



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:25 AM GMT

PDB ID : 3UNV
Title : Pantoea agglomerans Phenylalanine Aminomutase
Authors : Geiger, J.; Strom, S.
Deposited on : 2011-11-16
Resolution : 1.54 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

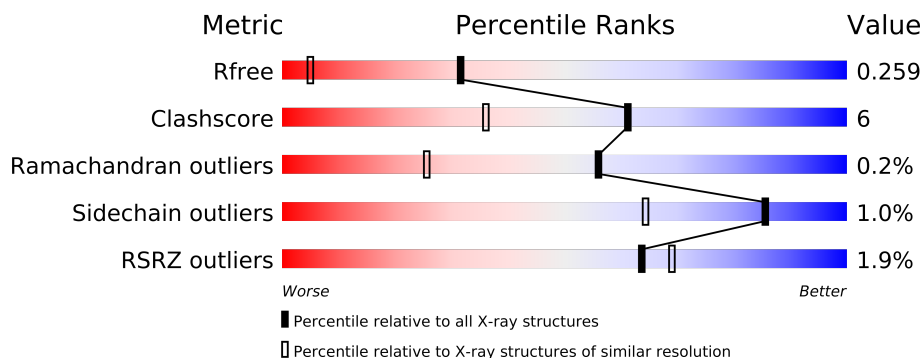
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.54 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}	66092	1031 (1.56-1.52)
Clashscore	79885	1155 (1.56-1.52)
Ramachandran outliers	78287	1127 (1.56-1.52)
Sidechain outliers	78261	1125 (1.56-1.52)
RSRZ outliers	66119	1031 (1.56-1.52)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	547	
1	B	547	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	A	1007	-	X
5	EDO	B	1003	-	X
5	EDO	B	1005	-	X
6	PO4	A	1008	-	X
6	PO4	A	550	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8538 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

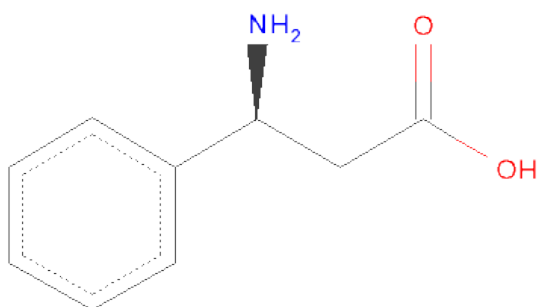
- Molecule 1 is a protein called AdmH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	1	3	0
			3981	2494	692	770	25			
1	B	514	Total	C	N	O	S	7	3	0
			3970	2489	689	767	25			

There are 16 discrepancies between the modelled and reference sequences:

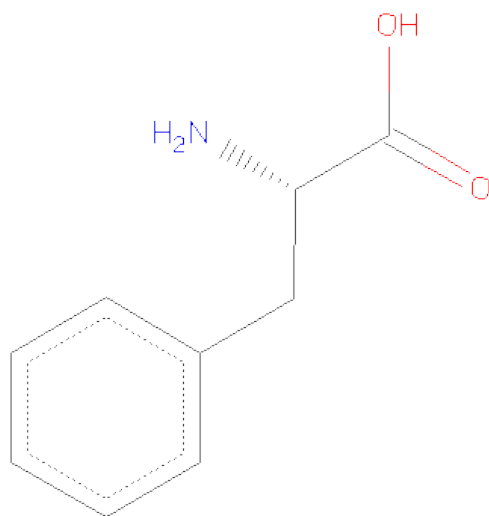
Chain	Residue	Modelled	Actual	Comment	Reference
A	542	LEU	-	EXPRESSION TAG	UNP Q84FL5
A	543	GLU	-	EXPRESSION TAG	UNP Q84FL5
A	544	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	545	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	546	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	547	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	548	HIS	-	EXPRESSION TAG	UNP Q84FL5
A	549	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	542	LEU	-	EXPRESSION TAG	UNP Q84FL5
B	543	GLU	-	EXPRESSION TAG	UNP Q84FL5
B	544	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	545	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	546	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	547	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	548	HIS	-	EXPRESSION TAG	UNP Q84FL5
B	549	HIS	-	EXPRESSION TAG	UNP Q84FL5

- Molecule 2 is (3S)-3-AMINO-3-PHENYLPROPANOICACID (three-letter code: SFE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			12	9	1	2		
2	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



