



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:47 AM UTC

PDB ID : 3A6G / pdb_00003a6g
Title : W154F mutant creatininase
Authors : Nakajima, Y.; Yamashita, K.; Ito, K.; Yoshimoto, T.
Deposited on : 2009-08-31
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
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

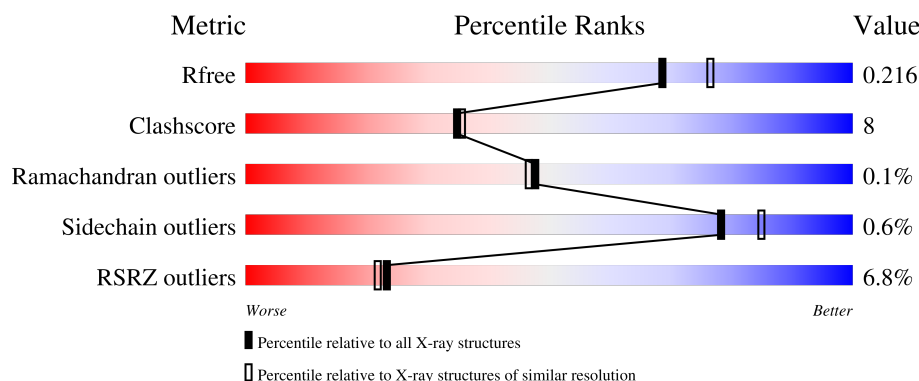
1 Overall quality at a glance

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	8% 78% 19% ..
1	B	260	6% 83% 13% ..
1	C	260	6% 79% 19% .
1	D	260	8% 81% 17% ..
1	E	260	5% 82% 16% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	260	7% 80% 18% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12321 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
			1940	1238	332	359	11			
1	B	253	Total	C	N	O	S	0	0	0
			1926	1229	328	358	11			
1	C	254	Total	C	N	O	S	0	0	0
			1944	1244	330	359	11			
1	D	257	Total	C	N	O	S	0	0	0
			1981	1269	336	365	11			
1	E	257	Total	C	N	O	S	0	0	0
			1981	1269	336	365	11			
1	F	257	Total	C	N	O	S	0	0	0
			1977	1266	335	365	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	PHE	TRP	engineered mutation	UNP P83772
B	154	PHE	TRP	engineered mutation	UNP P83772
C	154	PHE	TRP	engineered mutation	UNP P83772
D	154	PHE	TRP	engineered mutation	UNP P83772
E	154	PHE	TRP	engineered mutation	UNP P83772
F	154	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		

Continued on next page...

Continued from previous page...

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

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

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

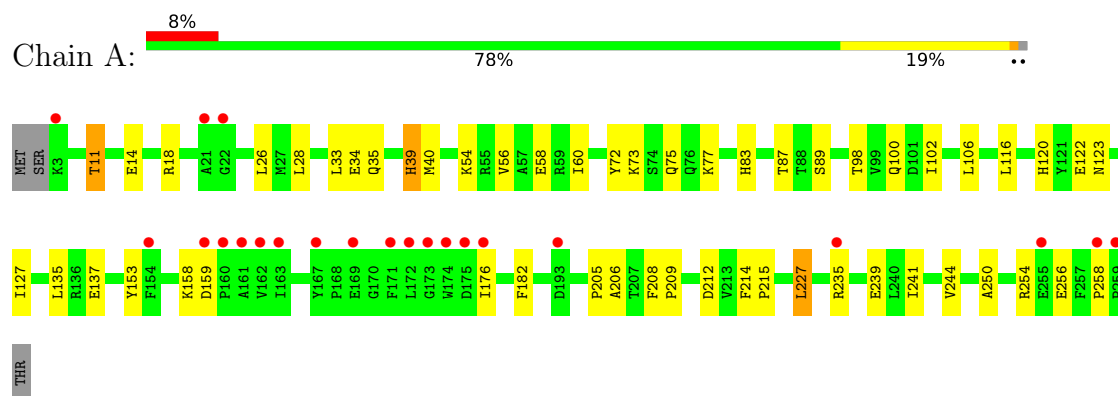
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total 97	O 97	0	0
4	B	96	Total 96	O 96	0	0
4	C	93	Total 93	O 93	0	0
4	D	98	Total 98	O 98	0	0
4	E	95	Total 95	O 95	0	0
4	F	81	Total 81	O 81	0	0

