W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2023 – 09:29 AM EDT

PDB ID	:	5K8P
Title	:	Zn2+/Tetrahedral intermediate-bound R289A 5-nitroanthranilate aminohydrolase
Authors	:	Kalyoncu, S.
Deposited on	:	2016-05-30
Resolution	:	2.20 Å(reported)

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

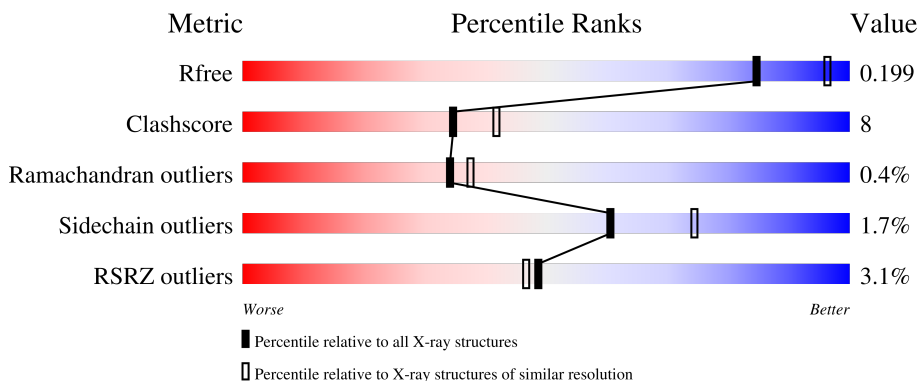|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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.
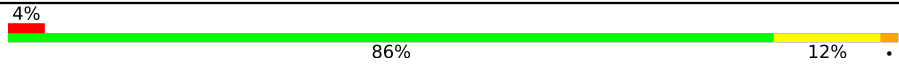
Metric	Percentile Ranks	Value
Rfree		0.199
Clashscore		8
Ramachandran outliers		0.4%
Sidechain outliers		1.7%
RSRZ outliers		3.1%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	425	4% — 82% / 16% / ••
1	B	425	2% — 87% / 11% / ••
1	C	425	3% — 84% / 14% / ••
1	D	425	5% — 84% / 16%
1	E	425	% — 89% / 10% / •

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	F	425	4% 86% 12%
1	G	425	3% 79% 19%
1	H	425	2% 87% 12%

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 27782 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 5-nitroanthranilic acid aminohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3229	2043	559	608	19			
1	B	421	Total	C	N	O	S	0	0	0
			3229	2043	559	608	19			
1	C	422	Total	C	N	O	S	0	0	0
			3235	2046	560	610	19			
1	D	425	Total	C	N	O	S	0	0	0
			3252	2056	563	613	20			
1	E	423	Total	C	N	O	S	0	0	0
			3239	2048	561	611	19			
1	F	425	Total	C	N	O	S	0	0	0
			3252	2056	563	613	20			
1	G	421	Total	C	N	O	S	0	0	0
			3229	2043	559	608	19			
1	H	422	Total	C	N	O	S	0	0	0
			3235	2046	560	610	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	ALA	ARG	engineered mutation	UNP D3WZ85
B	289	ALA	ARG	engineered mutation	UNP D3WZ85
C	289	ALA	ARG	engineered mutation	UNP D3WZ85
D	289	ALA	ARG	engineered mutation	UNP D3WZ85
E	289	ALA	ARG	engineered mutation	UNP D3WZ85
F	289	ALA	ARG	engineered mutation	UNP D3WZ85
G	289	ALA	ARG	engineered mutation	UNP D3WZ85
H	289	ALA	ARG	engineered mutation	UNP D3WZ85