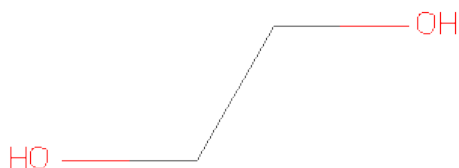
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			12	9	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



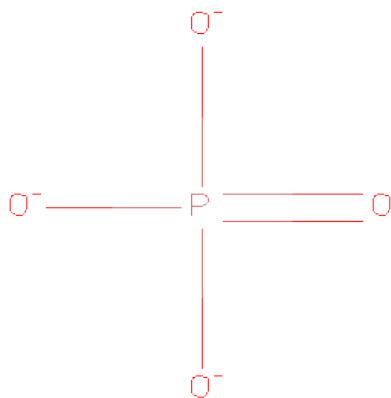
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 7 is water.

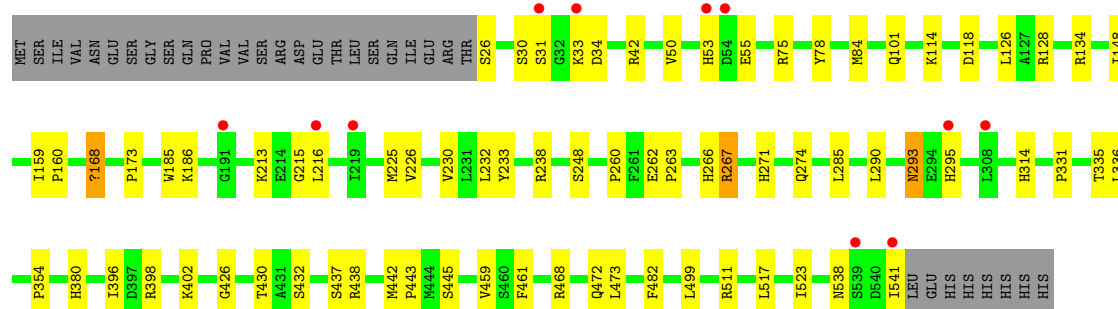
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	243	Total 243	O 243	0	0
7	B	248	Total 248	O 248	0	0

3 Residue-property plots

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.

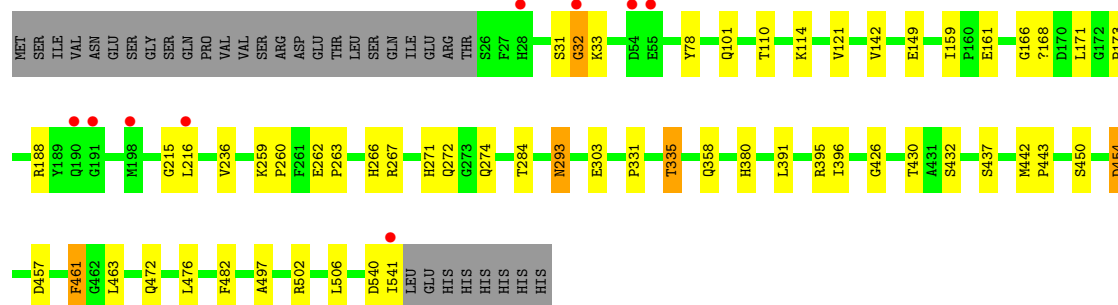
• Molecule 1: AdmH

Chain A: 



• Molecule 1: AdmH

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.96Å 185.84Å 72.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.54 27.81 – 1.54	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-1.54) 91.2 (27.81-1.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.204 , 0.247 0.213 , 0.259	Depositor DCC
R_{free} test set	7034 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	13 of 139966 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8538	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, SFE, EDO, KWS