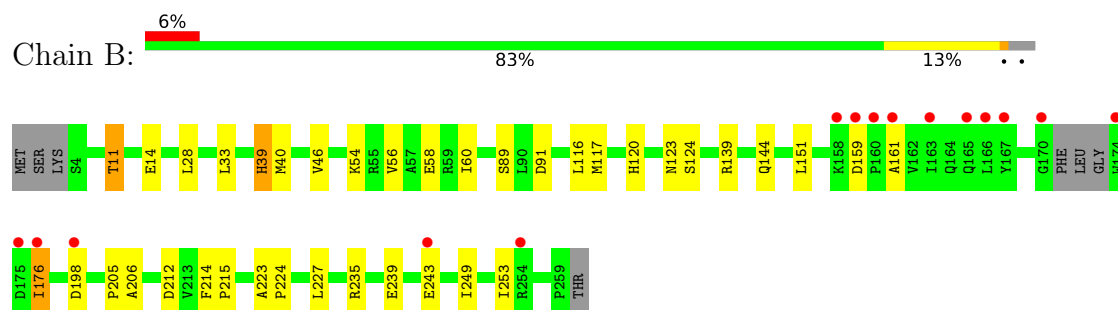
3 Residue-property plots [i](#)

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.

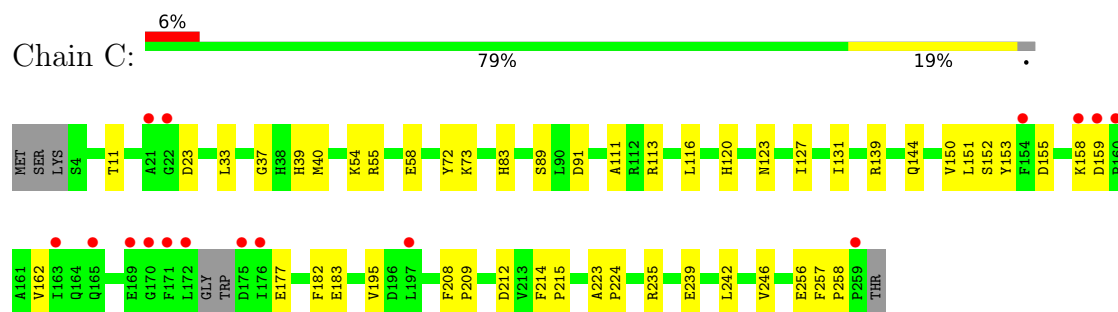
- Molecule 1: Creatinine amidohydrolase



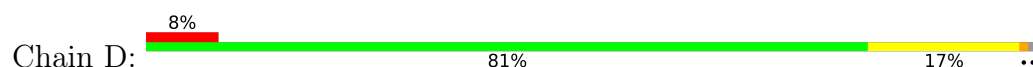
- Molecule 1: Creatinine amidohydrolase

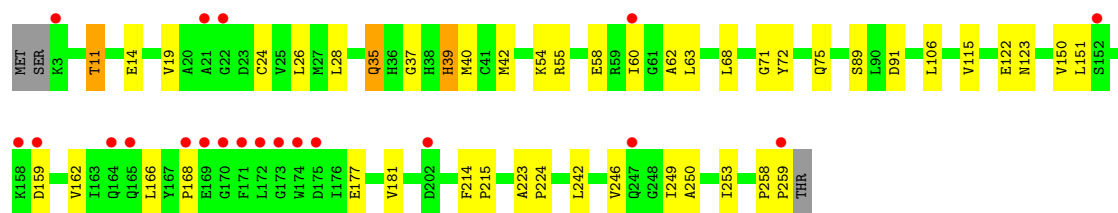


- Molecule 1: Creatinine amidohydrolase

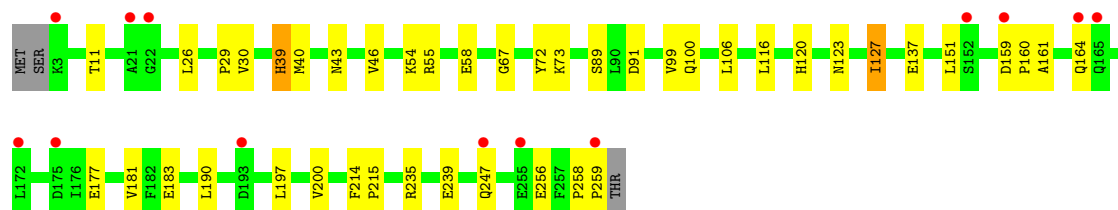
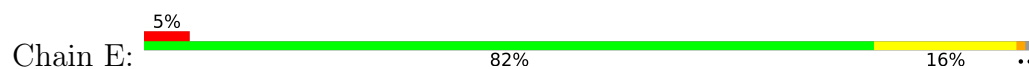


