



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 21, 2016 – 11:59 PM EDT

PDB ID : 5HSA
Title : Alcohol Oxidase AOX1 from Pichia Pastoris
Authors : Neumann, P.; Ficner, R.; Feussner, I.; Koch, C.
Deposited on : 2016-01-25
Resolution : 2.35 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
<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 : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

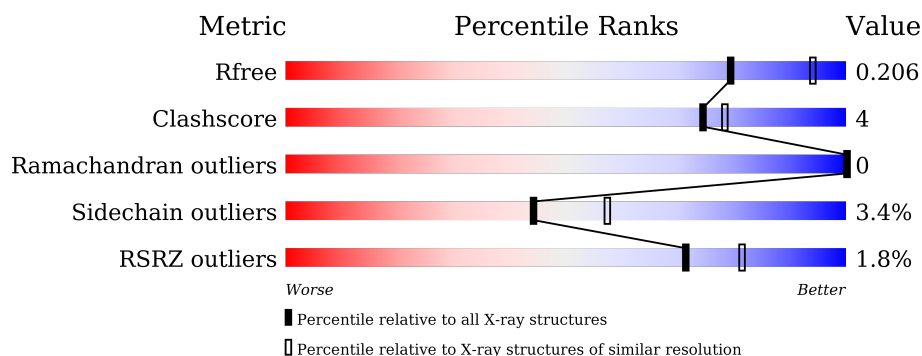
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	663	<div> <div></div> <div>89% 10% .</div> </div>
1	B	663	<div> <div>3%</div> <div>88% 11% .</div> </div>
1	C	663	<div> <div></div> <div>89% 10% .</div> </div>
1	D	663	<div> <div>4%</div> <div>90% 8% .</div> </div>
1	E	663	<div> <div>%</div> <div>89% 10% .</div> </div>
1	F	663	<div> <div>%</div> <div>89% 9% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	663	 % 89% 10%
1	H	663	 4% 88% 10%

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
3	P6G	B	702	-	-	-	X
3	P6G	B	703	-	-	-	X
3	P6G	C	702	-	-	-	X
3	P6G	C	703	-	-	-	X
3	P6G	E	702	-	-	-	X
3	P6G	F	703	-	-	-	X
4	PGE	A	703	-	-	-	X
4	PGE	B	704	-	-	-	X
4	PGE	C	704	-	-	-	X
4	PGE	D	703	-	-	-	X
4	PGE	E	703	-	-	-	X
4	PGE	G	702	-	-	-	X
4	PGE	G	703	-	-	-	X
7	GOL	F	705	-	-	-	X

2 Entry composition

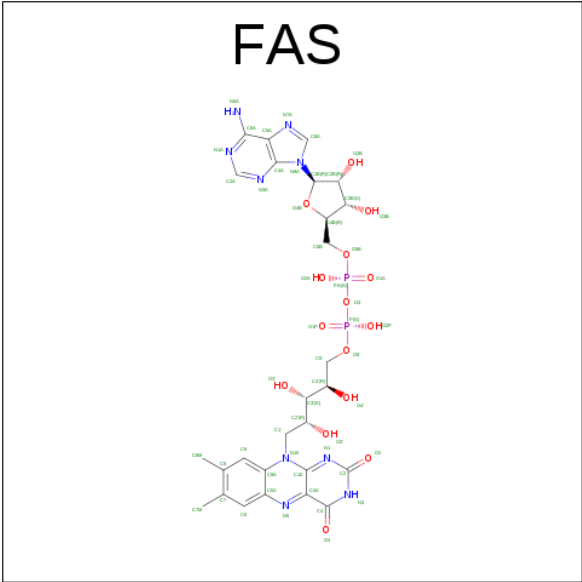
There are 9 unique types of molecules in this entry. The entry contains 44407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alcohol oxidase 1.

