



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:22 AM UTC

PDB ID : 4ZGE / pdb_00004zge
Title : Double Mutant H80W/H81W of Fe-Type Nitrile Hydratase from Comamonas testosteroni Ni1
Authors : Wu, R.; Martinez, S.; Holz, R.; Liu, D.
Deposited on : 2015-04-22
Resolution : 2.80 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

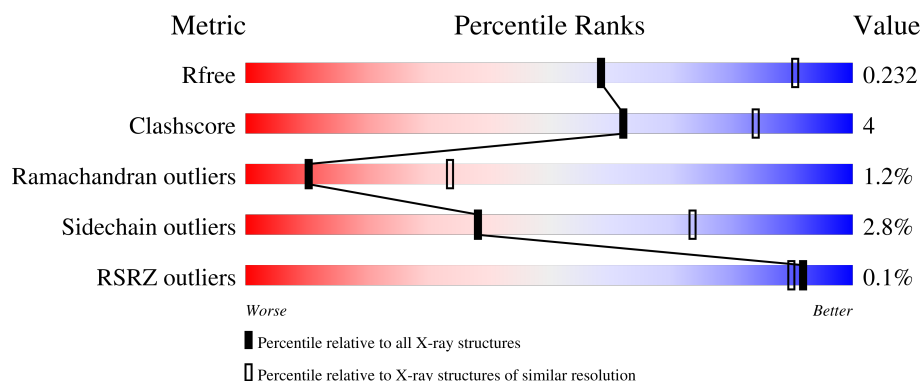
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	206	
1	C	206	
1	E	206	
1	G	206	
1	I	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	206	 86% 13%
1	M	206	 85% 13% .
1	O	206	 88% 11% .
2	B	206	 86% 13% .
2	D	206	 84% 14% .
2	F	206	 85% 13% .
2	H	206	 87% 11% .
2	J	206	 88% 10% .
2	L	206	 85% 13% .
2	N	206	 92% 8%
2	P	206	 90% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26101 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 Nitrile hydratase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			
1	C	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			
1	E	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			
1	G	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			
1	I	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			
1	K	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			
1	M	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			
1	O	206	Total	C	N	O	S	0	0	0
			1617	1036	266	306	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	TRP	HIS	engineered mutation	UNP J9PBS0
A	81	TRP	HIS	engineered mutation	UNP J9PBS0
C	80	TRP	HIS	engineered mutation	UNP J9PBS0
C	81	TRP	HIS	engineered mutation	UNP J9PBS0
E	80	TRP	HIS	engineered mutation	UNP J9PBS0
E	81	TRP	HIS	engineered mutation	UNP J9PBS0
G	80	TRP	HIS	engineered mutation	UNP J9PBS0
G	81	TRP	HIS	engineered mutation	UNP J9PBS0
I	80	TRP	HIS	engineered mutation	UNP J9PBS0
I	81	TRP	HIS	engineered mutation	UNP J9PBS0
K	80	TRP	HIS	engineered mutation	UNP J9PBS0
K	81	TRP	HIS	engineered mutation	UNP J9PBS0
M	80	TRP	HIS	engineered mutation	UNP J9PBS0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	81	TRP	HIS	engineered mutation	UNP J9PBS0
O	80	TRP	HIS	engineered mutation	UNP J9PBS0
O	81	TRP	HIS	engineered mutation	UNP J9PBS0

- Molecule 2 is a protein called Nitrile hydratase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	D	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	F	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	H	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	J	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	L	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	N	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			
2	P	206	Total	C	N	O	S	0	0	0
			1589	1017	271	293	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	PRO	ALA	conflict	UNP J9PBS1
D	112	PRO	ALA	conflict	UNP J9PBS1
F	112	PRO	ALA	conflict	UNP J9PBS1
H	112	PRO	ALA	conflict	UNP J9PBS1
J	112	PRO	ALA	conflict	UNP J9PBS1
L	112	PRO	ALA	conflict	UNP J9PBS1
N	112	PRO	ALA	conflict	UNP J9PBS1
P	112	PRO	ALA	conflict	UNP J9PBS1

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Fe 1	0	0
3	E	1	Total 1	Fe 1	0	0
3	G	1	Total 1	Fe 1	0	0
3	I	1	Total 1	Fe 1	0	0
3	K	1	Total 1	Fe 1	0	0
3	M	1	Total 1	Fe 1	0	0
3	O	1	Total 1	Fe 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	29	Total 29	O 29	0	0
4	C	22	Total 22	O 22	0	0
4	D	34	Total 34	O 34	0	0
4	E	24	Total 24	O 24	0	0
4	F	36	Total 36	O 36	0	0
4	G	25	Total 25	O 25	0	0
4	H	34	Total 34	O 34	0	0
4	I	20	Total 20	O 20	0	0
4	J	33	Total 33	O 33	0	0
4	K	25	Total 25	O 25	0	0
4	L	43	Total 43	O 43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	26	Total 26	O 26	0	0
4	N	25	Total 25	O 25	0	0
4	O	18	Total 18	O 18	0	0
4	P	28	Total 28	O 28	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: Nitrile hydratase alpha subunit