- Molecule 1: Creatinine amidohydrolase

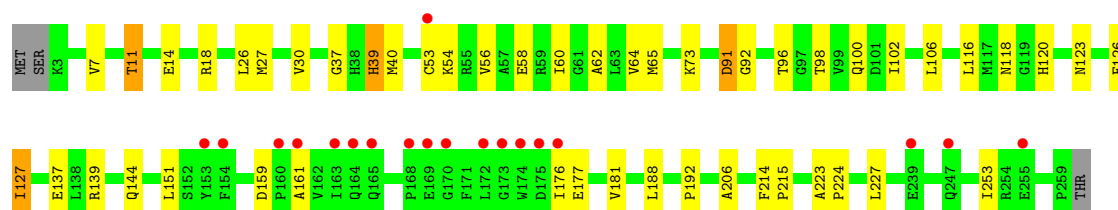
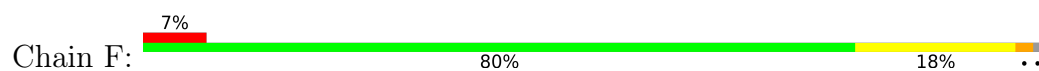




● Molecule 1: Creatinine amidohydrolase



● Molecule 1: Creatinine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.50Å 164.50Å 164.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.00) 99.9 (20.00-2.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.216 0.198 , 0.216	Depositor DCC
R_{free} test set	8660 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12321	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: ZN, MN

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	0.37	0/1985	0.88	6/2702 (0.2%)
1	B	0.38	0/1970	0.89	6/2681 (0.2%)
1	C	0.38	0/1989	0.88	8/2705 (0.3%)
1	D	0.36	0/2029	0.87	7/2760 (0.3%)
1	E	0.37	0/2029	0.89	7/2760 (0.3%)
1	F	0.36	0/2025	0.87	6/2756 (0.2%)
All	All	0.37	0/12027	0.88	40/16364 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	THR	N-CA-C	-6.54	101.71	110.55
1	E	11	THR	N-CA-C	-6.37	101.95	110.55
1	D	181	VAL	N-CA-C	6.32	116.49	110.42
1	D	11	THR	N-CA-C	-6.13	102.28	110.55
1	C	177	GLU	N-CA-C	5.79	119.61	112.54
1	E	181	VAL	N-CA-C	5.79	115.98	110.42
1	A	127	ILE	N-CA-C	-5.78	104.89	110.72
1	B	33	LEU	N-CA-C	-5.76	97.79	107.99
1	E	39	HIS	N-CA-C	5.71	120.40	113.38
1	F	177	GLU	N-CA-C	5.63	119.77	113.01
1	A	11	THR	N-CA-C	-5.61	102.22	110.52
1	B	11	THR	N-CA-C	-5.52	102.36	110.52
1	A	89	SER	N-CA-C	5.46	118.64	109.95
1	B	39	HIS	N-CA-C	5.46	120.09	113.38
1	A	33	LEU	N-CA-C	-5.43	98.37	107.99
1	D	89	SER	N-CA-C	5.39	118.52	109.95
1	B	89	SER	N-CA-C	5.39	118.52	109.95
1	C	89	SER	N-CA-C	5.38	118.50	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	ASP	N-CA-C	-5.35	103.32	110.55
1	E	91	ASP	N-CA-C	-5.34	103.34	110.55
1	E	89	SER	N-CA-C	5.34	118.44	109.95
1	C	127	ILE	N-CA-C	-5.33	105.33	110.72
1	F	127	ILE	N-CA-C	-5.30	105.36	110.72
1	F	91	ASP	N-CA-C	-5.29	103.40	110.55
1	C	91	ASP	N-CA-C	-5.27	103.57	110.53
1	F	39	HIS	N-CA-C	5.24	119.83	113.38
1	A	39	HIS	N-CA-C	5.24	119.83	113.38
1	F	11	THR	N-CA-C	-5.21	103.52	110.55
1	D	177	GLU	N-CA-C	5.18	118.86	112.54
1	B	91	ASP	N-CA-C	-5.18	103.56	110.55
1	E	127	ILE	N-CA-C	-5.17	105.67	110.53
1	D	39	HIS	N-CA-C	5.15	119.71	113.38
1	F	181	VAL	N-CA-C	5.12	115.74	110.36
1	E	177	GLU	N-CA-C	5.12	119.15	113.01
1	A	209	PRO	N-CA-C	-5.11	104.47	110.70
1	D	42	MET	N-CA-C	5.11	119.51	113.28
1	B	46	VAL	N-CA-C	-5.05	106.87	111.67
1	C	33	LEU	N-CA-C	-5.05	99.05	107.99
1	C	257	PHE	CA-C-N	5.04	123.34	119.66
1	C	257	PHE	C-N-CA	5.04	123.34	119.66