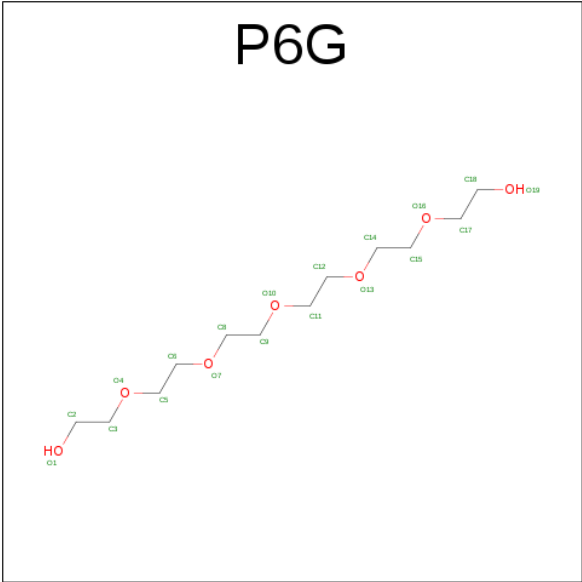
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	B	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	C	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	D	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	E	662	Total	C	N	O	S	0	1	0
			5206	3291	901	988	26			
1	F	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	G	662	Total	C	N	O	S	0	1	0
			5207	3292	901	988	26			
1	H	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			

- Molecule 2 is ARABINO-FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAS) (formula: C₂₇H₃₃N₉O₁₅P₂).



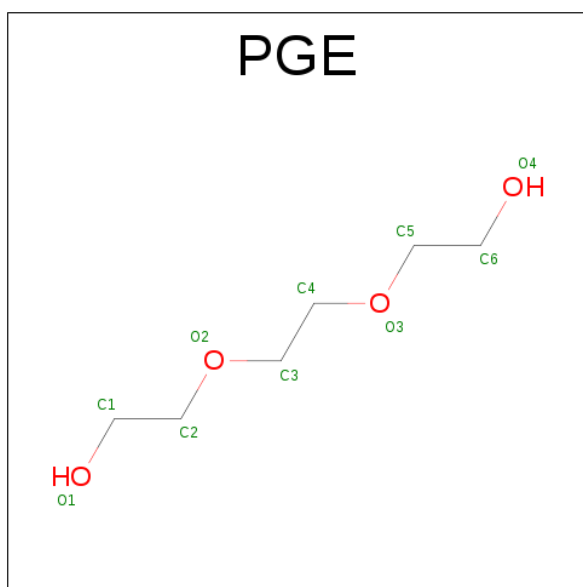
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



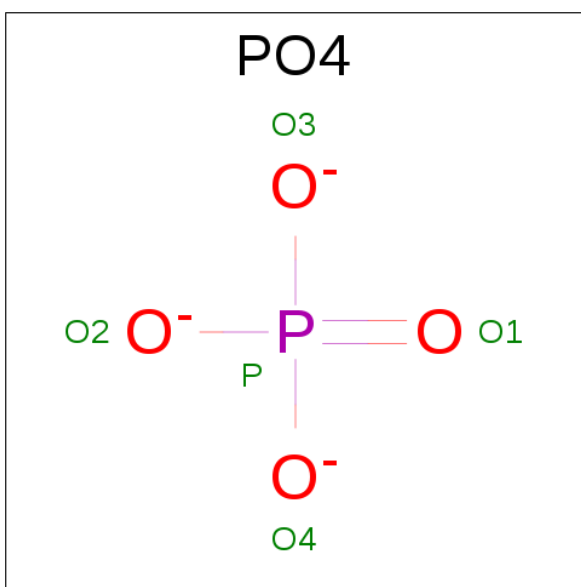
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		
3	D	1	Total	C	O	0	0
			19	12	7		
3	E	1	Total	C	O	0	0
			19	12	7		
3	F	1	Total	C	O	0	0
			19	12	7		
3	F	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		
4	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

