



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2016 – 02:28 PM EDT

PDB ID : 4Z10
Title : Inactive aurone synthase (polyphenol oxidase) co-crystallized with 1,4-resorcinol
Authors : Molitor, C.; Mauracher, S.G.; Rompel, A.
Deposited on : 2015-03-26
Resolution : 1.93 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

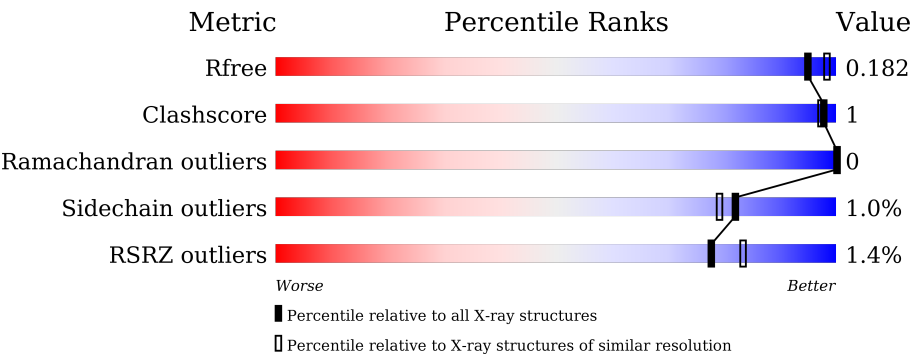
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.93 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}	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 $\leq 5\%$. 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	350	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>96%</div><div><div></div><div></div></div></div>
1	B	350	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>95%</div><div><div></div><div></div></div></div>
1	C	350	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>97%</div><div><div></div><div></div></div></div>
1	D	350	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>97%</div><div><div></div><div></div></div></div>
1	E	350	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>96%</div><div><div></div><div></div></div></div>
1	F	350	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>97%</div><div><div></div><div></div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	15	
2	H	15	
2	I	15	
2	J	15	
2	K	15	
2	L	15	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	RCO	A	602	-	-	-	X
4	RCO	A	604	-	-	-	X
4	RCO	D	602	-	-	-	X
4	RCO	D	603	-	-	-	X
5	GOL	A	605	-	-	-	X
5	GOL	B	605	-	-	-	X
5	GOL	B	606	-	-	-	X
5	GOL	C	604	-	-	-	X
5	GOL	C	605	-	-	-	X
5	GOL	D	604	-	-	-	X
6	ACT	K	501	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 34316 atoms, of which 15548 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 Aurone synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	347	Total	C	H	N	O	S	0	0	0
			5323	1763	2546	477	524	13			
1	B	347	Total	C	H	N	O	S	0	2	0
			5328	1765	2547	478	525	13			
1	C	347	Total	C	H	N	O	S	0	3	0
			5359	1770	2567	482	527	13			
1	D	347	Total	C	H	N	O	S	0	1	0
			5271	1752	2513	472	521	13			
1	E	347	Total	C	H	N	O	S	0	1	0
			5330	1763	2554	478	522	13			
1	F	350	Total	C	H	N	O	S	0	0	0
			5279	1761	2512	476	517	13			

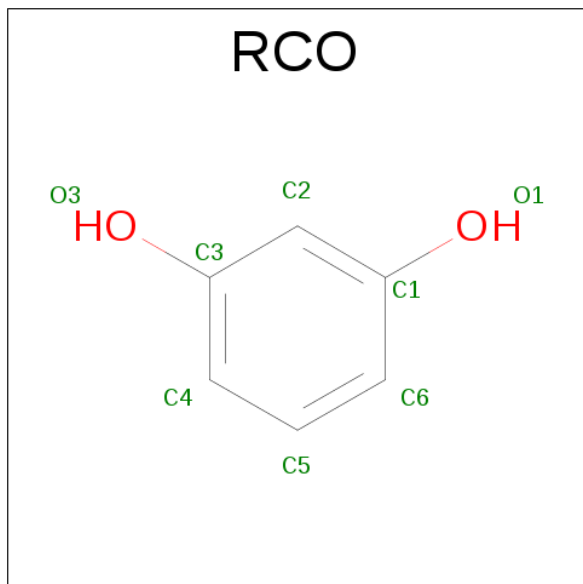
- Molecule 2 is a protein called Aurone synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	12	Total	C	H	N	O	S	0	0	0
			125	57	36	12	19	1			
2	H	10	Total	C	H	N	O	S	0	0	0
			91	44	22	10	14	1			
2	I	4	Total	C	H	N	O	S	0	0	0
			50	16	22	4	7	1			
2	J	4	Total	C	H	N	O	S	0	0	0
			50	16	22	4	7	1			
2	K	12	Total	C	H	N	O	S	0	0	0
			156	57	67	12	19	1			
2	L	4	Total	C	H	N	O	S	0	0	0
			38	14	15	4	4	1			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is RESORCINOL (three-letter code: RCO) (formula: C₆H₆O₂).