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	1940	0	1897	35	0
1	B	1926	0	1891	23	0
1	C	1944	0	1920	26	0
1	D	1981	0	1964	28	0
1	E	1981	0	1964	25	0
1	F	1977	0	1953	40	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	97	0	0	2	0
4	B	96	0	0	1	0
4	C	93	0	0	3	0
4	D	98	0	0	1	0
4	E	95	0	0	2	0
4	F	81	0	0	1	0
All	All	12321	0	11589	176	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 8.

All (176) 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:35:GLN:H	1:A:87:THR:HG22	1.33	0.92
1:D:60:ILE:HD11	1:D:250:ALA:HB1	1.53	0.90
1:F:176:ILE:HD11	1:F:206:ALA:HB3	1.64	0.78
1:A:87:THR:HG21	4:A:1066:HOH:O	1.84	0.75
1:F:53:CYS:SG	1:F:64:VAL:HG22	2.28	0.74
1:C:54:LYS:O	1:C:58:GLU:HG3	1.89	0.72
1:E:55:ARG:HG2	1:E:55:ARG:HH11	1.54	0.71
1:E:197:LEU:O	1:E:200:VAL:HG12	1.91	0.70
1:F:26:LEU:HD13	1:F:65:MET:HE3	1.73	0.69
1:A:176:ILE:HD13	1:A:205:PRO:HB3	1.74	0.69
1:D:54:LYS:O	1:D:58:GLU:HG3	1.93	0.69
1:E:30:VAL:HG11	1:E:127:ILE:HD11	1.76	0.68
1:F:188:LEU:O	1:F:192:PRO:HG3	1.94	0.67
1:A:176:ILE:HD11	1:A:206:ALA:N	2.11	0.66
1:C:235:ARG:O	1:C:239:GLU:HG2	1.94	0.66
1:D:72:TYR:H	1:D:123:ASN:ND2	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:O	1:A:239:GLU:HG3	1.97	0.64
1:A:35:GLN:H	1:A:87:THR:CG2	2.09	0.63
1:B:28:LEU:HD23	1:B:116:LEU:HD21	1.81	0.63
1:F:26:LEU:HD22	1:F:65:MET:HE2	1.81	0.62
1:A:176:ILE:HD11	1:A:206:ALA:H	1.66	0.60
1:F:159:ASP:OD2	1:F:161:ALA:HB3	2.02	0.60
1:D:26:LEU:HD23	1:D:106:LEU:HD22	1.84	0.59
1:F:27:MET:CE	1:F:60:ILE:HD11	2.33	0.59
1:D:62:ALA:C	1:D:63:LEU:HD12	2.28	0.59
1:A:35:GLN:N	1:A:87:THR:HG22	2.12	0.58
1:B:198:ASP:HB2	4:B:1486:HOH:O	2.04	0.57
1:D:249:ILE:O	1:D:253:ILE:HG12	2.04	0.57
1:F:27:MET:HE2	1:F:253:ILE:HD13	1.86	0.57
1:D:214:PHE:HA	1:D:215:PRO:C	2.29	0.57
1:F:27:MET:HB2	1:F:53:CYS:SG	2.44	0.57
1:A:54:LYS:O	1:A:58:GLU:HG3	2.04	0.57
1:B:159:ASP:OD2	1:B:161:ALA:HB3	2.04	0.57
1:F:54:LYS:O	1:F:58:GLU:HG3	2.05	0.57
1:B:235:ARG:O	1:B:239:GLU:HG3	2.04	0.57
1:C:120:HIS:HB3	1:C:123:ASN:ND2	2.21	0.56
1:D:26:LEU:CD2	1:D:106:LEU:HD22	2.34	0.56
1:F:139:ARG:HD3	1:F:144:GLN:HE21	1.71	0.56
