ALA	2.9
1	F	22	GLY	2.9
1	D	176	ILE	2.8
1	E	197	LEU	2.8
1	D	166	LEU	2.8
1	E	162	VAL	2.8
1	E	259	PRO	2.6
1	D	161	ALA	2.6
1	F	139	ARG	2.6
1	F	168	PRO	2.5
1	E	3	LYS	2.5
1	A	172	LEU	2.3
1	D	201	VAL	2.3
1	E	201	VAL	2.3
1	D	221	THR	2.3
1	E	168	PRO	2.3
1	C	164	GLN	2.3
1	B	19	VAL	2.3
1	A	176	ILE	2.2
1	C	3	LYS	2.2
1	E	167	TYR	2.2
1	A	139	ARG	2.1
1	D	199	ARG	2.1
1	E	221	THR	2.1
1	B	164	GLN	2.1
1	F	221	THR	2.1
1	E	141	ALA	2.1
1	F	166	LEU	2.1
1	B	196	ASP	2.1
1	E	198	ASP	2.1
1	E	165	GLN	2.1
1	B	200	VAL	2.0
1	D	168	PRO	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 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($\text{\AA}^2$)	Q<0.9
3	CRN	E	306	9/9	0.55	0.32	37,44,48,48	0
3	CRN	B	304	9/9	0.63	0.28	35,39,41,41	0
3	CRN	A	303	9/9	0.68	0.30	33,39,41,42	0
3	CRN	C	305	9/9	0.72	0.27	34,39,41,42	0
4	SO4	F	402	5/5	0.73	0.12	64,64,65,67	0
3	CRN	F	307	9/9	0.74	0.22	32,37,41,44	0
4	SO4	A	403	5/5	0.75	0.25	53,54,57,59	0
4	SO4	B	416	5/5	0.82	0.14	58,58,60,61	0
4	SO4	C	417	5/5	0.83	0.15	59,59,60,61	0
4	SO4	D	400	5/5	0.86	0.13	59,60,60,61	0
4	SO4	E	401	5/5	0.89	0.09	57,57,58,59	0
4	SO4	A	415	5/5	0.91	0.11	55,55,56,57	0
4	SO4	E	413	5/5	0.93	0.10	39,40,42,42	0
4	SO4	D	412	5/5	0.95	0.08	40,42,43,43	0
4	SO4	F	414	5/5	0.96	0.08	35,37,39,39	0
4	SO4	C	411	5/5	0.97	0.07	33,34,36,37	0
4	SO4	B	410	5/5	0.97	0.07	36,39,39,40	0
4	SO4	A	409	5/5	0.98	0.06	28,32,33,33	0
2	ZN	D	301	1/1	0.99	0.03	23,23,23,23	0
2	ZN	E	301	1/1	0.99	0.03	23,23,23,23	0
2	ZN	B	301	1/1	1.00	0.02	22,22,22,22	0
2	ZN	F	301	1/1	1.00	0.02	21,21,21,21	0
2	ZN	C	301	1/1	1.00	0.03	22,22,22,22	0
2	ZN	A	301	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.