Chain A: 



- Molecule 1: Nitrile hydratase alpha subunit

Chain C: 



- Molecule 1: Nitrile hydratase alpha subunit

Chain E: 



- Molecule 1: Nitrile hydratase alpha subunit

Chain G: 



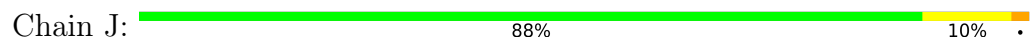
- Molecule 1: Nitrile hydratase alpha subunit

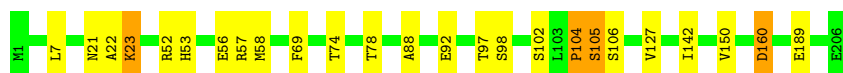
Chain I: 



- Molecule 1: Nitrile hydratase alpha subunit

Chain K: 





- Molecule 2: Nitrile hydratase beta subunit

Chain L: 85% 13% .



- Molecule 2: Nitrile hydratase beta subunit

Chain N: 92% 8%



- Molecule 2: Nitrile hydratase beta subunit

Chain P: 90% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	111.68Å 111.68Å 475.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.84 – 2.80 67.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.84-2.80) 94.0 (67.84-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.181 , 0.229 0.193 , 0.232	Depositor DCC
R_{free} test set	8196 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l 0.457 for h,-h-k,-l 0.457 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26101	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: FE, CSD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/1640	0.85	0/2243
1	C	0.52	0/1640	0.83	0/2243
1	E	0.51	0/1640	0.83	0/2243
1	G	0.52	0/1640	0.87	2/2243 (0.1%)
1	I	0.54	0/1640	0.88	2/2243 (0.1%)
1	K	0.53	0/1640	0.85	0/2243
1	M	0.52	0/1640	0.85	0/2243
1	O	0.50	0/1640	0.87	2/2243 (0.1%)
2	B	0.50	0/1636	0.84	0/2216
2	D	0.52	0/1636	0.91	1/2216 (0.0%)
2	F	0.51	0/1636	0.87	3/2216 (0.1%)
2	H	0.53	0/1636	0.87	4/2216 (0.2%)
2	J	0.52	0/1636	0.87	2/2216 (0.1%)
2	L	0.51	0/1636	0.86	3/2216 (0.1%)
2	N	0.50	0/1636	0.86	0/2216
2	P	0.50	0/1636	0.87	1/2216 (0.0%)
All	All	0.52	0/26208	0.86	20/35672 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	F	0	1
2	H	0	1
2	L	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	82	LYS	N-CA-C	-7.14	99.39	110.17
1	O	90	THR	CA-C-N	-6.20	113.57	120.45
1	O	90	THR	C-N-CA	-6.20	113.57	120.45
1	G	90	THR	CA-C-N	-5.94	113.69	119.87
1	G	90	THR	C-N-CA	-5.94	113.69	119.87

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	21	ASN	Peptide
2	F	21	ASN	Peptide
2	H	21	ASN	Peptide
2	L	21	ASN	Peptide

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	1617	0	1598	13	1
1	C	1617	0	1598	15	0
1	E	1617	0	1598	19	1
1	G	1617	0	1597	12	0
1	I	1617	0	1597	14	0
1	K	1617	0	1598	14	0
1	M	1617	0	1597	20	0
1	O	1617	0	1598	10	0
2	B	1589	0	1534	18	0
2	D	1589	0	1534	16	0
2	F	1589	0	1534	14	0
2	H	1589	0	1534	14	0
2	J	1589	0	1534	14	0
2	L	1589	0	1534	15	0
2	N	1589	0	1534	11	0
2	P	1589	0	1534	10	0
3	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
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
4	A	23	0	0	0	0
4	B	29	0	0	4	0
4	C	22	0	0	2	0
4	D	34	0	0	0	0
4	E	24	0	0	1	0
4	F	36	0	0	0	0
4	G	25	0	0	2	0
4	H	34	0	0	0	0
4	I	20	0	0	1	0
4	J	33	0	0	1	0
4	K	25	0	0	1	0
4	L	43	0	0	1	0
4	M	26	0	0	3	0
4	N	25	0	0	0	0
4	O	18	0	0	0	0
4	P	28	0	0	0	0
All	All	26101	0	25053	207	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 207 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:C:192:GLU:OE2	4:C:401:HOH:O	2.03	0.76
2:H:114:GLY:HA3	2:H:199:GLN:HE21	1.52	0.73
2:B:119:PHE:O	4:B:301:HOH:O	2.07	0.72
2:J:92:GLU:HG2	2:J:98:SER:HA	1.72	0.72
2:F:174:TYR:HE1	2:F:199:GLN:HG3	1.54	0.72