1:A:28:LEU:HD23	1:A:116:LEU:CD2	2.36	0.56
1:E:256:GLU:C	1:E:258:PRO:HD3	2.31	0.56
1:D:19:VAL:HG13	4:D:1406:HOH:O	2.05	0.56
1:B:214:PHE:HA	1:B:215:PRO:C	2.32	0.55
1:B:249:ILE:O	1:B:253:ILE:HG12	2.06	0.55
1:F:120:HIS:HB3	1:F:123:ASN:ND2	2.22	0.55
1:A:56:VAL:O	1:A:60:ILE:HG12	2.07	0.55
1:F:7:VAL:HG21	1:F:65:MET:HE2	1.89	0.55
1:E:55:ARG:HG2	1:E:55:ARG:NH1	2.22	0.55
1:F:30:VAL:CG1	1:F:118:ASN:HA	2.37	0.55
1:E:54:LYS:O	1:E:58:GLU:HG3	2.08	0.54
1:D:28:LEU:HD11	1:D:68:LEU:CD1	2.38	0.54
1:E:99:VAL:HG21	1:E:127:ILE:HD13	1.89	0.54
1:F:11:THR:OG1	1:F:14:GLU:HG3	2.08	0.54
1:B:176:ILE:HD11	1:B:206:ALA:N	2.22	0.54
1:E:214:PHE:HA	1:E:215:PRO:C	2.33	0.53
1:A:98:THR:O	1:A:102:ILE:HG12	2.08	0.53
1:C:214:PHE:HA	1:C:215:PRO:C	2.33	0.53
1:F:27:MET:HE1	1:F:56:VAL:HG12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HG13	1:A:227:LEU:HB3	1.91	0.53
1:B:54:LYS:O	1:B:58:GLU:HG3	2.10	0.52
1:E:55:ARG:HH21	1:E:190:LEU:CD2	2.23	0.52
1:C:155:ASP:O	1:C:158:LYS:HD2	2.09	0.52
1:F:27:MET:HE3	1:F:62:ALA:CB	2.40	0.52
1:E:120:HIS:HB3	1:E:123:ASN:ND2	2.25	0.52
1:F:151:LEU:C	1:F:151:LEU:HD12	2.35	0.52
1:A:214:PHE:HA	1:A:215:PRO:C	2.35	0.52
1:D:39:HIS:CD2	1:D:40:MET:HG3	2.45	0.52
1:F:30:VAL:HG13	1:F:118:ASN:HA	1.91	0.51
1:F:214:PHE:HA	1:F:215:PRO:C	2.35	0.51
1:C:256:GLU:C	1:C:258:PRO:HD3	2.36	0.51
1:B:151:LEU:C	1:B:151:LEU:HD12	2.36	0.50
1:A:28:LEU:HD23	1:A:116:LEU:HD21	1.93	0.50
1:F:30:VAL:HG13	1:F:30:VAL:O	2.12	0.50
1:E:43:ASN:O	1:E:46:VAL:HG12	2.12	0.50
1:F:18:ARG:HD3	4:F:1352:HOH:O	2.11	0.50
1:D:35:GLN:NE2	1:D:37:GLY:H	2.10	0.49
1:B:235:ARG:HG2	1:B:235:ARG:HH21	1.76	0.49
1:C:23:ASP:HB2	1:C:113:ARG:NH2	2.26	0.49
1:F:30:VAL:HG11	1:F:127:ILE:HD11	1.94	0.49
1:F:39:HIS:CD2	1:F:40:MET:HG3	2.47	0.49
1:A:120:HIS:HB3	1:A:123:ASN:ND2	2.28	0.49
1:B:11:THR:OG1	1:B:14:GLU:HG3	2.12	0.49
1:B:28:LEU:HD23	1:B:116:LEU:CD2	2.42	0.49
1:B:176:ILE:HD11	1:B:206:ALA:H	1.77	0.49
1:C:55:ARG:HH11	1:C:55:ARG:HG3	1.78	0.49
1:D:24:CYS:SG	1:D:63:LEU:HD13	2.53	0.49
1:F:96:THR:HG22	1:F:126:PHE:O	2.13	0.49
1:B:120:HIS:HB3	1:B:123:ASN:ND2	2.28	0.48
1:A:39:HIS:CD2	1:A:40:MET:HG3	2.48	0.48
