W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:07 am GMT

PDB ID : 4X1C
Title : Crystal structure of 4-OT from Pseudomonas putida mt-2 with an enamine adduct on the N-terminal proline at 1.7 Angstrom resolution
Authors : Thunnissen, A.M.W.H.; Poddar, H.
Deposited on : 2014-11-24
Resolution : 1.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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.
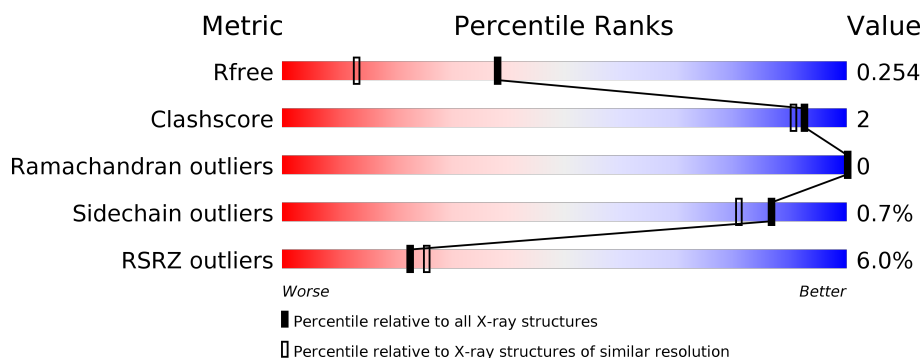
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	62	2% / 92% / · 6%
1	B	62	89% / · 10%
1	D	62	5% / 85% / 10% / 5%
1	E	62	3% / 90% / 5% 5%
1	F	62	2% / 87% / 5% 8%
1	I	62	6% / 89% / · 8%

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Mol	Chain	Length	Quality of chain
1	J	62	2% ... 87% ... 5% 8%
1	M	62	8% ... 87% ... 8%
1	N	62	16% ... 82% ... 11% 6%
1	O	62	21% ... 92% ... 6%
2	C	62	2% ... 90% ... 6%
2	G	62	5% ... 90% ... 8%
2	H	62	5% ... 97%
2	K	62	3% ... 89% ... 8%
2	L	62	5% ... 85% ... 6% 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6990 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 2-hydroxymuconate tautomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	58	Total	C	N	O	S	0	0	0
			441	275	78	87	1			
1	B	56	Total	C	N	O	S	0	2	0
			446	279	82	84	1			
1	D	59	Total	C	N	O	S	0	0	0
			450	281	80	88	1			
1	E	59	Total	C	N	O	S	0	0	0
			450	281	80	88	1			
1	F	57	Total	C	N	O	S	0	0	0
			435	272	77	85	1			
1	I	57	Total	C	N	O	S	0	0	0
			435	272	77	85	1			
1	J	57	Total	C	N	O	S	0	0	0
			435	272	77	85	1			
1	M	57	Total	C	N	O	S	0	0	0
			435	272	77	85	1			
1	N	58	Total	C	N	O	S	0	1	0
			447	279	79	88	1			
1	O	58	Total	C	N	O	S	0	0	0
			441	275	78	87	1			

- Molecule 2 is a protein called 2-hydroxymuconate tautomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	58	Total	C	N	O	S	0	0	0
			439	273	78	87	1			
2	G	61	Total	C	N	O	S	0	0	0
			466	290	85	90	1			
2	H	62	Total	C	N	O	S	0	0	0
			477	296	89	91	1			
2	K	57	Total	C	N	O	S	0	0	0
			433	270	77	85	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	57	Total 441	C 275	N 80	O 85	S 1	0	1	0