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	1.29	6/4016 (0.1%)	1.07	15/5433 (0.3%)
1	B	1.27	6/4023 (0.1%)	1.04	10/5444 (0.2%)
All	All	1.28	12/8039 (0.1%)	1.06	25/10877 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
All	All	0	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	TYR	CD2-CE2	5.82	1.48	1.39
1	B	461	PHE	CE1-CZ	5.76	1.48	1.37
1	B	149	GLU	CG-CD	5.68	1.60	1.51
1	B	335	THR	CB-CG2	-5.64	1.33	1.52
1	B	236	VAL	CB-CG2	5.55	1.64	1.52
1	A	336	LEU	N-CA	5.49	1.57	1.46
1	A	55	GLU	CG-CD	5.43	1.60	1.51
1	B	272	GLN	CG-CD	5.27	1.63	1.51
1	A	398	ARG	CG-CD	5.23	1.65	1.51
1	A	445	SER	CB-OG	5.16	1.49	1.42
1	A	262	GLU	CD-OE2	-5.12	1.20	1.25
1	B	395	ARG	CZ-NH1	5.06	1.39	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	A	267[A]	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	267[B]	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	267[A]	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	267[B]	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	134	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	511	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	B	188	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	395	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	126	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	A	438	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	B	463	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	B	454	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	188	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	128	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	B	395	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	118	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	457	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	391	LEU	CB-CG-CD1	5.42	120.21	111.00
1	A	225	MET	CG-SD-CE	5.37	108.79	100.20
1	A	75	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	468	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	476	LEU	CB-CG-CD2	-5.23	102.10	111.00
1	A	34	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	506	LEU	CB-CG-CD2	-5.14	102.26	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168[A]	KWS	Mainchain,Peptide
1	A	168[B]	KWS	Mainchain,Peptide
1	B	166	GLY	Mainchain
1	B	168	KWS	Mainchain,Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3981	0	3997	52	0
1	B	3970	0	3988	40	0
2	A	12	0	8	4	0
2	B	12	0	9	1	0
3	A	12	0	8	1	0
4	A	6	0	8	1	0
4	B	12	0	16	1	0
5	A	16	0	24	5	0
5	B	16	0	24	11	0
6	A	10	0	0	1	0
7	A	243	0	0	6	0
7	B	248	0	0	2	0
All	All	8538	0	8082	94	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (94) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:779:HOH:O	5:B:550:EDO:H22	1.59	1.01
1:B:454:ASP:OD1	5:B:1003:EDO:H21	1.68	0.92
1:A:538:ASN:O	1:A:541:ILE:HG22	1.81	0.81
1:B:266:HIS:HD2	1:B:274:GLN:HE21	1.33	0.77
1:A:266:HIS:HD2	1:A:274:GLN:HE21	1.32	0.74
1:A:271:HIS:HD2	4:A:1002:GOL:O2	1.70	0.74
1:B:78:TYR:OH	2:B:1000:SFE:HA2C	1.88	0.73
1:A:168[A]:KWS:HB2A	2:A:1000[A]:SFE:HD1	1.73	0.70
7:A:779:HOH:O	5:B:550:EDO:C2	2.25	0.70
1:A:538:ASN:O	1:A:541:ILE:CG2	2.41	0.69
1:A:238:ARG:HH22	5:A:1005:EDO:H22	1.57	0.68
1:B:259:LYS:O	1:B:262[B]:GLU:HG3	1.94	0.68
1:A:260:PRO:O	1:A:266:HIS:HE1	1.79	0.66
7:A:627:HOH:O	5:B:1003:EDO:H22	1.98	0.64
1:B:271:HIS:HD2	4:B:1001:GOL:O2	1.80	0.63
1:B:497:ALA:HB2	5:B:1004:EDO:H12	1.79	0.62
1:A:168[A]:KWS:HB2A	2:A:1000[A]:SFE:CD1	2.28	0.62
1:B:497:ALA:CB	5:B:1004:EDO:H12	2.30	0.61
1:A:168[A]:KWS:CB2	2:A:1000[A]:SFE:CD1	2.80	0.59
1:A:266:HIS:CD2	1:A:274:GLN:HE21	2.16	0.59