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is (6 {R})-6-azanyl-3-nitro-6-oxidanyl-cyclohexa-1,3-diene-1-carboxylic acid (three-letter code: 6R8) (formula: $C_7H_8N_2O_5$).
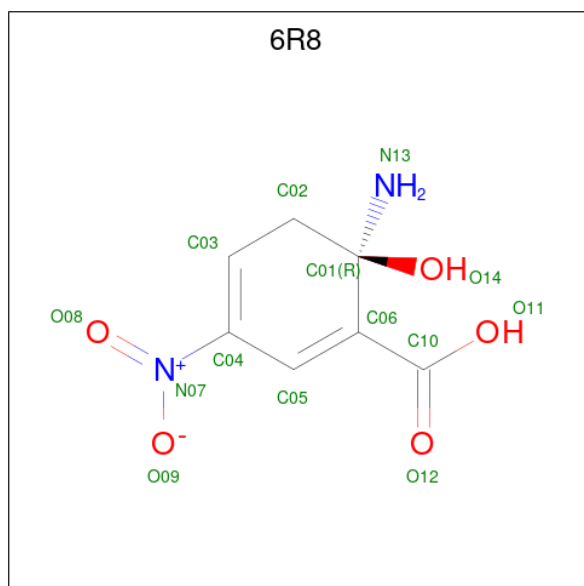
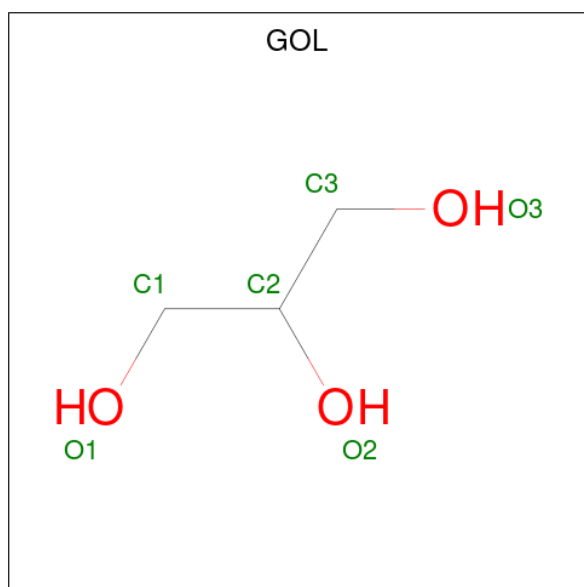| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 7	N 2	O 5	0	0
3	B	1	Total 14	C 7	N 2	O 5	0	0
3	C	1	Total 14	C 7	N 2	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total 14	C 7	N 2	O 5	0	0
3	G	1	Total 14	C 7	N 2	O 5	0	0
3	H	1	Total 14	C 7	N 2	O 5	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

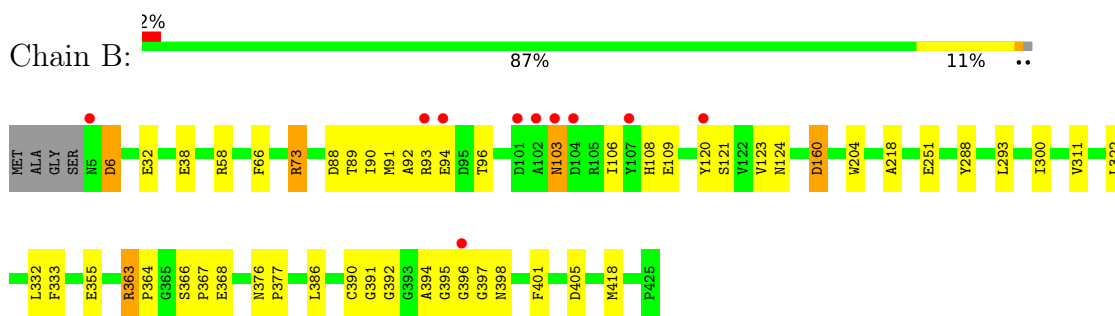| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	175	Total 175	O 175	0	0
5	B	249	Total 249	O 249	0	0
5	C	251	Total 251	O 251	0	0
5	D	235	Total 235	O 235	0	0
5	E	225	Total 225	O 225	0	0
5	F	233	Total 233	O 233	0	0
5	G	179	Total 179	O 179	0	0
5	H	195	Total 195	O 195	0	0