- Molecule 3 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).
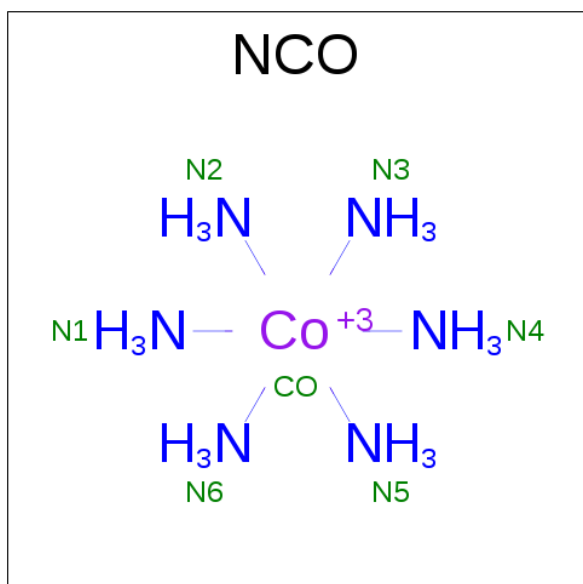
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 7	Co 1	N 6	0	0
3	F	1	Total 7	Co 1	N 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total 27	O 27	0	0
4	B	28	Total 28	O 28	0	0
4	C	33	Total 33	O 33	0	0
4	D	23	Total 23	O 23	0	0
4	E	26	Total 26	O 26	0	0
4	F	32	Total 32	O 32	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	18	Total 18	O 18	0	0
4	H	16	Total 16	O 16	0	0
4	I	23	Total 23	O 23	0	0
4	J	16	Total 16	O 16	0	0
4	K	17	Total 17	O 17	0	0
4	L	9	Total 9	O 9	0	0
4	M	13	Total 13	O 13	0	0
4	N	11	Total 11	O 11	0	0
4	O	13	Total 13	O 13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: 2-hydroxymuconate tautomerase
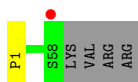
Chain A:

- Molecule 1: 2-hydroxymuconate tautomerase

Chain B:

- Molecule 1: 2-hydroxymuconate tautomerase

Chain D:

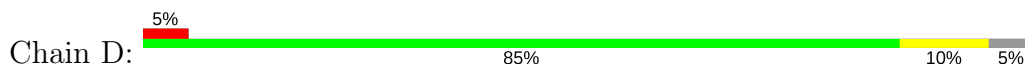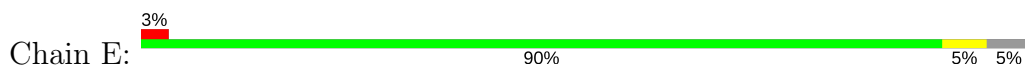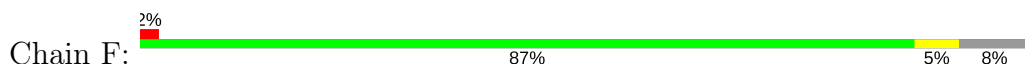- Molecule 1: 2-hydroxymuconate tautomerase

Chain E:

- Molecule 1: 2-hydroxymuconate tautomerase

Chain F:

- Molecule 1: 2-hydroxymuconate tautomerase

Chain I:

P1 E22 R29 S30 L31 P34 R39 A57 SER LYS VAL ARG ARG

• Molecule 1: 2-hydroxymuconate tautomerase

Chain J:

2%

87%　　　　　　　　　　　5%　　8%

P1 E9 E44 K47 A57 SER LYS VAL ARG ARG

• Molecule 1: 2-hydroxymuconate tautomerase

Chain M:

8%

87%　　　　　　　　　　　　　• •　　8%

P1 E25 A26 I27 S28 R29 D32 T36 I52 A57 SER LYS VAL ARG ARG

• Molecule 1: 2-hydroxymuconate tautomerase

Chain N:

16%

82%　　　　　　　　11%　　6%

P1 E9 E14 I20 R21 E22 E25 R29 D32 A33 P34 L35 T36 S37 V38 I42 T43 E44 E55 S58 LYS VAL ARG ARG

• Molecule 1: 2-hydroxymuconate tautomerase

Chain O:

21%

92%　　　　　　　　　　•　　6%

P1 Q15 R21 E22 V23 A26 L35 T36 S37 V38 K47 E55 L56 A57 S58 LYS VAL ARG ARG

• Molecule 2: 2-hydroxymuconate tautomerase

Chain C:

2%

90%　　　　　　　　　•　　6%

P1 E9 E44 A57 S58 LYS VAL ARG ARG

• Molecule 2: 2-hydroxymuconate tautomerase

Chain G:

5%

90%　　　　　　　　　8%　•

P1 I20 D32 I42 I52 K59 V60 R61 ARG

• Molecule 2: 2-hydroxymuconate tautomerase
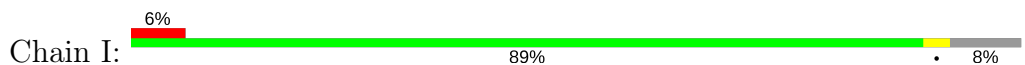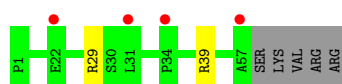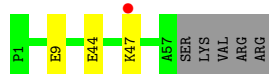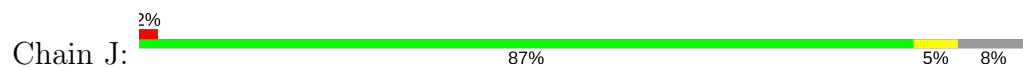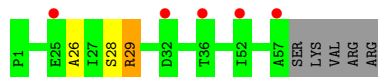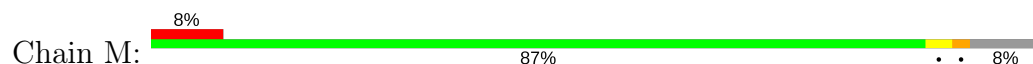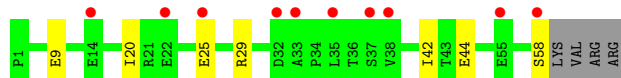
Chain H:

5%

97%　　　　　　　　　　　•

• Molecule 2: 2-hydroxymuconate tautomerase

Chain K:

• Molecule 2: 2-hydroxymuconate tautomerase

Chain L:
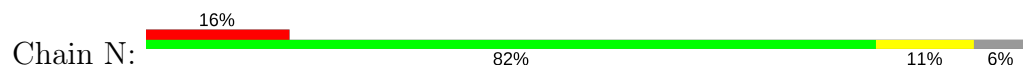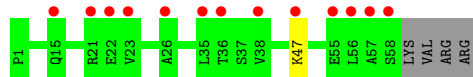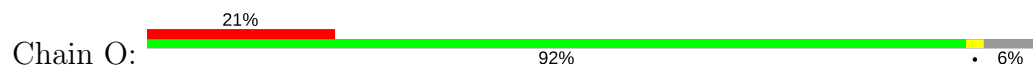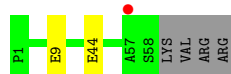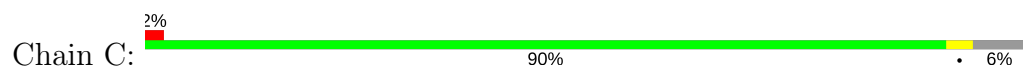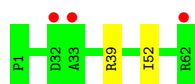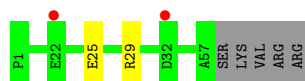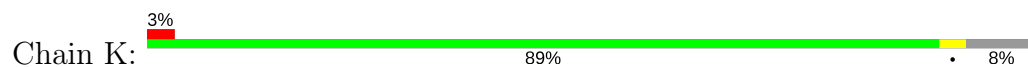
4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	55.29Å　85.13Å　170.91Å 90.00°　96.91°　90.00°	Depositor
Resolution (Å)	42.56　–　1.70 46.13　–　1.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (42.56-1.70) 95.0 (46.13-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.70Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196　,　0.227 0.236　,　0.254	Depositor DCC
R_{free} test set	4142 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6990	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: N80, NCO

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	0.27	0/435	0.50	0/584
1	B	0.28	0/446	0.51	0/597
1	D	0.27	0/444	0.53	0/595
1	E	0.26	0/444	0.51	0/595
1	F	0.36	0/429	0.56	0/576
1	I	0.34	0/429	0.53	0/576
1	J	0.25	0/429	0.47	0/576
1	M	0.98	2/429 (0.5%)	0.66	1/576 (0.2%)
1	N	0.28	0/444	0.53	0/596
1	O	0.24	0/435	0.45	0/584
2	C	0.28	0/443	0.53	0/595
2	G	0.25	0/470	0.46	0/630
2	H	0.34	0/481	0.54	0/644
2	K	0.37	0/437	0.51	0/587
2	L	0.25	0/448	0.49	0/601
All	All	0.38	2/6643 (0.0%)	0.52	1/8912 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	29	ARG	C-N	-15.62	0.98	1.34
1	M	28	SER	C-N	11.82	1.61	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	28	SER	C-N-CA	-7.42	103.14	121.70