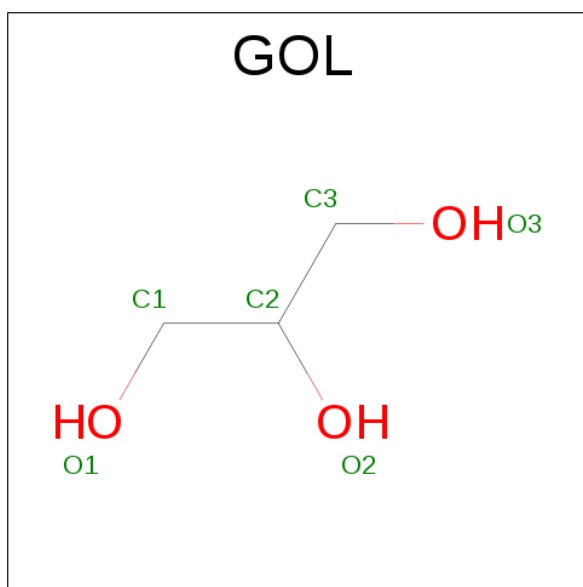


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	1
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	1
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	358	Total	O	0	2
			359	359		
9	B	226	Total	O	0	1
			226	226		
9	C	325	Total	O	0	3
			325	325		
9	D	178	Total	O	0	2
			178	178		
9	E	356	Total	O	0	0
			356	356		
9	F	300	Total	O	0	0
			300	300		

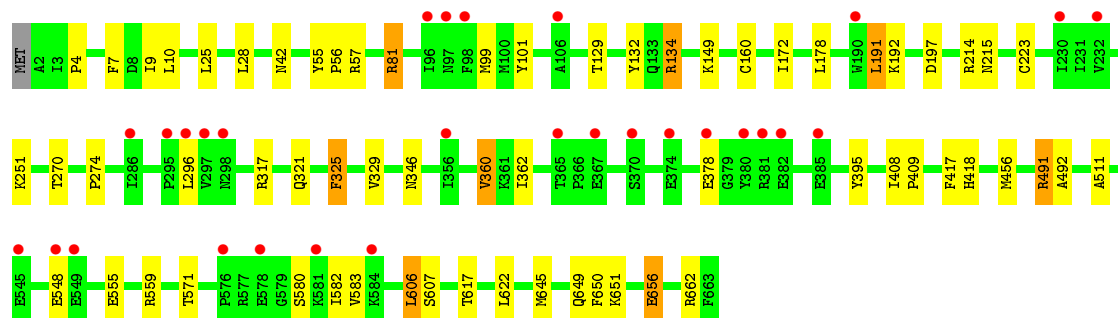
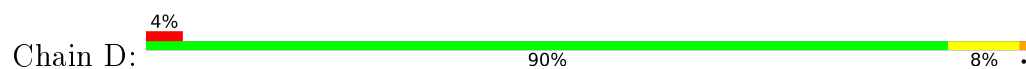
Continued on next page...

Continued from previous page...

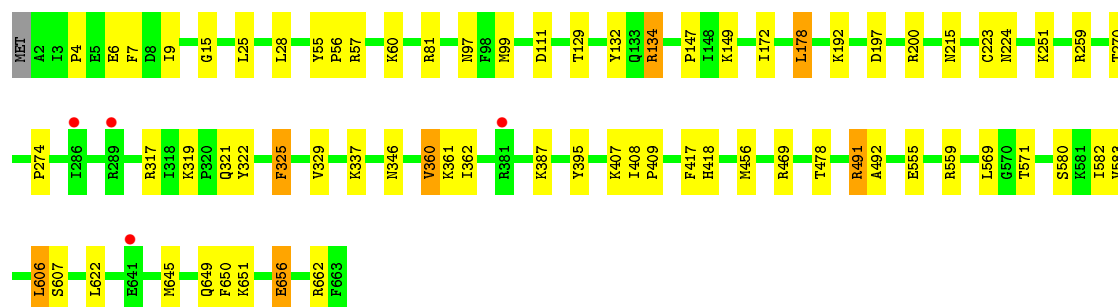
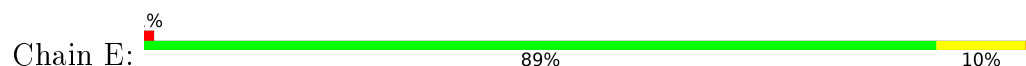
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	211	Total 211	O 211	0	0
9	H	129	Total 129	O 129	0	0