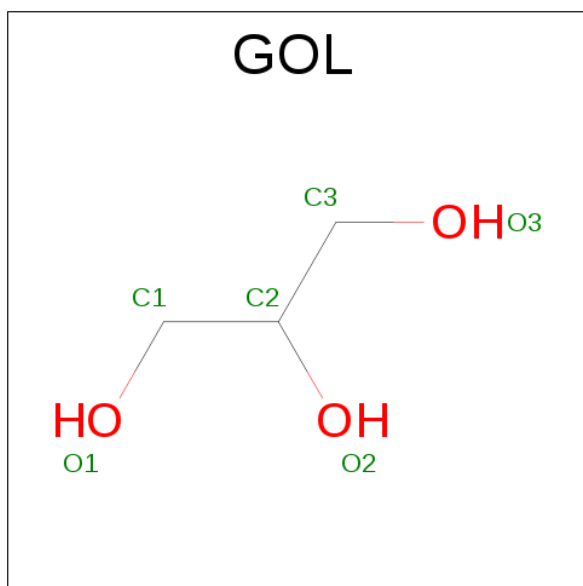
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 6 6 2	0	0
4	A	1	Total C H O 14 6 6 2	0	0
4	A	1	Total C H O 14 6 6 2	0	0
4	B	1	Total C H O 14 6 6 2	0	0
4	B	1	Total C H O 14 6 6 2	0	0
4	C	1	Total C H O 14 6 6 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			14	6	6	2		
4	D	1	Total	C	H	O	0	0
			14	6	6	2		
4	D	1	Total	C	H	O	0	0
			14	6	6	2		
4	E	1	Total	C	H	O	0	0
			14	6	6	2		
4	E	1	Total	C	H	O	0	0
			14	6	6	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



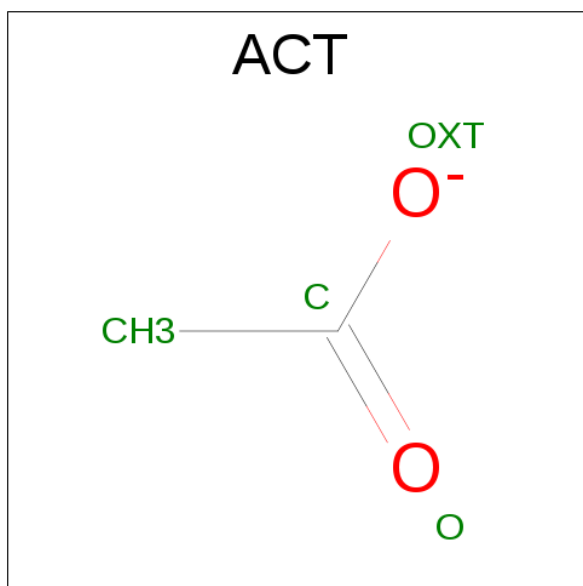
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	303	Total	O	0	0
			303	303		
7	G	8	Total	O	0	0
			8	8		
7	B	292	Total	O	0	0
			292	292		
7	H	7	Total	O	0	0
			7	7		
7	C	279	Total	O	0	0
			279	279		
7	I	2	Total	O	0	0
			2	2		
7	D	252	Total	O	0	0
			252	252		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	3	Total 3	O 3	0	0
7	E	272	Total 272	O 272	0	0
7	K	5	Total 5	O 5	0	0
7	F	228	Total 228	O 228	0	0