3 Residue-property plots ⓘ

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: 5-nitroanthranilic acid aminohydrolase
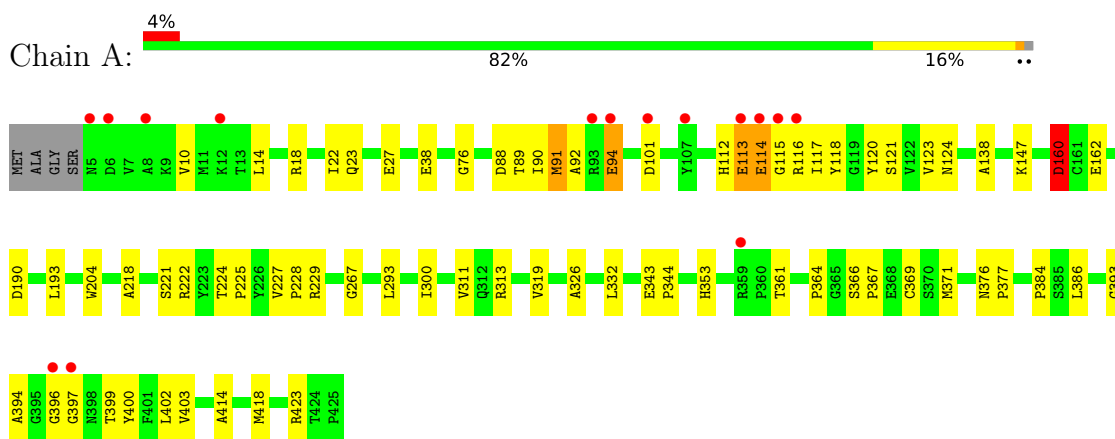
• Molecule 1: 5-nitroanthranilic acid aminohydrolase