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	441	0	453	1	0
1	B	446	0	470	0	0
1	D	450	0	467	4	0
1	E	450	0	467	2	0
1	F	435	0	449	1	1
1	I	435	0	449	1	0
1	J	435	0	449	2	0
1	M	435	0	447	1	0
1	N	447	0	461	3	0
1	O	441	0	454	1	0
2	C	439	0	453	2	0
2	G	466	0	488	4	0
2	H	477	0	501	3	0
2	K	433	0	448	0	0
2	L	441	0	461	4	0
3	B	7	0	0	0	0
3	F	7	0	0	1	0
4	A	27	0	0	1	0
4	B	28	0	0	0	0
4	C	33	0	0	0	0
4	D	23	0	0	1	0
4	E	26	0	0	0	0
4	F	32	0	0	0	0
4	G	18	0	0	0	0
4	H	16	0	0	0	0
4	I	23	0	0	0	0
4	J	16	0	0	0	0
4	K	17	0	0	0	0
4	L	9	0	0	0	0
4	M	13	0	0	0	0
4	N	11	0	0	0	0
4	O	13	0	0	0	0
All	All	6990	0	6917	24	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 2.

All (24) 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:F:25:GLU:OE2	3:F:101:NCO:N1	2.05	0.90
2:G:52:ILE:HG23	2:H:39:ARG:CZ	2.27	0.65
2:G:20:ILE:HG13	2:G:42:ILE:HD11	1.84	0.59
2:L:9:GLU:CG	2:L:44:GLU:HB3	2.40	0.52
1:D:52:ILE:HG23	1:E:39:ARG:NH1	2.26	0.50
2:H:52:ILE:HG23	1:I:39:ARG:CZ	2.43	0.49
4:A:106:HOH:O	1:D:1:N80:H9	2.13	0.47
1:N:20:ILE:HG13	1:N:42:ILE:HD11	1.95	0.47
1:J:9:GLU:HG2	1:J:44:GLU:HB3	1.96	0.47
2:L:9:GLU:HG2	2:L:44:GLU:HB3	1.96	0.46
2:C:9:GLU:HG2	2:C:44:GLU:HB3	1.98	0.45
1:N:9:GLU:HG2	1:N:44:GLU:HB3	1.99	0.45
2:L:20:ILE:HG13	2:L:42:ILE:HD11	1.99	0.45
1:A:1:N80:H9	4:D:120:HOH:O	2.17	0.45
2:G:52:ILE:HG23	2:H:39:ARG:NH1	2.32	0.44
1:M:26:ALA:HA	1:M:29:ARG:NH1	2.34	0.43
1:D:20:ILE:HG13	1:D:42:ILE:HD11	2.00	0.43
2:C:9:GLU:CG	2:C:44:GLU:HB3	2.49	0.42
1:E:20:ILE:HG13	1:E:42:ILE:HD11	2.02	0.41
1:D:47:LYS:HB3	1:D:58:SER:HB3	2.03	0.41
1:N:25:GLU:HG2	1:N:29:ARG:HH11	1.85	0.41
2:G:60:VAL:HG23	2:G:61:ARG:HG2	2.02	0.41
2:L:9:GLU:HG3	2:L:44:GLU:HB3	2.01	0.41
1:J:47:LYS:NZ	1:O:47:LYS:HD2	2.36	0.40

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:F:29:ARG:NH1	1:F:32:ASP:OD1[2_455]	1.66	0.54

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	56/62 (90%)	56 (100%)	0	0	100	100
1	B	56/62 (90%)	56 (100%)	0	0	100	100
1	D	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	E	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
1	F	55/62 (89%)	55 (100%)	0	0	100	100
1	I	55/62 (89%)	55 (100%)	0	0	100	100
1	J	55/62 (89%)	55 (100%)	0	0	100	100
1	M	55/62 (89%)	55 (100%)	0	0	100	100
1	N	57/62 (92%)	57 (100%)	0	0	100	100
1	O	56/62 (90%)	56 (100%)	0	0	100	100
2	C	56/62 (90%)	56 (100%)	0	0	100	100
2	G	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
2	H	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
2	K	55/62 (89%)	55 (100%)	0	0	100	100
2	L	56/62 (90%)	56 (100%)	0	0	100	100
All	All	845/930 (91%)	841 (100%)	4 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	47/51 (92%)	47 (100%)	0	100	100
1	B	48/51 (94%)	46 (96%)	2 (4%)	34	14
1	D	48/51 (94%)	48 (100%)	0	100	100
1	E	48/51 (94%)	48 (100%)	0	100	100
1	F	46/51 (90%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	46/51 (90%)	45 (98%)	1 (2%)	57	38
1	J	46/51 (90%)	46 (100%)	0	100	100
1	M	46/51 (90%)	46 (100%)	0	100	100
1	N	48/51 (94%)	47 (98%)	1 (2%)	59	40
1	O	47/51 (92%)	47 (100%)	0	100	100
2	C	48/52 (92%)	48 (100%)	0	100	100
2	G	51/52 (98%)	51 (100%)	0	100	100
2	H	52/52 (100%)	52 (100%)	0	100	100
2	K	47/52 (90%)	45 (96%)	2 (4%)	33	13
2	L	48/52 (92%)	48 (100%)	0	100	100
All	All	716/770 (93%)	710 (99%)	6 (1%)	87	78