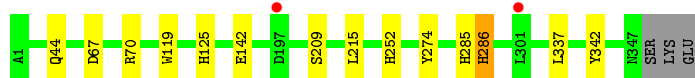
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Aurone synthase



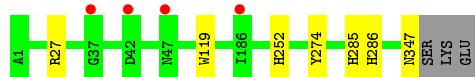
- Molecule 1: Aurone synthase



- Molecule 1: Aurone synthase



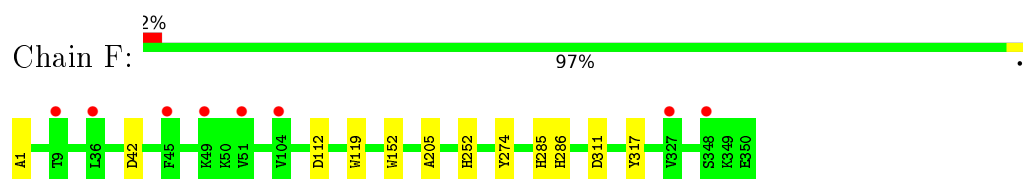
- Molecule 1: Aurone synthase



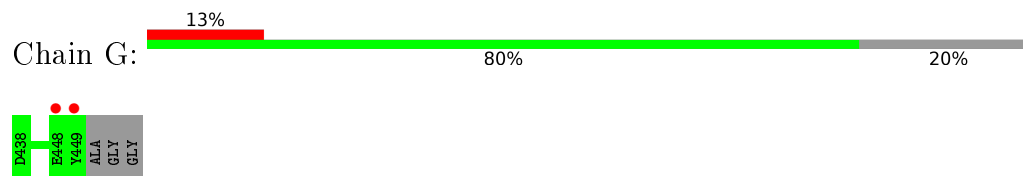
- Molecule 1: Aurone synthase



- Molecule 1: Aurone synthase



- Molecule 2: Aurone synthase



- Molecule 2: Aurone synthase



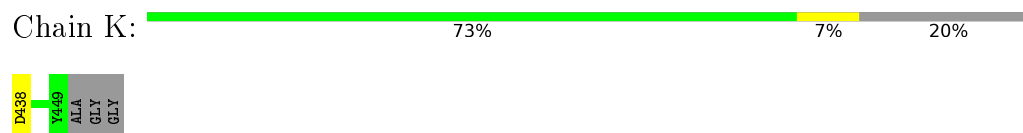
- Molecule 2: Aurone synthase



- Molecule 2: Aurone synthase



- Molecule 2: Aurone synthase



- Molecule 2: Aurone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.10Å 137.10Å 209.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.92 – 1.93 48.92 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.92-1.93) 100.0 (48.92-1.93)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.92Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.144 , 0.179 0.149 , 0.182	Depositor DCC
R_{free} test set	16547 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 52.4	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	6 of 170782 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	34316	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.2624e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, HS8, RCO, CU, ACT

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	0.33	0/2847	0.49	0/3881
1	B	0.32	0/2851	0.49	0/3887
1	C	0.33	0/2862	0.48	0/3902
1	D	0.32	0/2828	0.47	0/3860
1	E	0.32	0/2846	0.48	0/3880
1	F	0.30	0/2837	0.46	0/3871
2	G	0.31	0/92	0.50	0/127
2	H	0.28	0/71	0.50	0/98
2	I	0.25	0/28	0.52	0/38
2	J	0.21	0/28	0.47	0/38
2	K	0.28	0/92	0.47	0/127
2	L	0.22	0/23	0.34	0/31
All	All	0.32	0/17405	0.48	0/23740

There are no bond length outliers.

There are no bond angle outliers.