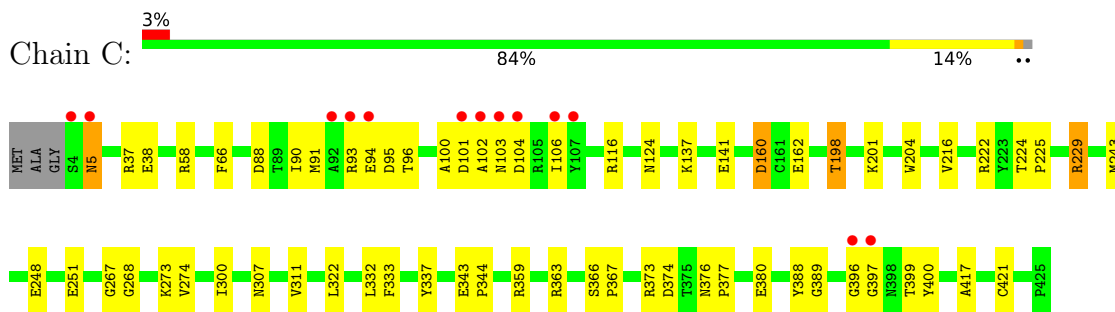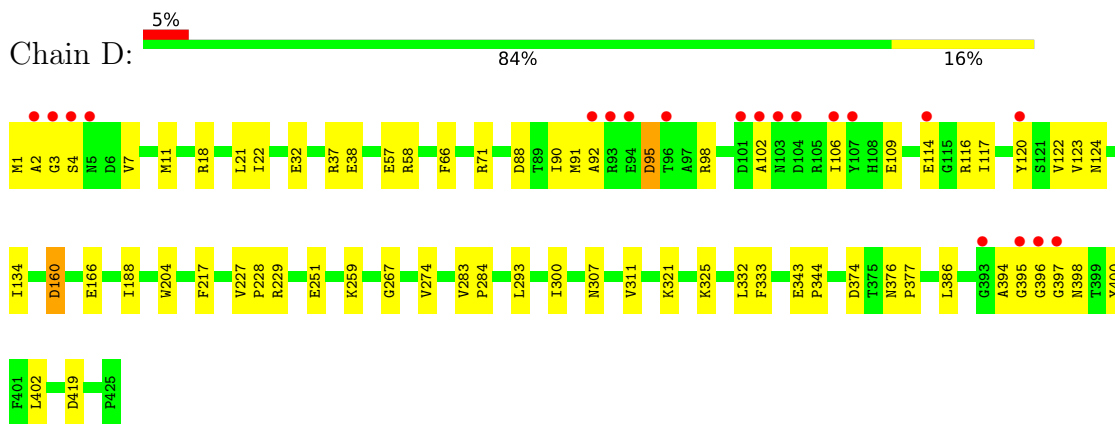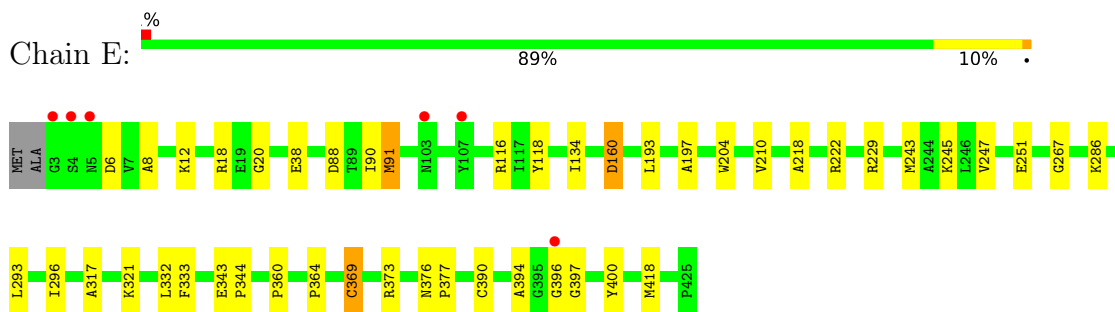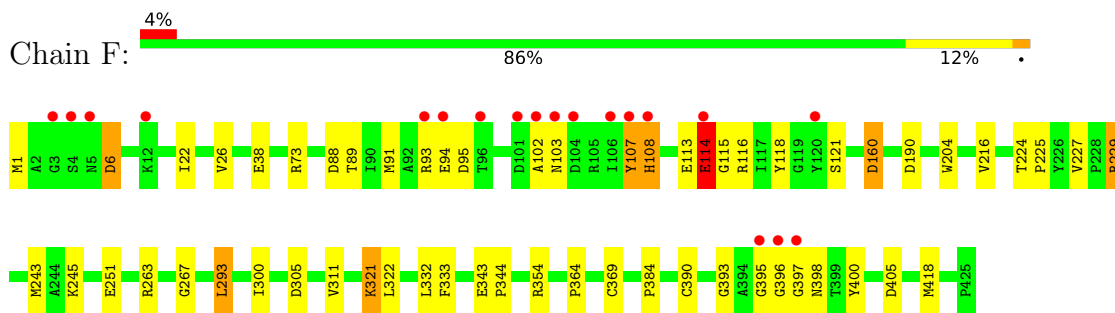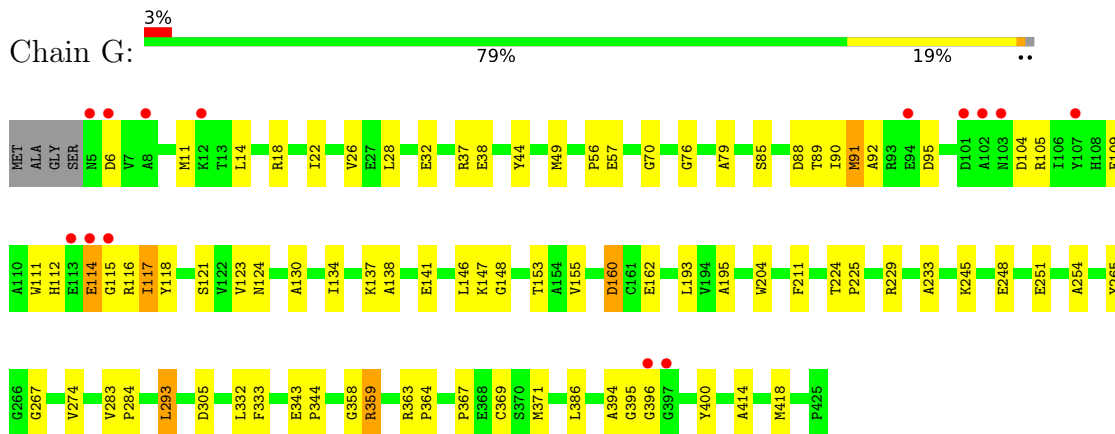