1:A:101:GLN:HE21	1:A:215:GLY:H	1.50	0.59
1:A:232:LEU:HD23	1:A:541:ILE:CD1	2.33	0.58
1:B:101:GLN:HE21	1:B:215:GLY:H	1.51	0.58
1:A:523:ILE:HG12	1:B:110:THR:HG22	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:ARG:HH21	5:A:1005:EDO:C1	2.17	0.57
1:A:314:HIS:HE1	7:A:769:HOH:O	1.89	0.55
1:A:380:HIS:HD2	7:A:750:HOH:O	1.89	0.55
1:A:293:ASN:HD22	1:A:295:HIS:H	1.54	0.55
1:A:293:ASN:HD21	1:A:295:HIS:HB3	1.71	0.54
1:B:114:LYS:O	1:B:161:GLU:HG3	2.07	0.54
1:A:437:SER:HA	1:A:472:GLN:HE22	1.73	0.54
1:B:31:SER:O	1:B:32:GLY:O	2.25	0.53
1:A:78:TYR:OH	2:A:1000[A]:SFE:HA2C	2.08	0.53
1:A:232:LEU:HD23	1:A:541:ILE:HD11	1.91	0.53
1:B:101:GLN:HE21	1:B:215:GLY:N	2.07	0.52
1:A:293:ASN:ND2	1:A:295:HIS:H	2.08	0.52
1:B:442:MET:SD	1:B:443:PRO:HD2	2.50	0.52
1:B:260:PRO:O	1:B:266:HIS:HE1	1.93	0.51
1:A:101:GLN:HE21	1:A:215:GLY:N	2.08	0.51
1:A:248:SER:HB3	1:A:285:LEU:HD21	1.93	0.51
1:A:293:ASN:HD22	1:A:293:ASN:C	2.15	0.50
1:A:30:SER:HA	1:A:53:HIS:HB3	1.92	0.50
7:A:627:HOH:O	5:B:1003:EDO:C2	2.55	0.49
1:A:442:MET:SD	1:A:443:PRO:HD2	2.52	0.49
1:B:380:HIS:HD2	7:B:635:HOH:O	1.95	0.49
1:B:497:ALA:H	5:B:1004:EDO:C1	2.26	0.49
1:B:266:HIS:CD2	1:B:274:GLN:HE21	2.22	0.49
1:A:232:LEU:CD2	1:A:541:ILE:HD11	2.44	0.47
1:A:78:TYR:CE1	1:A:84:MET:HA	2.50	0.46
1:A:293:ASN:HD22	1:A:295:HIS:N	2.13	0.46
1:B:331:PRO:O	1:B:335:THR:HG22	2.15	0.46
1:A:473:LEU:HD23	1:A:541:ILE:HD11	1.98	0.45
1:A:232:LEU:HD23	1:A:541:ILE:HD12	1.97	0.45
5:A:1007:EDO:H21	6:A:1008:PO4:O3	2.15	0.45
1:B:142:VAL:HG23	7:B:681:HOH:O	2.15	0.45
1:B:426:GLY:HA3	1:B:482:PHE:CZ	2.51	0.45
1:B:284:THR:HG23	1:B:502:ARG:HB3	1.99	0.45
1:A:263:PRO:O	1:A:267[B]:ARG:HG3	2.17	0.45
1:B:437:SER:HA	1:B:472:GLN:HE22	1.82	0.45
1:B:454:ASP:OD1	5:B:1003:EDO:C2	2.53	0.44
1:A:213:LYS:HE2	1:A:354:PRO:HD2	1.99	0.44
1:A:426:GLY:HA3	1:A:482:PHE:CZ	2.52	0.44
1:B:101:GLN:HE22	1:B:216:LEU:H	1.65	0.43
1:A:432:SER:HA	1:B:461:PHE:CE1	2.53	0.43
1:A:226:VAL:O	1:A:230:VAL:HG13	2.18	0.43
1:A:159:ILE:HA	1:A:160:PRO:HD3	1.88	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:159:ILE:HG21	1:B:173:PRO:HB3	2.01	0.43
1:A:168[A]:KWS:HG2	1:A:459:VAL:HA	2.01	0.42
1:A:42:ARG:HH21	5:A:1005:EDO:H11	1.84	0.42
1:A:159:ILE:HG23	1:A:173:PRO:HA	2.01	0.42
1:A:396:ILE:HD13	1:A:430:THR:HG21	2.01	0.42
1:B:262[B]:GLU:HA	1:B:263:PRO:HD3	1.93	0.42
1:A:461:PHE:CE1	1:B:432:SER:HA	2.55	0.42
1:B:259:LYS:N	1:B:260:PRO:CD	2.83	0.42
1:B:497:ALA:H	5:B:1004:EDO:H11	1.85	0.41
1:B:450:SER:O	5:B:1003:EDO:O1	2.34	0.41
1:A:168[B]:KWS:HB2	3:A:1001[B]:PHE:HB2	1.83	0.41
1:A:50:VAL:HB	1:A:148:ILE:HG23	2.02	0.41
1:B:396:ILE:HD13	1:B:430:THR:HG21	2.03	0.41
1:A:260:PRO:O	1:A:266:HIS:CE1	2.67	0.41
1:A:331:PRO:O	1:A:335:THR:HG22	2.21	0.41
1:B:267[B]:ARG:HD2	1:B:267[B]:ARG:HH21	1.62	0.41
1:A:185:TRP:CG	1:A:186:LYS:N	2.88	0.41
1:B:541:ILE:O	1:B:541:ILE:HG23	2.20	0.41
1:A:168[B]:KWS:HG2	1:A:459:VAL:HA	2.02	0.41
1:A:101:GLN:NE2	1:A:216:LEU:H	2.19	0.41
1:B:159:ILE:HG23	1:B:173:PRO:HA	2.03	0.41
1:B:358:GLN:HE21	1:B:358:GLN:HB3	1.72	0.41
1:B:171:LEU:HA	1:B:171:LEU:HD23	1.94	0.40
1:B:121:VAL:HG22	1:B:159:ILE:HD12	2.03	0.40
1:B:101:GLN:NE2	1:B:216:LEU:H	2.20	0.40
1:A:114:LYS:H	5:A:1006:EDO:C2	2.34	0.40
1:A:290:LEU:HD12	1:A:499:LEU:HD23	2.04	0.40
1:B:293:ASN:HD22	1:B:293:ASN:C	2.24	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	513/547 (94%)	503 (98%)	10 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	514/547 (94%)	502 (98%)	10 (2%)	2 (0%)	43 16
All	All	1027/1094 (94%)	1005 (98%)	20 (2%)	2 (0%)	56 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	LYS
1	B	32	GLY