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29[A]	ARG
1	B	29[B]	ARG
1	I	29	ARG
2	K	25	GLU
2	K	29	ARG
1	N	58	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	N80	A	1	-	8,9,10	1.02	0	4,11,13	2.89	2 (50%)
1	N80	B	1	1	8,9,10	0.80	0	4,11,13	2.01	1 (25%)
1	N80	D	1	1	8,9,10	0.94	1 (12%)	4,11,13	1.95	1 (25%)
1	N80	E	1	1	8,9,10	0.92	0	4,11,13	1.96	1 (25%)
1	N80	F	1	1	8,9,10	0.85	0	4,11,13	1.71	1 (25%)
1	N80	I	1	1	8,9,10	0.95	1 (12%)	4,11,13	2.31	2 (50%)
1	N80	J	1	1	8,9,10	0.91	0	4,11,13	1.97	1 (25%)
1	N80	M	1	-	8,9,10	1.49	2 (25%)	4,11,13	2.86	2 (50%)
1	N80	N	1	-	8,9,10	1.25	1 (12%)	4,11,13	2.64	2 (50%)
1	N80	O	1	1	8,9,10	1.14	1 (12%)	4,11,13	2.21	1 (25%)

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	N80	A	1	-	-	0/0/14/16	0/1/1/1
1	N80	B	1	1	-	0/0/14/16	0/1/1/1
1	N80	D	1	1	-	0/0/14/16	0/1/1/1
1	N80	E	1	1	-	0/0/14/16	0/1/1/1
1	N80	F	1	1	-	0/0/14/16	0/1/1/1
1	N80	I	1	1	-	0/0/14/16	0/1/1/1
1	N80	J	1	1	-	0/0/14/16	0/1/1/1
1	N80	M	1	-	-	0/0/14/16	0/1/1/1
1	N80	N	1	-	-	0/0/14/16	0/1/1/1
1	N80	O	1	1	-	0/0/14/16	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1	N80	CA-N	-2.66	1.45	1.47
1	M	1	N80	CA-N	-2.18	1.45	1.47
1	D	1	N80	CA-C	2.02	1.52	1.50
1	I	1	N80	CA-C	2.09	1.53	1.50
1	O	1	N80	CA-C	2.84	1.54	1.50
1	M	1	N80	CA-C	2.88	1.54	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	N80	O-C-CA	-3.98	112.04	124.50
1	A	1	N80	O-C-CA	-3.91	112.25	124.50
1	M	1	N80	CD-N-CAD	-3.79	111.42	123.23
1	O	1	N80	CD-N-CAD	-3.72	111.62	123.23
1	M	1	N80	O-C-CA	-3.53	113.42	124.50
1	A	1	N80	CD-N-CAD	-3.51	112.27	123.23
1	I	1	N80	CD-N-CAD	-3.34	112.82	123.23
1	J	1	N80	CD-N-CAD	-3.17	113.33	123.23
1	B	1	N80	CD-N-CAD	-3.14	113.43	123.23
1	E	1	N80	CD-N-CAD	-3.07	113.66	123.23
1	N	1	N80	CB-CA-C	-2.92	108.69	112.70
1	D	1	N80	CD-N-CAD	-2.83	114.41	123.23
1	I	1	N80	CB-CA-C	-2.40	109.40	112.70
1	F	1	N80	CB-CA-C	-2.14	109.75	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	N80	1	0
1	D	1	N80	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	$\#|Z| > 2$
3	NCO	B	101	-	6,6,6	0.41	0	0,15,15	0.00	-
3	NCO	F	101	-	6,6,6	0.15	0	0,15,15	0.00	-

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	NCO	B	101	-	-	0/0/0/0	0/0/0/0
3	NCO	F	101	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	101	NCO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	3
1	A	1
1	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	28:SER	C	29:ARG	N	1.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1:N80	C	2:ILE	N	1.18
1	N	1:N80	C	2:ILE	N	1.16
1	M	1:N80	C	2:ILE	N	1.09
1	M	29:ARG	C	30:SER	N	0.98