• Molecule 1: 5-nitroanthranilic acid aminohydrolase

• Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain D:

● Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain E:

● Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain F:

● Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain G:

● Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain H:
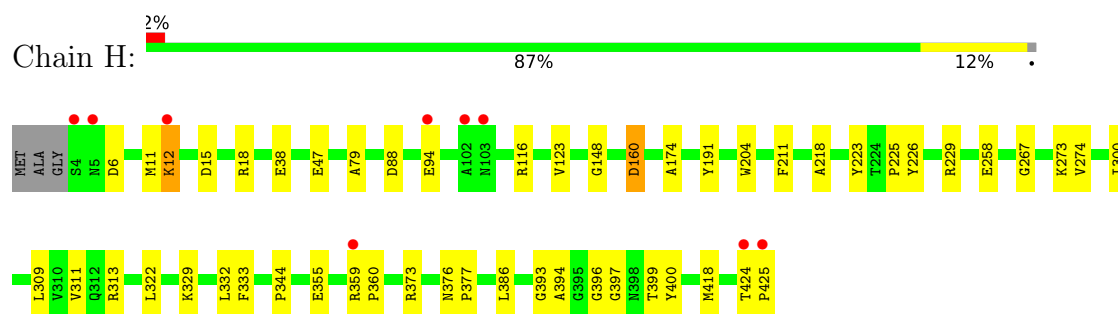
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	185.88Å 247.63Å 247.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.16 – 2.20 37.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	60.3 (37.16-2.20) 94.0 (37.17-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.174 , 0.204 0.173 , 0.199	Depositor DCC
R_{free} test set	2000 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 37.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27782	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.31% 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 $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 6R8, ZN

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	0.42	0/3303	0.56	0/4484
1	B	0.44	0/3303	0.54	0/4484
1	C	0.45	0/3309	0.56	1/4492 (0.0%)
1	D	0.43	0/3326	0.56	0/4514
1	E	0.44	1/3313 (0.0%)	0.54	0/4497
1	F	0.43	0/3326	0.57	1/4514 (0.0%)
1	G	0.42	0/3303	0.55	0/4484
1	H	0.44	0/3309	0.55	0/4492
All	All	0.43	1/26492 (0.0%)	0.55	2/35961 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	369	CYS	CB-SG	-5.93	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	229	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	229	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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	3229	0	3157	61	0
1	B	3229	0	3157	39	0
1	C	3235	0	3162	56	0
1	D	3252	0	3182	64	0
1	E	3239	0	3165	40	0
1	F	3252	0	3182	56	0
1	G	3229	0	3157	87	0
1	H	3235	0	3162	45	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
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	14	0	0	2	0
3	B	14	0	0	0	0
3	C	14	0	0	1	0
3	E	14	0	0	0	0
3	G	14	0	0	0	0
3	H	14	0	0	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	6	0	8	1	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	A	175	0	0	2	0
5	B	249	0	0	3	0
5	C	251	0	0	2	0
5	D	235	0	0	8	0
5	E	225	0	0	5	0
5	F	233	0	0	6	1
5	G	179	0	0	7	1
5	H	195	0	0	4	0
All	All	27782	0	25388	426	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 8.

The worst 5 of 426 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:H:373:ARG:NH1	3:H:502:6R8:O11	1.90	1.03
1:E:38:GLU:HG2	1:E:88:ASP:HB3	1.46	0.97
1:G:49:MET:HE2	1:G:56:PRO:HB3	1.45	0.95
1:A:116:ARG:HD2	1:A:400:TYR:CD2	2.10	0.87
1:D:2:ALA:HB2	1:D:419:ASP:HB2	1.55	0.87

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)
5:F:797:HOH:O	5:G:763:HOH:O[6_445]	2.15	0.05