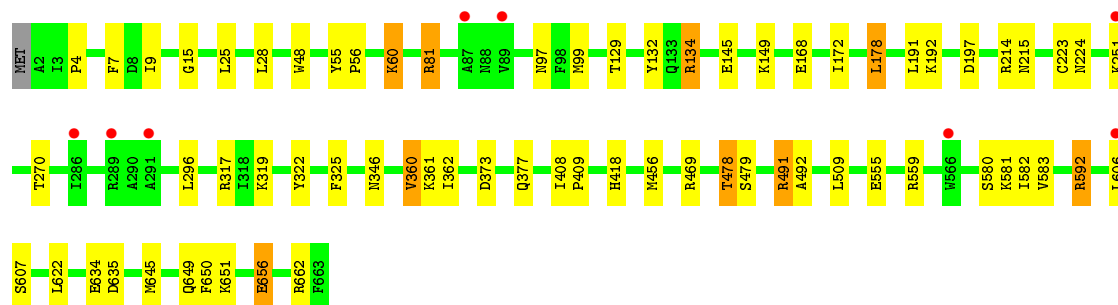
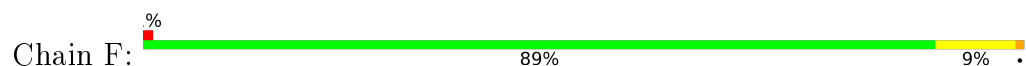
• Molecule 1: Alcohol oxidase 1



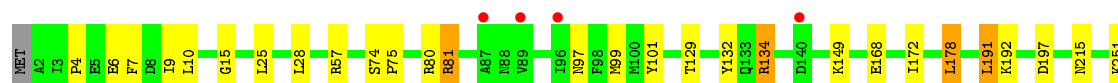
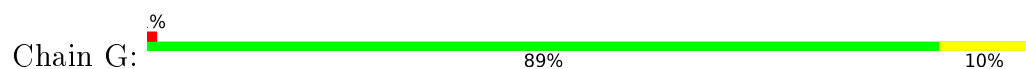
• Molecule 1: Alcohol oxidase 1

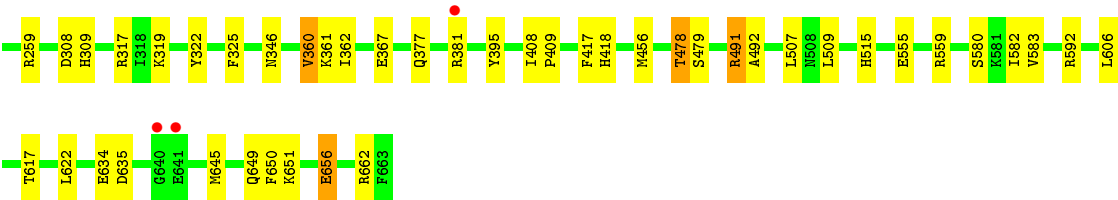


• Molecule 1: Alcohol oxidase 1

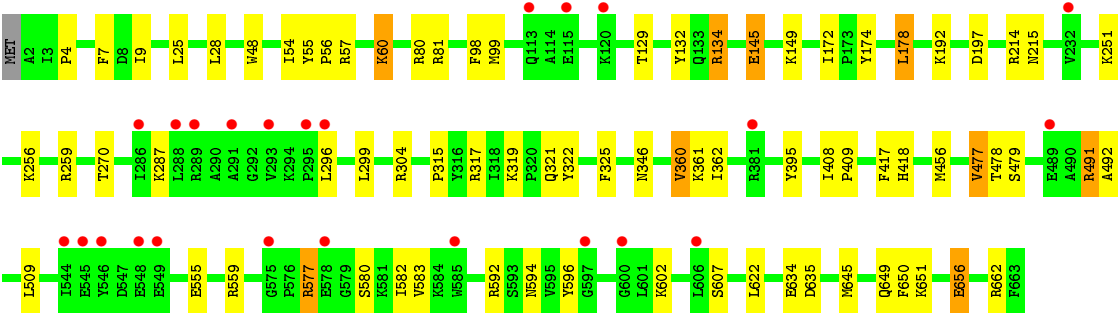
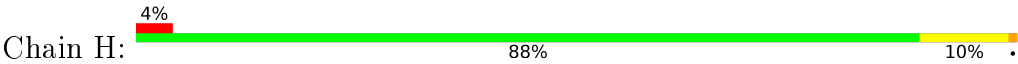