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	2777	2546	2574	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2781	2547	2572	10	0
1	C	2792	2567	2580	5	0
1	D	2758	2513	2534	4	0
1	E	2776	2554	2572	6	0
1	F	2767	2512	2545	5	0
2	G	89	36	71	0	0
2	H	69	22	58	1	0
2	I	28	22	21	2	0
2	J	28	22	21	0	0
2	K	89	67	71	1	0
2	L	23	15	14	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	24	18	18	0	0
4	B	16	12	12	0	0
4	C	16	12	12	0	0
4	D	16	12	12	1	0
4	E	16	12	12	0	0
5	A	6	8	8	0	0
5	B	18	24	24	2	0
5	C	12	16	16	2	0
5	D	6	8	8	1	0
6	K	4	3	3	0	0
7	A	303	0	0	1	0
7	B	292	0	0	1	0
7	C	279	0	0	1	0
7	D	252	0	0	1	0
7	E	272	0	0	0	0
7	F	228	0	0	1	0
7	G	8	0	0	0	0
7	H	7	0	0	0	0
7	I	2	0	0	2	0
7	J	3	0	0	0	0
7	K	5	0	0	0	0
All	All	18768	15548	15758	35	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 1.

All (35) 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:B:44:GLN:H	5:B:605:GOL:H12	1.51	0.75
2:I:443:THR:N	7:I:501:HOH:O	2.23	0.70
1:B:44:GLN:H	5:B:605:GOL:C1	2.11	0.62
1:E:152:TRP:HE1	1:E:285:HIS:HD1	1.51	0.57
1:D:252:HS8:HE1	1:D:286:HIS:NE2	2.21	0.55
1:F:152:TRP:HE1	1:F:285:HIS:HD1	1.54	0.55
1:C:152:TRP:HE1	1:C:285:HIS:HD1	1.53	0.54
1:C:110:ASP:O	7:C:701:HOH:O	2.18	0.53
1:F:1:ALA:N	1:F:311:ASP:OD1	2.34	0.53
1:B:252:HS8:HE1	1:B:286:HIS:NE2	2.24	0.51
1:B:209:SER:HG	2:H:438:ASP:N	2.07	0.51
1:E:209:SER:HG	2:K:438:ASP:N	2.09	0.50
1:E:148:PRO:HG2	1:E:284:ILE:HD12	1.94	0.50
1:F:252:HS8:HE1	1:F:286:HIS:NE2	2.26	0.49
1:B:142:GLU:OE1	7:B:701:HOH:O	2.19	0.49
2:I:443:THR:N	7:I:502:HOH:O	2.47	0.48
1:C:44:GLN:H	5:C:605:GOL:C3	2.28	0.47
1:D:347:ASN:O	7:D:701:HOH:O	2.20	0.46
1:B:215:LEU:HD23	4:D:602:RCO:H5	1.96	0.46
1:A:252:HS8:HE1	1:A:286:HIS:NE2	2.30	0.46
1:B:337:LEU:HD22	1:B:342:TYR:CZ	2.52	0.45
1:A:213:ARG:HA	1:A:217:ARG:HB3	1.99	0.45
1:E:252:HS8:HE1	1:E:286:HIS:NE2	2.32	0.44
1:B:252:HS8:HD1	1:B:285:HIS:HE2	1.66	0.44
1:B:67:ASP:OD1	1:B:70:ARG:NH2	2.52	0.43
1:E:201:GLN:HG2	1:F:205:ALA:HB2	2.00	0.43
1:C:44:GLN:H	5:C:605:GOL:H32	1.84	0.42
1:C:296:TRP:CH2	1:C:304:HIS:HA	2.54	0.42
1:D:27:ARG:HH22	5:D:604:GOL:C1	2.32	0.42
1:E:127:TRP:CE2	1:E:334:CYS:HB3	2.55	0.42
1:D:252:HS8:HD1	1:D:285:HIS:HE2	1.69	0.41
1:A:339:LYS:NZ	7:A:721:HOH:O	2.52	0.41
1:F:112:ASP:OD2	7:F:801:HOH:O	2.22	0.41
1:B:125:HIS:CD2	1:B:286:HIS:CE1	3.09	0.40
1:A:75:MET:HG2	1:A:86:PHE:N	2.37	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	344/350 (98%)	335 (97%)	9 (3%)	0	100	100
1	B	346/350 (99%)	335 (97%)	11 (3%)	0	100	100
1	C	347/350 (99%)	338 (97%)	9 (3%)	0	100	100
1	D	345/350 (99%)	337 (98%)	8 (2%)	0	100	100
1	E	345/350 (99%)	336 (97%)	9 (3%)	0	100	100