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	419/425 (99%)	403 (96%)	13 (3%)	3 (1%)	22	22
1	B	419/425 (99%)	406 (97%)	11 (3%)	2 (0%)	29	31
1	C	420/425 (99%)	405 (96%)	13 (3%)	2 (0%)	29	31
1	D	423/425 (100%)	403 (95%)	19 (4%)	1 (0%)	47	55
1	E	421/425 (99%)	408 (97%)	11 (3%)	2 (0%)	29	31
1	F	423/425 (100%)	409 (97%)	12 (3%)	2 (0%)	29	31
1	G	419/425 (99%)	399 (95%)	19 (4%)	1 (0%)	47	55
1	H	420/425 (99%)	407 (97%)	11 (3%)	2 (0%)	29	31
All	All	3364/3400 (99%)	3240 (96%)	109 (3%)	15 (0%)	34	37

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	C	101	ASP
1	F	114	GLU
1	F	160	ASP
1	A	160	ASP

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	328/330 (99%)	322 (98%)	6 (2%)	59	72
1	B	328/330 (99%)	321 (98%)	7 (2%)	53	67
1	C	329/330 (100%)	323 (98%)	6 (2%)	59	72
1	D	330/330 (100%)	328 (99%)	2 (1%)	86	93
1	E	329/330 (100%)	327 (99%)	2 (1%)	86	93
1	F	330/330 (100%)	322 (98%)	8 (2%)	49	62
1	G	328/330 (99%)	321 (98%)	7 (2%)	53	67
1	H	329/330 (100%)	323 (98%)	6 (2%)	59	72
All	All	2631/2640 (100%)	2587 (98%)	44 (2%)	60	74

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	160	ASP
1	G	160	ASP
1	F	293	LEU
1	G	104	ASP
1	G	359	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	103	ASN

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Mol	Chain	Res	Type
1	F	108	HIS
1	G	112	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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 Counts	Bond lengths RMSZ	Bond lengths #$|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles #$|Z| > 2$
4	GOL	B	503	-	5,5,5	0.38	0	5,5,5	0.53	0
4	GOL	H	503	-	5,5,5	0.44	0	5,5,5	0.34	0
3	6R8	E	502	2	9,14,14	4.50	3 (33%)	8,21,21	2.34	3 (37%)
4	GOL	D	502	-	5,5,5	0.45	0	5,5,5	0.24	0
3	6R8	B	502	2	9,14,14	4.52	4 (44%)	8,21,21	2.10	2 (25%)
4	GOL	E	503	-	5,5,5	0.48	0	5,5,5	0.50	0
4	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.44	0
4	GOL	G	503	-	5,5,5	0.44	0	5,5,5	0.24	0
3	6R8	C	502	2	9,14,14	4.46	3 (33%)	8,21,21	2.15	1 (12%)
3	6R8	A	502	2	9,14,14	4.37	3 (33%)	8,21,21	2.19	1 (12%)
3	6R8	H	502	2	9,14,14	4.37	3 (33%)	8,21,21	2.20	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GOL	F	502	-	5,5,5	0.43	0	5,5,5	0.50	0
4	GOL	C	503	-	5,5,5	0.48	0	5,5,5	0.27	0
3	6R8	G	502	2	9,14,14	4.35	3 (33%)	8,21,21	2.15	2 (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
4	GOL	B	503	-	-	4/4/4/4	-
4	GOL	H	503	-	-	2/4/4/4	-
3	6R8	E	502	2	-	6/6/24/24	0/1/1/1
4	GOL	D	502	-	-	2/4/4/4	-
3	6R8	B	502	2	-	6/6/24/24	0/1/1/1
4	GOL	E	503	-	-	4/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
4	GOL	G	503	-	-	1/4/4/4	-
3	6R8	C	502	2	-	6/6/24/24	0/1/1/1
3	6R8	A	502	2	-	6/6/24/24	0/1/1/1
3	6R8	H	502	2	-	4/6/24/24	0/1/1/1
4	GOL	F	502	-	-	1/4/4/4	-
4	GOL	C	503	-	-	4/4/4/4	-
3	6R8	G	502	2	-	6/6/24/24	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	6R8	O08-N07	9.86	1.39	1.22
3	C	502	6R8	O08-N07	9.77	1.39	1.22
3	E	502	6R8	O08-N07	9.63	1.39	1.22
3	G	502	6R8	O08-N07	9.59	1.39	1.22
3	A	502	6R8	O08-N07	9.50	1.39	1.22