• Molecule 1: Alcohol oxidase 1





● Molecule 1: Alcohol oxidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.10Å 165.19Å 164.31Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	40.88 – 2.35 45.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.88-2.35) 98.7 (45.67-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.177 , 0.205 0.175 , 0.206	Depositor DCC
R_{free} test set	12268 reflections (4.82%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 254642 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	44407	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, PGE, CL, FAS, PO4, P6G, CA

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	0.29	0/5341	0.46	0/7245
1	B	0.27	0/5341	0.46	0/7245
1	C	0.29	0/5341	0.47	0/7245
1	D	0.26	0/5341	0.45	0/7245
1	E	0.30	0/5348	0.47	0/7255
1	F	0.28	0/5341	0.46	0/7245
1	G	0.27	0/5349	0.46	0/7256
1	H	0.26	0/5341	0.45	0/7245
All	All	0.28	0/42743	0.46	0/57981

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 [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	5199	0	5013	45	0
1	B	5199	0	5013	43	0
1	C	5199	0	5013	50	0
1	D	5199	0	5013	36	0
1	E	5206	0	5021	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5199	0	5013	45	0
1	G	5207	0	5023	45	0
1	H	5199	0	5013	47	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
2	E	53	0	31	3	0
2	F	53	0	31	3	0
2	G	53	0	31	3	0
2	H	53	0	31	1	0
3	A	19	0	26	1	0
3	B	38	0	52	10	0
3	C	38	0	52	13	0
3	D	19	0	26	1	0
3	E	19	0	26	4	0
3	F	38	0	52	8	0
4	A	10	0	14	2	0
4	B	20	0	28	1	0
4	C	10	0	14	1	0
4	D	10	0	14	0	0
4	E	10	0	14	0	0
4	G	20	0	28	0	0
4	H	10	0	14	1	0
5	A	5	0	0	1	0
5	F	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
7	C	6	0	8	0	0
7	F	6	0	8	2	0
8	C	1	0	0	0	0
9	A	359	0	0	3	0
9	B	226	0	0	2	0
9	C	325	0	0	4	0
9	D	178	0	0	3	0
9	E	356	0	0	3	0
9	F	300	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	211	0	0	0	0
9	H	129	0	0	1	0
All	All	44407	0	40746	334	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 4.

The worst 5 of 334 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:CYS:H	3:B:702:P6G:H62	1.36	0.89
3:C:703:P6G:H111	1:D:42:ASN:HD22	1.48	0.77
1:C:479:SER:HB2	3:F:702:P6G:H62	1.66	0.75
1:C:649:GLN:NE2	1:C:651:LYS:HG2	2.03	0.73
5:F:704:PO4:O3	9:F:801:HOH:O	2.08	0.71

There are no symmetry-related clashes.

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	660/663 (100%)	637 (96%)	23 (4%)	0	100	100
1	B	660/663 (100%)	635 (96%)	25 (4%)	0	100	100
1	C	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	D	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	E	661/663 (100%)	639 (97%)	22 (3%)	0	100	100
1	F	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	G	661/663 (100%)	639 (97%)	22 (3%)	0	100	100
1	H	660/663 (100%)	638 (97%)	22 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5282/5304 (100%)	5102 (97%)	180 (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	560/561 (100%)	545 (97%)	15 (3%)	52	67
1	B	560/561 (100%)	541 (97%)	19 (3%)	44	57
1	C	560/561 (100%)	538 (96%)	22 (4%)	39	51
1	D	560/561 (100%)	540 (96%)	20 (4%)	42	55
1	E	561/561 (100%)	544 (97%)	17 (3%)	48	62
1	F	560/561 (100%)	540 (96%)	20 (4%)	42	55
1	G	561/561 (100%)	544 (97%)	17 (3%)	48	62
1	H	560/561 (100%)	539 (96%)	21 (4%)	40	52
All	All	4482/4488 (100%)	4331 (97%)	151 (3%)	44	57