1:F:73:LYS:NZ	1:F:91:ASP:HA	2.28	0.48
1:A:34:GLU:HA	1:A:87:THR:HG22	1.96	0.48
1:E:159:ASP:OD2	1:E:161:ALA:HB3	2.13	0.48
1:C:153:TYR:HE1	1:C:182:PHE:HE1	1.61	0.47
1:B:56:VAL:O	1:B:60:ILE:HG12	2.14	0.47
1:C:212:ASP:HB2	1:D:150:VAL:HG13	1.95	0.47
1:F:116:LEU:HD22	1:F:127:ILE:HG23	1.96	0.47
1:A:75:GLN:HG2	1:A:122:GLU:HG2	1.96	0.47
1:F:37:GLY:HA2	1:F:224:PRO:O	2.15	0.46
1:E:183:GLU:HG3	4:E:1186:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLY:HA2	1:C:224:PRO:O	2.16	0.46
1:D:166:LEU:C	1:D:168:PRO:HD3	2.40	0.46
1:E:100:GLN:NE2	1:E:137:GLU:OE2	2.48	0.46
1:A:256:GLU:C	1:A:258:PRO:HD3	2.40	0.46
1:A:153:TYR:HE1	1:A:182:PHE:HE1	1.63	0.46
1:C:39:HIS:CD2	1:C:40:MET:HG3	2.50	0.46
1:C:152:SER:HB2	1:C:155:ASP:OD2	2.16	0.46
1:F:223:ALA:HB3	1:F:224:PRO:HD3	1.98	0.46
1:A:11:THR:OG1	1:A:14:GLU:HG3	2.17	0.45
1:B:139:ARG:HG3	1:B:144:GLN:HE21	1.81	0.45
1:C:242:LEU:O	1:C:246:VAL:HG23	2.17	0.45
1:D:55:ARG:HG3	1:D:55:ARG:HH11	1.81	0.45
1:E:160:PRO:O	1:E:164:GLN:HG3	2.16	0.45
1:F:27:MET:CB	1:F:53:CYS:SG	3.05	0.45
1:E:151:LEU:C	1:E:151:LEU:HD12	2.42	0.45
1:A:83:HIS:H	1:A:83:HIS:CD2	2.34	0.45
1:C:40:MET:HG2	1:C:195:VAL:HG22	1.98	0.45
1:F:92:GLY:O	1:F:96:THR:HG23	2.17	0.45
1:D:11:THR:OG1	1:D:14:GLU:HG3	2.17	0.44
1:D:159:ASP:OD2	1:D:162:VAL:HG23	2.17	0.44
1:E:247:GLN:NE2	4:E:1510:HOH:O	2.51	0.44
1:E:39:HIS:CD2	1:E:40:MET:HG3	2.52	0.44
1:C:111:ALA:HB1	4:C:1502:HOH:O	2.17	0.44
1:D:242:LEU:O	1:D:246:VAL:HG23	2.17	0.44
1:A:158:LYS:O	1:A:159:ASP:C	2.61	0.43
1:A:241:ILE:O	1:A:244:VAL:HG12	2.17	0.43
1:C:183:GLU:HG3	4:C:1473:HOH:O	2.16	0.43
1:E:235:ARG:NH1	1:E:239:GLU:OE2	2.51	0.43
1:C:139:ARG:HD3	1:C:144:GLN:HE21	1.82	0.43
1:D:258:PRO:HA	1:D:259:PRO:HD3	1.85	0.43
1:B:39:HIS:CD2	1:B:40:MET:HG3	2.53	0.43
1:A:153:TYR:CD1	1:A:153:TYR:C	2.96	0.43
1:B:176:ILE:HD13	1:B:205:PRO:HB3	2.01	0.43
1:D:75:GLN:HG2	1:D:122:GLU:HG2	2.01	0.43
1:C:151:LEU:HD12	1:C:151:LEU:C	2.44	0.43
1:A:100:GLN:NE2	1:A:137:GLU:OE2	2.50	0.43
1:A:77:LYS:HE2	1:A:208:PHE:HB3	2.00	0.43
1:B:223:ALA:HB3	1:B:224:PRO:HD3	2.01	0.43
1:C:83:HIS:CD2	1:C:83:HIS:H	2.37	0.43