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	437/469 (93%)	431 (99%)	6 (1%)	78 50
1	B	436/469 (93%)	433 (99%)	3 (1%)	91 76
All	All	873/938 (93%)	864 (99%)	9 (1%)	85 64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	31	SER
1	A	33	LYS
1	A	293	ASN
1	A	402	LYS
1	A	517	LEU
1	B	293	ASN
1	B	303	GLU
1	B	540	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	58	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	101	GLN
1	A	102	ASN
1	A	143	ASN
1	A	184	GLN
1	A	266	HIS
1	A	271	HIS
1	A	293	ASN
1	A	314	HIS
1	A	358	GLN
1	A	380	HIS
1	A	404	ASN
1	A	456	GLN
1	A	472	GLN
1	B	48	GLN
1	B	58	ASN
1	B	101	GLN
1	B	102	ASN
1	B	136	ASN
1	B	184	GLN
1	B	266	HIS
1	B	271	HIS
1	B	293	ASN
1	B	295	HIS
1	B	358	GLN
1	B	380	HIS
1	B	404	ASN
1	B	456	GLN
1	B	472	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

3 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	KWS	A	168[A]	1,2	15,15,16	7.21	9 (60%)	19,21,23	3.97	11 (57%)
1	KWS	A	168[B]	1,3	15,15,16	7.16	8 (53%)	19,21,23	3.98	13 (68%)
1	KWS	B	168	1,2	15,15,16	7.75	7 (46%)	19,21,23	3.23	10 (52%)