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	378	GLU
1	E	325	PHE
1	H	317	ARG
1	D	456	MET
1	E	57	ARG

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

Mol	Chain	Res	Type
1	B	215	ASN
1	F	556	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 9 are monoatomic - leaving 30 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
2	FAS	A	701	-	52,58,58	1.34	5 (9%)	52,89,89	2.12	10 (19%)
3	P6G	A	702	-	18,18,18	0.47	0	17,17,17	0.40	0
4	PGE	A	703	-	9,9,9	0.33	0	8,8,8	0.36	0
5	PO4	A	704[B]	-	4,4,4	0.79	0	6,6,6	0.24	0
2	FAS	B	701	-	52,58,58	1.34	6 (11%)	52,89,89	2.19	9 (17%)
3	P6G	B	702	-	18,18,18	0.50	0	17,17,17	0.38	0
3	P6G	B	703	-	18,18,18	0.45	0	17,17,17	0.52	0
4	PGE	B	704	-	9,9,9	0.34	0	8,8,8	0.31	0
4	PGE	B	705	-	9,9,9	0.34	0	8,8,8	0.30	0
2	FAS	C	701	-	52,58,58	1.32	5 (9%)	52,89,89	2.11	10 (19%)
3	P6G	C	702	-	18,18,18	0.46	0	17,17,17	0.43	0
3	P6G	C	703	-	18,18,18	0.51	0	17,17,17	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	C	704	-	9,9,9	0.39	0	8,8,8	0.22	0
7	GOL	C	705[B]	6	5,5,5	0.36	0	5,5,5	0.23	0
2	FAS	D	701	-	52,58,58	1.34	6 (11%)	52,89,89	2.18	8 (15%)
3	P6G	D	702	-	18,18,18	0.48	0	17,17,17	0.32	0
4	PGE	D	703	-	9,9,9	0.34	0	8,8,8	0.31	0
2	FAS	E	701	-	52,58,58	1.38	6 (11%)	52,89,89	2.06	10 (19%)
3	P6G	E	702	-	18,18,18	0.49	0	17,17,17	0.41	0
4	PGE	E	703	-	9,9,9	0.39	0	8,8,8	0.24	0
2	FAS	F	701	-	52,58,58	1.33	5 (9%)	52,89,89	2.26	9 (17%)
3	P6G	F	702	-	18,18,18	0.46	0	17,17,17	0.46	0
3	P6G	F	703	-	18,18,18	0.47	0	17,17,17	0.40	0
5	PO4	F	704	-	4,4,4	0.54	0	6,6,6	0.23	0
7	GOL	F	705	-	5,5,5	0.33	0	5,5,5	0.33	0
2	FAS	G	701	-	52,58,58	1.33	5 (9%)	52,89,89	2.19	11 (21%)
4	PGE	G	702	-	9,9,9	0.35	0	8,8,8	0.24	0
4	PGE	G	703	-	9,9,9	0.35	0	8,8,8	0.27	0
2	FAS	H	701	-	52,58,58	1.34	5 (9%)	52,89,89	2.17	11 (21%)
4	PGE	H	702	-	9,9,9	0.34	0	8,8,8	0.27	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
2	FAS	A	701	-	-	0/30/50/50	0/6/6/6
3	P6G	A	702	-	-	0/16/16/16	0/0/0/0
4	PGE	A	703	-	-	0/7/7/7	0/0/0/0
5	PO4	A	704[B]	-	-	0/0/0/0	0/0/0/0
2	FAS	B	701	-	-	0/30/50/50	0/6/6/6
3	P6G	B	702	-	-	0/16/16/16	0/0/0/0
3	P6G	B	703	-	-	0/16/16/16	0/0/0/0
4	PGE	B	704	-	-	0/7/7/7	0/0/0/0
4	PGE	B	705	-	-	0/7/7/7	0/0/0/0
2	FAS	C	701	-	-	0/30/50/50	0/6/6/6
3	P6G	C	702	-	-	0/16/16/16	0/0/0/0
3	P6G	C	703	-	-	0/16/16/16	0/0/0/0
4	PGE	C	704	-	-	0/7/7/7	0/0/0/0
7	GOL	C	705[B]	6	-	0/4/4/4	0/0/0/0
2	FAS	D	701	-	-	0/30/50/50	0/6/6/6
3	P6G	D	702	-	-	0/16/16/16	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	D	703	-	-	0/7/7/7	0/0/0/0
2	FAS	E	701	-	-	0/30/50/50	0/6/6/6
3	P6G	E	702	-	-	0/16/16/16	0/0/0/0
4	PGE	E	703	-	-	0/7/7/7	0/0/0/0
2	FAS	F	701	-	-	0/30/50/50	0/6/6/6
3	P6G	F	702	-	-	0/16/16/16	0/0/0/0
3	P6G	F	703	-	-	0/16/16/16	0/0/0/0
5	PO4	F	704	-	-	0/0/0/0	0/0/0/0
7	GOL	F	705	-	-	0/4/4/4	0/0/0/0
2	FAS	G	701	-	-	0/30/50/50	0/6/6/6
4	PGE	G	702	-	-	0/7/7/7	0/0/0/0
4	PGE	G	703	-	-	0/7/7/7	0/0/0/0
2	FAS	H	701	-	-	0/30/50/50	0/6/6/6
4	PGE	H	702	-	-	0/7/7/7	0/0/0/0