1	F	347/350 (99%)	334 (96%)	13 (4%)	0	100	100
2	G	10/15 (67%)	10 (100%)	0	0	100	100
2	H	8/15 (53%)	8 (100%)	0	0	100	100
2	I	2/15 (13%)	2 (100%)	0	0	100	100
2	J	2/15 (13%)	2 (100%)	0	0	100	100
2	K	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
2	L	2/15 (13%)	2 (100%)	0	0	100	100
All	All	2108/2190 (96%)	2048 (97%)	60 (3%)	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	292/304 (96%)	288 (99%)	4 (1%)	74	68
1	B	292/304 (96%)	289 (99%)	3 (1%)	82	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	293/304 (96%)	290 (99%)	3 (1%)	82	79
1	D	287/304 (94%)	285 (99%)	2 (1%)	88	87
1	E	291/304 (96%)	289 (99%)	2 (1%)	88	87
1	F	284/304 (93%)	280 (99%)	4 (1%)	74	68
2	G	10/11 (91%)	10 (100%)	0	100	100
2	H	8/11 (73%)	8 (100%)	0	100	100
2	I	4/11 (36%)	4 (100%)	0	100	100
2	J	4/11 (36%)	4 (100%)	0	100	100
2	K	10/11 (91%)	10 (100%)	0	100	100
2	L	2/11 (18%)	2 (100%)	0	100	100
All	All	1777/1890 (94%)	1759 (99%)	18 (1%)	82	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	119	TRP
1	A	274	TYR
1	A	286	HIS
1	B	119	TRP
1	B	274	TYR
1	B	286	HIS
1	C	119	TRP
1	C	274	TYR
1	C	286	HIS
1	D	119	TRP
1	D	274	TYR
1	E	119	TRP
1	E	274	TYR
1	F	42	ASP
1	F	119	TRP
1	F	274	TYR
1	F	317	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	HS8	A	252	1	8,14,15	4.29	2 (25%)	7,20,22	1.82	3 (42%)
1	HS8	B	252	1	8,14,15	4.33	2 (25%)	7,20,22	1.75	2 (28%)
1	HS8	C	252	1	8,14,15	2.19	3 (37%)	7,20,22	0.84	0
1	HS8	D	252	1	8,14,15	2.15	3 (37%)	7,20,22	0.86	0
1	HS8	E	252	1	8,14,15	4.36	2 (25%)	7,20,22	1.82	2 (28%)
1	HS8	F	252	1	8,14,15	2.13	3 (37%)	7,20,22	0.89	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	HS8	A	252	1	-	0/4/12/14	0/1/1/1
1	HS8	B	252	1	-	0/4/12/14	0/1/1/1
1	HS8	C	252	1	-	0/4/12/14	0/1/1/1
1	HS8	D	252	1	-	0/4/12/14	0/1/1/1
1	HS8	E	252	1	-	0/4/12/14	0/1/1/1
1	HS8	F	252	1	-	0/4/12/14	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	HS8	O1-S	-3.62	1.36	1.42
1	D	252	HS8	O1-S	-3.57	1.36	1.42
1	E	252	HS8	O3-S	-3.39	1.37	1.42
1	F	252	HS8	O1-S	-3.31	1.37	1.42
1	F	252	HS8	O3-S	-3.21	1.37	1.42
1	B	252	HS8	O3-S	-3.17	1.37	1.42
1	A	252	HS8	O3-S	-3.13	1.37	1.42
1	C	252	HS8	O3-S	-3.11	1.37	1.42
1	D	252	HS8	O3-S	-3.07	1.37	1.42
1	D	252	HS8	O2-S	3.17	1.62	1.44
1	F	252	HS8	O2-S	3.23	1.62	1.44
1	C	252	HS8	O2-S	3.28	1.62	1.44
1	A	252	HS8	O1-S	11.43	1.61	1.42
1	B	252	HS8	O1-S	11.56	1.61	1.42
1	E	252	HS8	O1-S	11.57	1.61	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	HS8	O1-S-NE2	-3.01	99.53	107.78
1	E	252	HS8	O1-S-NE2	-2.77	100.20	107.78
1	B	252	HS8	O1-S-NE2	-2.61	100.64	107.78
1	A	252	HS8	CG-CD2-NE2	-2.12	106.13	108.96
1	A	252	HS8	O2-S-O3	2.99	126.96	111.62