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	6R8	C01-C02-C03	4.90	122.05	113.06
3	G	502	6R8	C01-C02-C03	4.88	122.02	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	6R8	C01-C02-C03	4.87	122.00	113.06
3	A	502	6R8	C01-C02-C03	4.82	121.90	113.06
3	H	502	6R8	C01-C02-C03	4.77	121.81	113.06

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	6R8	C01-C06-C10-O11
3	A	502	6R8	C05-C06-C10-O11
3	A	502	6R8	C01-C06-C10-O12
3	A	502	6R8	C05-C06-C10-O12
3	A	502	6R8	C03-C04-N07-O08

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	502	GOL	1	0
3	C	502	6R8	1	0
3	A	502	6R8	2	0
3	H	502	6R8	1	0
4	F	502	GOL	1	0
4	C	503	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	421/425 (99%)	-0.33	15 (3%)	42	41	19, 30, 63, 95	0
1	B	421/425 (99%)	-0.48	10 (2%)	59	56	17, 26, 58, 106	0
1	C	422/425 (99%)	-0.50	13 (3%)	49	47	17, 25, 55, 105	0
1	D	425/425 (100%)	-0.35	20 (4%)	31	30	17, 26, 71, 123	0
1	E	423/425 (99%)	-0.50	6 (1%)	75	73	18, 26, 52, 80	0
1	F	425/425 (100%)	-0.35	19 (4%)	33	32	17, 26, 70, 128	0
1	G	421/425 (99%)	-0.21	14 (3%)	46	44	18, 31, 67, 102	0
1	H	422/425 (99%)	-0.46	9 (2%)	63	61	18, 28, 55, 87	0
All	All	3380/3400 (99%)	-0.40	106 (3%)	49	47	17, 27, 63, 128	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	93	ARG	8.7
1	D	3	GLY	8.5
1	F	107	TYR	8.4
1	D	102	ALA	8.3
1	D	397	GLY	7.8

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides 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	6R8	C	502	14/14	0.79	0.29	34,47,56,56	0
3	6R8	B	502	14/14	0.81	0.25	40,46,56,61	0
3	6R8	E	502	14/14	0.86	0.23	36,42,57,59	0
3	6R8	G	502	14/14	0.87	0.18	42,52,62,63	0
3	6R8	A	502	14/14	0.88	0.18	41,46,55,62	0
4	GOL	E	503	6/6	0.90	0.18	25,31,38,38	0
4	GOL	B	503	6/6	0.91	0.14	22,31,35,35	0
4	GOL	A	503	6/6	0.91	0.17	25,33,34,41	0
3	6R8	H	502	14/14	0.92	0.16	33,40,49,54	0
2	ZN	D	501	1/1	0.92	0.06	38,38,38,38	1
4	GOL	F	502	6/6	0.93	0.15	27,30,36,40	0
2	ZN	F	501	1/1	0.94	0.08	39,39,39,39	1
4	GOL	D	502	6/6	0.95	0.12	29,31,33,37	0
2	ZN	A	501	1/1	0.95	0.07	38,38,38,38	1
2	ZN	G	501	1/1	0.95	0.04	67,67,67,67	0
4	GOL	H	503	6/6	0.95	0.10	23,29,32,37	0
4	GOL	G	503	6/6	0.96	0.15	27,33,37,38	0
4	GOL	C	503	6/6	0.97	0.10	28,29,31,33	0
2	ZN	H	501	1/1	0.98	0.05	34,34,34,34	1
2	ZN	C	501	1/1	0.98	0.06	30,30,30,30	1
2	ZN	B	501	1/1	0.98	0.06	33,33,33,33	1
2	ZN	E	501	1/1	0.99	0.08	33,33,33,33	1

6.5 Other polymers ⓘ

There are no such residues in this entry.