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:NZ	1:E:206:GLY:O[1_655]	2.11	0.09

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	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	55
1	C	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	12	38
1	E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	38
1	G	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	38
1	I	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	12	38
1	K	202/206 (98%)	193 (96%)	6 (3%)	3 (2%)	8	28
1	M	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	55
1	O	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	55
2	B	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	24	55
2	D	204/206 (99%)	192 (94%)	7 (3%)	5 (2%)	4	16
2	F	204/206 (99%)	192 (94%)	8 (4%)	4 (2%)	6	21
2	H	204/206 (99%)	191 (94%)	9 (4%)	4 (2%)	6	21
2	J	204/206 (99%)	192 (94%)	8 (4%)	4 (2%)	6	21
2	L	204/206 (99%)	193 (95%)	7 (3%)	4 (2%)	6	21
2	N	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	12	38
2	P	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	12	38
All	All	3248/3296 (98%)	3080 (95%)	128 (4%)	40 (1%)	10	34

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	103	SER
2	D	106	SER
1	I	103	SER
1	M	103	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	172/172 (100%)	166 (96%)	6 (4%)	32	67
1	C	172/172 (100%)	169 (98%)	3 (2%)	53	83
1	E	172/172 (100%)	166 (96%)	6 (4%)	32	67
1	G	172/172 (100%)	167 (97%)	5 (3%)	37	73
1	I	172/172 (100%)	168 (98%)	4 (2%)	44	78
1	K	172/172 (100%)	168 (98%)	4 (2%)	44	78
1	M	172/172 (100%)	168 (98%)	4 (2%)	44	78
1	O	172/172 (100%)	165 (96%)	7 (4%)	27	62
2	B	164/165 (99%)	158 (96%)	6 (4%)	30	65
2	D	164/165 (99%)	157 (96%)	7 (4%)	26	60
2	F	164/165 (99%)	157 (96%)	7 (4%)	26	60
2	H	164/165 (99%)	160 (98%)	4 (2%)	43	77
2	J	164/165 (99%)	162 (99%)	2 (1%)	63	87
2	L	164/165 (99%)	158 (96%)	6 (4%)	30	65
2	N	164/165 (99%)	163 (99%)	1 (1%)	78	92
2	P	164/165 (99%)	161 (98%)	3 (2%)	51	82
All	All	2688/2696 (100%)	2613 (97%)	75 (3%)	38	73