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	57/62 (91%)	-0.04	1 (1%)	69	74	21, 32, 51, 74	0
1	B	55/62 (88%)	0.04	0	100	100	21, 33, 50, 62	0
1	D	58/62 (93%)	-0.04	3 (5%)	28	31	22, 37, 60, 73	0
1	E	58/62 (93%)	0.25	2 (3%)	46	52	23, 37, 61, 83	0
1	F	56/62 (90%)	0.11	1 (1%)	69	74	23, 36, 57, 67	0
1	I	56/62 (90%)	0.42	4 (7%)	17	20	27, 45, 70, 81	0
1	J	56/62 (90%)	0.24	1 (1%)	69	74	26, 46, 71, 80	0
1	M	56/62 (90%)	0.73	5 (8%)	10	12	26, 53, 78, 83	0
1	N	57/62 (91%)	0.85	10 (17%)	2	2	30, 51, 76, 81	0
1	O	57/62 (91%)	1.27	13 (22%)	1	1	38, 67, 86, 100	0
2	C	58/62 (93%)	0.08	1 (1%)	70	75	20, 34, 58, 75	0
2	G	61/62 (98%)	0.26	3 (4%)	30	35	26, 38, 59, 77	0
2	H	62/62 (100%)	0.45	3 (4%)	31	36	26, 44, 68, 78	0
2	K	57/62 (91%)	0.49	2 (3%)	44	50	29, 47, 67, 78	0
2	L	57/62 (91%)	0.80	3 (5%)	27	31	29, 55, 74, 79	0
All	All	861/930 (92%)	0.39	52 (6%)	23	25	20, 42, 75, 100	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	58	SER	4.6
1	O	55	GLU	4.6
1	N	32	ASP	4.0
1	E	58	SER	3.8
2	K	22	GLU	3.4
2	L	47	LYS	3.2
2	L	57	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	55	GLU	2.9
1	M	57	ALA	2.9
1	O	36	THR	2.9
1	O	22	GLU	2.9
2	H	62	ARG	2.8
1	A	58	SER	2.8
1	E	59	LYS	2.8
1	O	35	LEU	2.8
1	J	47	LYS	2.8
2	G	59	LYS	2.8
1	D	57	ALA	2.7
1	O	21	ARG	2.6
2	C	57	ALA	2.5
1	N	37	SER	2.5
2	H	32	ASP	2.5
2	K	32	ASP	2.5
1	D	59	LYS	2.4
2	H	33	ALA	2.4
1	F	29	ARG	2.4
1	N	33	ALA	2.4
1	O	58	SER	2.4
2	G	60	VAL	2.4
1	M	25	GLU	2.3
1	N	25	GLU	2.3
1	O	26	ALA	2.3
1	M	32	ASP	2.3
1	N	38	VAL	2.3
1	O	47	LYS	2.3
1	O	56	LEU	2.2
1	O	57	ALA	2.2
1	I	57	ALA	2.2
1	N	35	LEU	2.1
1	O	15	GLN	2.1
1	I	34	PRO	2.1
1	N	14	GLU	2.1
1	O	38	VAL	2.1
1	M	52	ILE	2.1
1	M	36	THR	2.1
1	I	31	LEU	2.1
1	I	22	GLU	2.0
1	O	23	VAL	2.0
1	D	58	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	15	GLN	2.0
2	G	32	ASP	2.0
1	N	22	GLU	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	N80	F	1	9/10	0.91	0.10	-	25,34,68,80	0
1	N80	E	1	9/10	0.93	0.10	-	25,36,56,71	0
1	N80	O	1	9/10	0.81	0.13	-	44,52,65,71	0
1	N80	B	1	9/10	0.95	0.08	-	21,28,57,62	0
1	N80	A	1	9/10	0.96	0.07	-	22,30,49,68	0
1	N80	N	1	9/10	0.73	0.14	-	37,44,54,63	0
1	N80	M	1	9/10	0.84	0.13	-	30,40,70,71	0
1	N80	J	1	9/10	0.95	0.09	-	30,33,67,69	0
1	N80	I	1	9/10	0.84	0.12	-	36,49,69,75	0
1	N80	D	1	9/10	0.94	0.10	-	23,31,56,74	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	NCO	B	101	7/7	0.97	0.17	1.64	32,42,55,63	0
3	NCO	F	101	7/7	0.95	0.19	0.98	43,47,80,93	0

6.5 Other polymers ⓘ

There are no such residues in this entry.