1	B	252	HS8	O2-S-O3	3.15	127.78	111.62
1	E	252	HS8	O2-S-O3	3.26	128.31	111.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	252	HS8	1	0
1	B	252	HS8	2	0
1	D	252	HS8	2	0
1	E	252	HS8	1	0
1	F	252	HS8	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	RCO	A	602	-	8,8,8	4.64	5 (62%)	10,10,10	0.52	0
4	RCO	A	603	-	8,8,8	4.60	5 (62%)	10,10,10	0.28	0
4	RCO	A	604	-	8,8,8	4.59	4 (50%)	10,10,10	0.31	0
5	GOL	A	605	-	5,5,5	0.33	0	5,5,5	0.16	0
4	RCO	B	602	-	8,8,8	4.53	4 (50%)	10,10,10	0.29	0
4	RCO	B	603	-	8,8,8	4.68	4 (50%)	10,10,10	0.46	0
5	GOL	B	604	-	5,5,5	0.34	0	5,5,5	0.24	0
5	GOL	B	605	-	5,5,5	0.20	0	5,5,5	0.35	0
5	GOL	B	606	-	5,5,5	0.34	0	5,5,5	0.25	0
4	RCO	C	602	-	8,8,8	4.59	4 (50%)	10,10,10	0.36	0
4	RCO	C	603	-	8,8,8	4.56	4 (50%)	10,10,10	0.32	0
5	GOL	C	604	-	5,5,5	0.35	0	5,5,5	0.44	0
5	GOL	C	605	-	5,5,5	0.21	0	5,5,5	0.42	0
4	RCO	D	602	-	8,8,8	4.61	4 (50%)	10,10,10	0.34	0
4	RCO	D	603	-	8,8,8	4.51	4 (50%)	10,10,10	0.32	0
5	GOL	D	604	-	5,5,5	0.27	0	5,5,5	0.45	0
4	RCO	E	602	-	8,8,8	4.63	4 (50%)	10,10,10	0.32	0
4	RCO	E	603	-	8,8,8	4.56	4 (50%)	10,10,10	0.27	0
6	ACT	K	501	-	0,3,3	0.00	-	0,3,3	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
4	RCO	A	602	-	-	0/0/0/0	0/1/1/1
4	RCO	A	603	-	-	0/0/0/0	0/1/1/1
4	RCO	A	604	-	-	0/0/0/0	0/1/1/1
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0
4	RCO	B	602	-	-	0/0/0/0	0/1/1/1
4	RCO	B	603	-	-	0/0/0/0	0/1/1/1
5	GOL	B	604	-	-	0/4/4/4	0/0/0/0
5	GOL	B	605	-	-	0/4/4/4	0/0/0/0
5	GOL	B	606	-	-	0/4/4/4	0/0/0/0
4	RCO	C	602	-	-	0/0/0/0	0/1/1/1
4	RCO	C	603	-	-	0/0/0/0	0/1/1/1
5	GOL	C	604	-	-	0/4/4/4	0/0/0/0
5	GOL	C	605	-	-	0/4/4/4	0/0/0/0
4	RCO	D	602	-	-	0/0/0/0	0/1/1/1
4	RCO	D	603	-	-	0/0/0/0	0/1/1/1
5	GOL	D	604	-	-	0/4/4/4	0/0/0/0
4	RCO	E	602	-	-	0/0/0/0	0/1/1/1
4	RCO	E	603	-	-	0/0/0/0	0/1/1/1
6	ACT	K	501	-	-	0/0/0/0	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	RCO	C2-C1	-2.90	1.34	1.39
4	B	602	RCO	C2-C1	-2.62	1.35	1.39
4	C	602	RCO	C2-C1	-2.60	1.35	1.39
4	A	604	RCO	C2-C1	-2.51	1.35	1.39
4	B	603	RCO	C2-C1	-2.49	1.35	1.39
4	D	603	RCO	C2-C1	-2.48	1.35	1.39
4	E	603	RCO	C2-C1	-2.47	1.35	1.39
4	D	602	RCO	C2-C1	-2.46	1.35	1.39
4	A	603	RCO	C2-C1	-2.39	1.35	1.39
4	E	602	RCO	C2-C1	-2.25	1.35	1.39
4	C	603	RCO	C2-C1	-2.16	1.35	1.39
4	A	603	RCO	C4-C3	-2.03	1.34	1.38
4	A	602	RCO	O1-C1	2.10	1.42	1.37
4	D	603	RCO	C6-C1	6.32	1.51	1.38
4	E	602	RCO	C6-C1	6.37	1.51	1.38
4	A	603	RCO	C6-C1	6.38	1.51	1.38
4	A	604	RCO	C6-C1	6.42	1.51	1.38
4	C	603	RCO	C6-C1	6.43	1.51	1.38
4	B	602	RCO	C6-C1	6.43	1.51	1.38
4	B	602	RCO	C5-C4	6.44	1.51	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	RCO	C6-C1	6.46	1.51	1.38