1:D:223:ALA:N	1:D:224:PRO:HD2	2.34	0.43
1:F:98:THR:O	1:F:102:ILE:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ALA:HB3	1:C:224:PRO:HD3	2.01	0.42
1:D:115:VAL:HG21	1:D:253:ILE:HD12	2.00	0.42
1:F:30:VAL:HG11	1:F:127:ILE:CD1	2.49	0.42
1:A:83:HIS:HE1	4:A:1105:HOH:O	2.02	0.42
1:D:68:LEU:HD12	1:D:68:LEU:N	2.34	0.42
1:E:26:LEU:HD13	1:E:106:LEU:HD22	2.01	0.42
1:E:258:PRO:HA	1:E:259:PRO:HD3	1.92	0.42
1:F:53:CYS:SG	1:F:64:VAL:CG2	3.03	0.42
1:F:53:CYS:SG	1:F:64:VAL:HG13	2.59	0.42
1:E:55:ARG:NH1	1:E:55:ARG:CG	2.83	0.42
1:F:100:GLN:NE2	1:F:137:GLU:OE2	2.50	0.42
1:E:72:TYR:CG	1:E:73:LYS:N	2.88	0.42
1:F:26:LEU:HD13	1:F:106:LEU:HD22	2.02	0.42
1:C:159:ASP:OD2	1:C:162:VAL:HG23	2.20	0.42
1:E:29:PRO:HG2	1:E:67:GLY:CA	2.48	0.42
1:F:7:VAL:HG21	1:F:65:MET:CE	2.51	0.41
1:C:83:HIS:HE1	4:C:1167:HOH:O	2.03	0.41
1:C:208:PHE:HB3	1:C:209:PRO:HD2	2.02	0.41
1:D:151:LEU:HD12	1:D:151:LEU:C	2.45	0.41
1:C:131:ILE:CD1	1:C:150:VAL:HG21	2.51	0.41
1:E:26:LEU:CD1	1:E:106:LEU:HD22	2.50	0.41
1:D:63:LEU:HD12	1:D:63:LEU:N	2.34	0.41
1:A:26:LEU:HD13	1:A:106:LEU:HD22	2.03	0.41
1:B:117:MET:HE2	1:B:249:ILE:HD13	2.03	0.41
1:C:72:TYR:CG	1:C:73:LYS:N	2.89	0.41
1:B:176:ILE:HG13	1:B:227:LEU:HB3	2.02	0.41
1:F:176:ILE:CD1	1:F:227:LEU:HB3	2.50	0.41
1:A:26:LEU:CD1	1:A:106:LEU:HD22	2.51	0.41
1:A:72:TYR:CG	1:A:73:LYS:N	2.88	0.41
1:A:176:ILE:CD1	1:A:205:PRO:HB3	2.48	0.41
1:B:239:GLU:O	1:B:243:GLU:HG3	2.21	0.41
1:A:18:ARG:HD2	1:A:18:ARG:HA	1.88	0.41
1:F:176:ILE:HG13	1:F:227:LEU:O	2.21	0.40
1:A:250:ALA:O	1:A:254:ARG:HG3	2.21	0.40
1:D:71:GLY:HA3	1:D:123:ASN:HD21	1.86	0.40
1:B:176:ILE:HG12	1:B:176:ILE:O	2.21	0.40
1:D:72:TYR:H	1:D:123:ASN:HD21	1.64	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%)	246 (96%)	9 (4%)	0	100	100
1	B	249/260 (96%)	240 (96%)	7 (3%)	2 (1%)	16	11
1	C	250/260 (96%)	243 (97%)	7 (3%)	0	100	100
1	D	255/260 (98%)	250 (98%)	5 (2%)	0	100	100
1	E	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
1	F	255/260 (98%)	251 (98%)	4 (2%)	0	100	100
All	All	1519/1560 (97%)	1479 (97%)	38 (2%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	176	ILE
1	B	124	SER