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	188	VAL
2	L	160	ASP
1	O	37	MET
1	E	108	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	126	HIS
2	J	194	HIS
2	P	199	GLN
2	L	126	HIS
2	H	5	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	A	102	3,1	4,7,8	0.74	0	1,8,10	2.96	1 (100%)
1	CSD	G	104	3,1	4,7,8	0.93	0	1,8,10	1.21	0
1	CSD	M	102	3,1	4,7,8	0.69	0	1,8,10	3.01	1 (100%)
1	CSD	O	102	3,1	4,7,8	0.66	0	1,8,10	3.07	1 (100%)
1	CSD	E	102	3,1	4,7,8	0.64	0	1,8,10	2.03	1 (100%)
1	CSD	E	104	3,1	4,7,8	0.87	0	1,8,10	1.04	0
1	CSD	M	104	3,1	4,7,8	1.05	0	1,8,10	1.06	0
1	CSD	K	102	3,1	4,7,8	0.53	0	1,8,10	3.14	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	I	102	3,1	4,7,8	0.78	0	1,8,10	2.79	1 (100%)
1	CSD	K	104	3,1	4,7,8	0.89	0	1,8,10	0.75	0
1	CSD	A	104	3,1	4,7,8	0.91	0	1,8,10	0.40	0
1	CSD	O	104	3,1	4,7,8	0.87	0	1,8,10	2.31	1 (100%)
1	CSD	C	104	3,1	4,7,8	0.97	0	1,8,10	1.58	0
1	CSD	G	102	3,1	4,7,8	0.67	0	1,8,10	1.34	0
1	CSD	C	102	3,1	4,7,8	0.61	0	1,8,10	2.34	1 (100%)
1	CSD	I	104	3,1	4,7,8	0.93	0	1,8,10	1.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	102	3,1	-	1/2/6/8	-
1	CSD	G	104	3,1	-	1/2/6/8	-
1	CSD	M	102	3,1	-	0/2/6/8	-
1	CSD	O	102	3,1	-	0/2/6/8	-
1	CSD	E	102	3,1	-	0/2/6/8	-
1	CSD	E	104	3,1	-	0/2/6/8	-
1	CSD	M	104	3,1	-	1/2/6/8	-
1	CSD	K	102	3,1	-	0/2/6/8	-
1	CSD	I	102	3,1	-	0/2/6/8	-
1	CSD	K	104	3,1	-	1/2/6/8	-
1	CSD	A	104	3,1	-	0/2/6/8	-
1	CSD	O	104	3,1	-	0/2/6/8	-
1	CSD	C	104	3,1	-	0/2/6/8	-
1	CSD	G	102	3,1	-	0/2/6/8	-
1	CSD	C	102	3,1	-	0/2/6/8	-
1	CSD	I	104	3,1	-	0/2/6/8	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	102	CSD	OD1-SG-CB	3.14	111.38	105.60
1	O	102	CSD	OD1-SG-CB	3.07	111.26	105.60
1	M	102	CSD	OD1-SG-CB	3.01	111.15	105.60
1	A	102	CSD	OD1-SG-CB	2.96	111.06	105.60
1	I	102	CSD	OD1-SG-CB	2.79	110.74	105.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	102	CSD	N-CA-CB-SG
1	G	104	CSD	CA-CB-SG-OD1
1	K	104	CSD	CA-CB-SG-OD1
1	M	104	CSD	CA-CB-SG-OD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	102	CSD	1	0
1	C	102	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	204/206 (99%)	-1.65	1 (0%) 87 82	31, 45, 65, 100	0
1	C	204/206 (99%)	-1.61	0 100 100	32, 47, 70, 87	1 (0%)
1	E	204/206 (99%)	-1.58	0 100 100	35, 46, 69, 82	1 (0%)
1	G	204/206 (99%)	-1.63	0 100 100	33, 47, 71, 81	1 (0%)
1	I	204/206 (99%)	-1.64	0 100 100	33, 45, 64, 84	0
1	K	204/206 (99%)	-1.61	0 100 100	34, 47, 71, 83	1 (0%)
1	M	204/206 (99%)	-1.62	1 (0%) 87 82	32, 46, 63, 104	0
1	O	204/206 (99%)	-1.64	1 (0%) 87 82	33, 45, 65, 97	0
2	B	206/206 (100%)	-1.62	0 100 100	31, 46, 75, 92	0
2	D	206/206 (100%)	-1.61	0 100 100	32, 45, 75, 86	0
2	F	206/206 (100%)	-1.59	0 100 100	31, 45, 75, 88	0
2	H	206/206 (100%)	-1.62	0 100 100	32, 45, 73, 89	0
2	J	206/206 (100%)	-1.63	0 100 100	32, 46, 74, 89	0
2	L	206/206 (100%)	-1.60	0 100 100	33, 45, 74, 84	0
2	N	206/206 (100%)	-1.62	0 100 100	30, 46, 74, 90	0
2	P	206/206 (100%)	-1.57	0 100 100	31, 47, 75, 94	0
All	All	3280/3296 (99%)	-1.61	3 (0%) 92 90	30, 46, 72, 104	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ALA	3.1
1	M	207	ALA	2.8
1	O	207	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	A	102	8/9	1.00	0.02	40,43,47,48	0
1	CSD	A	104	8/9	1.00	0.03	48,50,52,53	0
1	CSD	C	102	8/9	1.00	0.02	39,43,50,50	0
1	CSD	C	104	8/9	1.00	0.03	45,48,50,53	0
1	CSD	E	102	8/9	1.00	0.02	41,47,53,55	0
1	CSD	E	104	8/9	1.00	0.02	46,48,53,55	0
1	CSD	G	102	8/9	1.00	0.02	40,46,49,49	0
1	CSD	G	104	8/9	1.00	0.02	49,51,53,54	0
1	CSD	I	102	8/9	1.00	0.02	40,44,49,51	0
1	CSD	I	104	8/9	1.00	0.02	48,50,54,55	0
1	CSD	K	102	8/9	1.00	0.02	41,44,50,53	0
1	CSD	K	104	8/9	1.00	0.02	46,48,54,54	0
1	CSD	M	102	8/9	1.00	0.02	40,43,47,49	0
1	CSD	M	104	8/9	1.00	0.03	45,46,47,48	0
1	CSD	O	102	8/9	1.00	0.02	36,44,45,45	0
1	CSD	O	104	8/9	1.00	0.03	49,52,55,55	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	FE	A	301	1/1	1.00	0.01	42,42,42,42	0
3	FE	C	301	1/1	1.00	0.01	51,51,51,51	0
3	FE	E	301	1/1	1.00	0.01	55,55,55,55	0
3	FE	G	301	1/1	1.00	0.01	55,55,55,55	0
3	FE	I	301	1/1	1.00	0.01	45,45,45,45	0
3	FE	K	301	1/1	1.00	0.01	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FE	M	301	1/1	1.00	0.01	47,47,47,47	0
3	FE	O	301	1/1	1.00	0.01	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.