4	C	603	RCO	C5-C4	6.47	1.51	1.38
4	D	602	RCO	C6-C1	6.50	1.51	1.38
4	E	603	RCO	C6-C1	6.51	1.51	1.38
4	D	602	RCO	C5-C4	6.51	1.51	1.38
4	A	603	RCO	C5-C4	6.53	1.51	1.38
4	B	603	RCO	C6-C1	6.59	1.52	1.38
4	E	602	RCO	C5-C4	6.60	1.51	1.38
4	D	603	RCO	C5-C4	6.63	1.51	1.38
4	E	603	RCO	C5-C4	6.65	1.51	1.38
4	A	604	RCO	C5-C4	6.67	1.51	1.38
4	A	602	RCO	C5-C4	6.79	1.52	1.38
4	A	602	RCO	C6-C1	6.79	1.52	1.38
4	C	602	RCO	C5-C4	6.96	1.52	1.38
4	B	603	RCO	C5-C4	7.02	1.52	1.38
4	A	602	RCO	C2-C3	7.68	1.51	1.39
4	C	602	RCO	C2-C3	7.70	1.51	1.39
4	D	603	RCO	C2-C3	7.79	1.51	1.39
4	B	602	RCO	C2-C3	7.83	1.51	1.39
4	E	603	RCO	C2-C3	7.85	1.51	1.39
4	C	603	RCO	C2-C3	8.08	1.51	1.39
4	A	604	RCO	C2-C3	8.09	1.51	1.39
4	B	603	RCO	C2-C3	8.14	1.51	1.39
4	D	602	RCO	C2-C3	8.14	1.51	1.39
4	A	603	RCO	C2-C3	8.19	1.51	1.39
4	E	602	RCO	C2-C3	8.33	1.52	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	605	GOL	2	0
5	C	605	GOL	2	0
4	D	602	RCO	1	0
5	D	604	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	346/350 (98%)	-0.18	5 (1%) 78 83	20, 30, 48, 77	0
1	B	346/350 (98%)	-0.21	2 (0%) 90 93	20, 31, 48, 79	0
1	C	346/350 (98%)	-0.25	4 (1%) 81 86	19, 31, 50, 76	0
1	D	346/350 (98%)	-0.19	4 (1%) 81 86	20, 34, 52, 78	0
1	E	346/350 (98%)	-0.14	2 (0%) 90 93	20, 31, 50, 69	0
1	F	349/350 (99%)	-0.08	8 (2%) 64 72	21, 37, 56, 66	0
2	G	12/15 (80%)	0.50	2 (16%) 2 3	39, 43, 60, 71	0
2	H	10/15 (66%)	0.25	0 100 100	40, 45, 59, 101	0
2	I	4/15 (26%)	1.39	1 (25%) 1 1	46, 54, 59, 84	0
2	J	4/15 (26%)	1.59	1 (25%) 1 1	47, 54, 65, 76	0
2	K	12/15 (80%)	0.12	0 100 100	36, 38, 49, 50	0
2	L	4/15 (26%)	0.72	0 100 100	47, 50, 61, 68	0
All	All	2125/2190 (97%)	-0.16	29 (1%) 78 83	19, 32, 52, 101	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	36	LEU	3.7
1	D	47	ASN	3.6
1	D	186	ILE	3.4
1	F	49	LYS	3.3
1	E	47	ASN	3.1
1	C	47	ASN	3.0
1	A	300	ARG	3.0
1	B	197	ASP	2.9
1	F	104	VAL	2.8
2	I	443	THR	2.7
2	G	449	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	9	THR	2.6
1	F	45	PHE	2.6
1	E	36	LEU	2.6
1	C	37	GLY	2.5
1	B	301	LEU	2.5
1	D	37	GLY	2.4
1	F	327	VAL	2.4
1	F	51	VAL	2.3
1	C	263	THR	2.2
1	C	300[A]	ARG	2.2
1	A	47	ASN	2.2
1	A	305	VAL	2.2
1	D	42	ASP	2.1
1	F	348	SER	2.1
2	J	445	CYS	2.1
2	G	448	GLU	2.1
1	A	301	LEU	2.1
1	A	37	GLY	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	HS8	C	252	14/15	0.97	0.10	-	24,27,41,43	4
1	HS8	A	252	14/15	0.96	0.15	-	20,24,41,47	4
1	HS8	E	252	14/15	0.96	0.13	-	21,24,44,46	4
1	HS8	F	252	14/15	0.95	0.09	-	23,28,46,49	4
1	HS8	D	252	14/15	0.97	0.12	-	26,29,47,48	4
1	HS8	B	252	14/15	0.96	0.12	-	23,28,41,47	4