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	201/215 (94%)	198 (98%)	3 (2%)	57	64
1	B	203/215 (94%)	202 (100%)	1 (0%)	81	87
1	C	206/215 (96%)	205 (100%)	1 (0%)	81	87
1	D	211/215 (98%)	210 (100%)	1 (0%)	81	87
1	E	211/215 (98%)	210 (100%)	1 (0%)	81	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	210/215 (98%)	210 (100%)	0	100	100
All	All	1242/1290 (96%)	1235 (99%)	7 (1%)	78	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	212	ASP
1	A	227	LEU
1	B	212	ASP
1	C	116	LEU
1	D	35	GLN
1	E	116	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	76	GLN
1	A	83	HIS
1	B	75	GLN
1	B	144	GLN
1	C	83	HIS
1	C	144	GLN
1	C	247	GLN
1	D	35	GLN
1	D	76	GLN
1	D	123	ASN
1	D	165	GLN
1	E	76	GLN
1	E	164	GLN
1	F	76	GLN
1	F	144	GLN
1	F	165	GLN
1	F	247	GLN

5.3.3 RNA ⓘ

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 [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 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%)	0.06	22 (8%)	16 15	10, 18, 44, 54	0
1	B	253/260 (97%)	-0.07	15 (5%)	28 27	10, 18, 46, 57	0
1	C	254/260 (97%)	0.05	16 (6%)	26 24	10, 20, 46, 59	0
1	D	257/260 (98%)	0.07	20 (7%)	19 18	11, 19, 43, 53	0
1	E	257/260 (98%)	-0.04	13 (5%)	33 32	11, 19, 39, 46	0
1	F	257/260 (98%)	0.07	19 (7%)	20 19	10, 19, 46, 53	0
All	All	1535/1560 (98%)	0.02	105 (6%)	23 22	10, 19, 44, 59	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	PHE	6.5
1	A	175	ASP	6.4
1	B	175	ASP	5.5
1	A	172	LEU	5.3
1	B	176	ILE	5.2
1	C	172	LEU	5.2
1	B	174	TRP	5.0
1	B	170	GLY	4.9
1	F	53	CYS	4.9
1	C	21	ALA	4.8
1	A	163	ILE	4.7
1	F	176	ILE	4.7
1	D	259	PRO	4.5
1	E	3	LYS	4.5
1	A	174	TRP	4.4
1	A	171	PHE	4.4
1	C	22	GLY	4.2
1	E	259	PRO	4.1
1	F	175	ASP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	169	GLU	3.9
1	A	176	ILE	3.7
1	F	154	PHE	3.7
1	F	164	GLN	3.7
1	A	159	ASP	3.7
1	D	158	LYS	3.7
1	A	3	LYS	3.6
1	C	171	PHE	3.6
1	B	158	LYS	3.6
1	A	21	ALA	3.5
1	D	172	LEU	3.5
1	F	161	ALA	3.4
1	E	164	GLN	3.3
1	A	154	PHE	3.3
1	D	247	GLN	3.2
1	C	175	ASP	3.2
1	D	171	PHE	3.2
1	A	173	GLY	3.1
1	A	160	PRO	3.1
1	B	161	ALA	3.1
1	E	21	ALA	3.1
1	F	172	LEU	3.0
1	F	169	GLU	3.0
1	D	3	LYS	3.0
1	D	164	GLN	3.0
1	B	198	ASP	3.0
1	B	167	TYR	3.0
1	D	22	GLY	2.9
1	E	247	GLN	2.9
1	B	166	LEU	2.9
1	D	175	ASP	2.8
1	A	259	PRO	2.8
1	D	60	ILE	2.8
1	E	255	GLU	2.7
1	C	259	PRO	2.7
1	F	247	GLN	2.7
1	F	255	GLU	2.7
1	F	153	TYR	2.7
1	C	170	GLY	2.7
1	F	174	TRP	2.7
1	D	165	GLN	2.6
1	B	163	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	165	GLN	2.6
1	F	165	GLN	2.6
1	D	152	SER	2.6
1	B	160	PRO	2.5
1	C	197	LEU	2.5
1	E	152	SER	2.5
1	C	163	ILE	2.5
1	A	255	GLU	2.4
1	C	159	ASP	2.4
1	A	162	VAL	2.4
1	D	174	TRP	2.4
1	D	159	ASP	2.4
1	D	202	ASP	2.4
1	C	158	LYS	2.4
1	F	239	GLU	2.3
1	A	235	ARG	2.3
1	A	169	GLU	2.3
1	C	160	PRO	2.3
1	F	160	PRO	2.3
1	D	21	ALA	2.3
1	E	172	LEU	2.3
1	C	165	GLN	2.2
1	B	254	ARG	2.2
1	F	168	PRO	2.2
1	F	170	GLY	2.2
1	B	243	GLU	2.2
1	C	169	GLU	2.2
1	D	168	PRO	2.1
1	E	22	GLY	2.1
1	F	173	GLY	2.1
1	B	159	ASP	2.1
1	F	163	ILE	2.1
1	A	193	ASP	2.1
1	A	258	PRO	2.1
1	C	176	ILE	2.1
1	A	161	ALA	2.1
1	E	175	ASP	2.1
1	D	170	GLY	2.1
1	E	159	ASP	2.0
1	A	22	GLY	2.0
1	A	167	TYR	2.0
1	E	165	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	193	ASP	2.0
1	D	173	GLY	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(Å ²)	Q<0.9
2	MN	C	300	1/1	0.99	0.04	24,24,24,24	0
2	MN	D	300	1/1	0.99	0.06	25,25,25,25	0
2	MN	F	300	1/1	0.99	0.06	26,26,26,26	0
3	ZN	A	301	1/1	0.99	0.09	32,32,32,32	0
3	ZN	C	301	1/1	0.99	0.07	34,34,34,34	0
3	ZN	D	301	1/1	0.99	0.06	31,31,31,31	0
3	ZN	F	301	1/1	0.99	0.09	30,30,30,30	0
3	ZN	B	301	1/1	1.00	0.08	30,30,30,30	0
2	MN	E	300	1/1	1.00	0.04	22,22,22,22	0
2	MN	A	300	1/1	1.00	0.05	23,23,23,23	0
3	ZN	E	301	1/1	1.00	0.05	30,30,30,30	0
2	MN	B	300	1/1	1.00	0.05	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.