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAS	C9A-N10	2.12	1.41	1.38
2	D	701	FAS	C9A-N10	2.26	1.42	1.38
2	E	701	FAS	C10-N10	2.27	1.41	1.39
2	G	701	FAS	C8-C7	2.84	1.48	1.41
2	C	701	FAS	C8-C7	2.84	1.48	1.41

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	FAS	N3A-C2A-N1A	-6.91	123.44	128.87
2	G	701	FAS	N3A-C2A-N1A	-6.81	123.52	128.87
2	F	701	FAS	N3A-C2A-N1A	-6.79	123.54	128.87
2	E	701	FAS	N3A-C2A-N1A	-6.76	123.56	128.87
2	H	701	FAS	N3A-C2A-N1A	-6.70	123.61	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAS	2	0
3	A	702	P6G	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	PGE	2	0
5	A	704[B]	PO4	1	0
3	B	702	P6G	6	0
3	B	703	P6G	4	0
4	B	704	PGE	1	0
2	C	701	FAS	2	0
3	C	702	P6G	5	0
3	C	703	P6G	8	0
4	C	704	PGE	1	0
2	D	701	FAS	1	0
3	D	702	P6G	1	0
2	E	701	FAS	3	0
3	E	702	P6G	4	0
2	F	701	FAS	3	0
3	F	702	P6G	4	0
3	F	703	P6G	4	0
5	F	704	PO4	1	0
7	F	705	GOL	2	0
2	G	701	FAS	3	0
2	H	701	FAS	1	0
4	H	702	PGE	1	0