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
5	GOL	A	605	6/6	0.85	0.21	12.02	44,60,70,72	0
4	RCO	A	602	8/8	0.81	0.20	9.07	44,49,59,62	0
5	GOL	D	604	6/6	0.66	0.20	7.31	45,58,64,70	0
5	GOL	B	605	6/6	0.83	0.27	6.88	41,50,57,59	0
5	GOL	B	606	6/6	0.82	0.26	6.07	55,67,71,75	0
5	GOL	C	605	6/6	0.65	0.33	6.06	39,48,59,65	0
4	RCO	D	603	8/8	0.81	0.19	4.89	42,50,61,68	0
4	RCO	A	604	8/8	0.90	0.27	4.00	39,43,52,52	0
6	ACT	K	501	4/4	0.81	0.18	3.37	65,67,78,78	0
4	RCO	D	602	8/8	0.70	0.22	3.23	53,62,72,78	0
5	GOL	C	604	6/6	0.82	0.22	3.22	55,67,79,83	0
4	RCO	E	603	8/8	0.91	0.13	1.38	34,41,50,61	0
4	RCO	E	602	8/8	0.96	0.15	1.36	33,39,47,47	0
4	RCO	B	602	8/8	0.90	0.16	1.04	38,46,58,61	0
4	RCO	B	603	8/8	0.89	0.18	0.74	31,39,50,51	0
5	GOL	B	604	6/6	0.92	0.15	0.57	30,44,54,56	0
4	RCO	C	602	8/8	0.92	0.13	0.28	32,38,51,53	0
3	CU	B	601	1/1	1.00	0.08	0.11	27,27,27,27	0
4	RCO	A	603	8/8	0.95	0.16	-0.01	29,36,48,52	0
3	CU	D	601	1/1	1.00	0.09	-0.09	29,29,29,29	0
3	CU	A	601	1/1	1.00	0.09	-0.21	27,27,27,27	0
4	RCO	C	603	8/8	0.90	0.16	-0.25	30,37,48,54	0
3	CU	C	601	1/1	1.00	0.08	-1.38	27,27,27,27	0
3	CU	E	601	1/1	1.00	0.07	-1.62	26,26,26,26	0
3	CU	F	700	1/1	0.99	0.06	-2.63	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.