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	662/663 (99%)	-0.25	3 (0%) 91 96	20, 34, 55, 70	0
1	B	662/663 (99%)	0.05	18 (2%) 58 70	25, 45, 73, 100	0
1	C	662/663 (99%)	-0.25	2 (0%) 94 97	22, 35, 53, 70	0
1	D	662/663 (99%)	0.16	29 (4%) 38 52	30, 52, 76, 102	0
1	E	662/663 (99%)	-0.28	4 (0%) 90 95	21, 34, 54, 91	0
1	F	662/663 (99%)	-0.15	8 (1%) 81 89	22, 41, 66, 86	0
1	G	662/663 (99%)	-0.09	7 (1%) 82 90	26, 44, 63, 87	0
1	H	662/663 (99%)	0.23	24 (3%) 46 60	34, 57, 86, 113	0
All	All	5296/5304 (99%)	-0.07	95 (1%) 71 81	20, 42, 70, 113	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	597	GLY	4.2
1	D	296	LEU	3.4
1	E	641	GLU	3.3
1	H	296	LEU	3.3
1	H	291	ALA	3.3

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 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	P6G	F	703	19/19	0.81	0.30	13.15	71,74,75,76	0
4	PGE	G	702	10/10	0.86	0.33	11.79	56,59,59,60	0
3	P6G	B	702	19/19	0.76	0.37	10.76	67,68,79,79	0
4	PGE	G	703	10/10	0.82	0.38	9.15	69,69,71,71	0
3	P6G	E	702	19/19	0.78	0.32	8.71	67,69,74,74	0
3	P6G	C	702	19/19	0.87	0.30	8.63	64,67,71,71	0
3	P6G	C	703	19/19	0.80	0.29	7.76	67,75,77,77	0
7	GOL	F	705	6/6	0.68	0.19	4.94	59,61,61,61	0
4	PGE	C	704	10/10	0.76	0.21	4.72	53,61,65,65	0
4	PGE	D	703	10/10	0.83	0.17	4.13	64,67,70,70	0
4	PGE	E	703	10/10	0.87	0.18	3.46	50,54,58,58	0
4	PGE	B	704	10/10	0.83	0.17	3.27	65,67,70,71	0
4	PGE	A	703	10/10	0.90	0.15	2.33	55,56,61,61	0
3	P6G	B	703	19/19	0.95	0.15	2.17	42,47,52,52	0
3	P6G	F	702	19/19	0.95	0.13	1.38	36,38,41,42	0
7	GOL	C	705[B]	6/6	0.90	0.14	1.29	48,50,51,51	6
4	PGE	B	705	10/10	0.92	0.13	1.21	54,55,57,58	0
4	PGE	H	702	10/10	0.87	0.15	1.09	67,68,69,69	0
3	P6G	A	702	19/19	0.96	0.13	0.83	29,34,37,37	0
3	P6G	D	702	19/19	0.94	0.14	0.71	49,52,55,56	0
2	FAS	E	701	53/53	0.98	0.19	0.64	28,29,32,34	0
5	PO4	F	704	5/5	0.90	0.15	0.51	46,50,51,52	0
2	FAS	D	701	53/53	0.95	0.19	0.50	41,45,49,50	0
2	FAS	F	701	53/53	0.97	0.19	0.46	36,40,45,48	0
2	FAS	C	701	53/53	0.98	0.17	0.44	25,28,30,35	0
2	FAS	A	701	53/53	0.98	0.17	0.36	28,30,35,37	0
2	FAS	G	701	53/53	0.97	0.19	0.33	31,33,36,37	0
2	FAS	B	701	53/53	0.95	0.19	0.31	40,43,52,52	0
2	FAS	H	701	53/53	0.95	0.17	0.13	45,48,58,59	0
6	CA	A	705	1/1	0.96	0.12	-	64,64,64,64	0
6	CA	F	706	1/1	0.87	0.12	-	89,89,89,89	0
6	CA	B	706	1/1	0.98	0.13	-	76,76,76,76	0
6	CA	C	708	1/1	0.91	0.14	-	97,97,97,97	0
6	CA	E	704	1/1	0.85	0.12	-	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	PO4	A	704[B]	5/5	0.98	0.15	-	39,41,43,44	5
6	CA	D	704	1/1	0.83	0.11	-	97,97,97,97	0
8	CL	C	706	1/1	0.91	0.08	-	84,84,84,84	0
6	CA	C	707	1/1	0.95	0.16	-	76,76,76,76	0
6	CA	G	704	1/1	0.81	0.22	-	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.