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	KWS	A	168[A]	1,2	-	0/8/27/28	0/1/1/1
1	KWS	A	168[B]	1,3	-	0/8/27/28	0/1/1/1
1	KWS	B	168	1,2	-	0/8/27/28	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	KWS	O-C	26.03	1.29	1.11
1	A	168[A]	KWS	O-C	23.36	1.27	1.11
1	A	168[B]	KWS	O-C	22.54	1.27	1.11
1	B	168	KWS	O2-C2	11.04	1.47	1.23
1	A	168[B]	KWS	O2-C2	10.75	1.46	1.23
1	A	168[A]	KWS	O2-C2	10.32	1.45	1.23
1	A	168[A]	KWS	CB2-CA2	8.06	1.53	1.34
1	A	168[B]	KWS	CB2-CA2	7.32	1.51	1.34
1	B	168	KWS	CB2-CA2	6.26	1.49	1.34
1	A	168[B]	KWS	CA2-N2	-4.88	1.34	1.38
1	B	168	KWS	CA3-C	4.68	1.54	1.48
1	A	168[B]	KWS	C2-N3	-4.35	1.30	1.39
1	A	168[B]	KWS	CA-N	4.09	1.62	1.47
1	A	168[A]	KWS	C2-N3	-3.88	1.31	1.39
1	B	168	KWS	C2-N3	-3.84	1.31	1.39
1	A	168[A]	KWS	CA3-C	3.79	1.53	1.48
1	A	168[B]	KWS	CA3-C	3.54	1.53	1.48
1	B	168	KWS	CA-C1	-3.41	1.45	1.51
1	A	168[A]	KWS	CA-C1	-3.38	1.45	1.51
1	A	168[B]	KWS	CA-C1	-3.37	1.46	1.51
1	A	168[A]	KWS	CA2-C2	-3.00	1.36	1.43
1	B	168	KWS	CA2-C2	-2.56	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168[A]	KWS	C1-N3	-2.21	1.33	1.37
1	A	168[A]	KWS	CA3-N3	2.17	1.48	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168[A]	KWS	C2-CA2-N2	-10.18	101.06	108.96
1	A	168[B]	KWS	C2-CA2-N2	-9.50	101.58	108.96
1	B	168	KWS	C2-CA2-N2	-8.28	102.53	108.96
1	A	168[B]	KWS	CB-CA-N	7.83	119.39	109.22
1	A	168[A]	KWS	O2-C2-CA2	-6.19	127.38	130.96
1	A	168[A]	KWS	CB2-CA2-C2	5.87	131.81	122.29
1	A	168[A]	KWS	CA2-C2-N3	5.74	115.53	104.40
1	A	168[B]	KWS	CB2-CA2-C2	5.51	131.22	122.29
1	B	168	KWS	CA2-C2-N3	4.83	113.77	104.40
1	B	168	KWS	O2-C2-CA2	-4.75	128.21	130.96
1	B	168	KWS	CA2-N2-C1	4.41	109.21	105.36
1	A	168[B]	KWS	O2-C2-CA2	-4.30	128.47	130.96
1	A	168[A]	KWS	CA3-N3-C2	4.29	126.13	123.46
1	A	168[B]	KWS	CA2-C2-N3	4.26	112.66	104.40
1	A	168[A]	KWS	CA2-N2-C1	4.17	109.00	105.36
1	A	168[B]	KWS	CA2-N2-C1	4.06	108.91	105.36
1	A	168[B]	KWS	CG2-CB-CA	-3.64	105.80	112.56
1	B	168	KWS	CB2-CA2-C2	3.58	128.10	122.29
1	A	168[A]	KWS	O2-C2-N3	-3.57	117.02	124.71
1	A	168[B]	KWS	CA3-N3-C2	3.53	125.66	123.46
1	A	168[B]	KWS	C1-CA-N	-3.41	101.92	109.07
1	A	168[A]	KWS	CG2-CB-CA	-3.33	106.39	112.56
1	B	168	KWS	CB-CA-N	3.30	113.50	109.22
1	B	168	KWS	O2-C2-N3	-3.14	117.96	124.71
1	A	168[A]	KWS	CB-CA-N	3.10	113.24	109.22
1	B	168	KWS	CA3-N3-C2	2.81	125.21	123.46
1	A	168[B]	KWS	CA3-N3-C1	2.74	130.44	124.64
1	A	168[B]	KWS	O2-C2-N3	-2.73	118.82	124.71
1	B	168	KWS	CA3-N3-C1	2.70	130.35	124.64
1	A	168[A]	KWS	C2-N3-C1	-2.69	102.69	108.63
1	A	168[A]	KWS	CA3-N3-C1	2.68	130.32	124.64
1	A	168[B]	KWS	N3-C1-N2	2.37	113.25	111.51
1	A	168[B]	KWS	C2-N3-C1	-2.37	103.40	108.63
1	B	168	KWS	C2-N3-C1	-2.02	104.17	108.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	$\# Z > 2$
2	SFE	A	1000[A]	1	12,12,12	1.38	1 (8%)	15,15,15	1.81	4 (26%)
3	PHE	A	1001[B]	1	12,12,12	0.68	0	15,15,15	1.19	2 (13%)
4	GOL	A	1002	-	5,5,5	0.57	0	5,5,5	0.45	0
5	EDO	A	1004	-	3,3,3	0.75	0	2,2,2	0.88	0
5	EDO	A	1005	-	3,3,3	0.50	0	2,2,2	0.88	0
5	EDO	A	1006	-	3,3,3	0.12	0	2,2,2	1.28	0
5	EDO	A	1007	-	3,3,3	0.65	0	2,2,2	0.33	0
6	PO4	A	1008	-	4,4,4	0.35	0	6,6,6	0.34	0
6	PO4	A	550	-	4,4,4	1.39	1 (25%)	6,6,6	0.35	0
2	SFE	B	1000	1	12,12,12	1.16	1 (8%)	15,15,15	1.35	3 (20%)
4	GOL	B	1001	-	5,5,5	0.85	0	5,5,5	0.74	0
4	GOL	B	1002	-	5,5,5	0.17	0	5,5,5	0.77	0
5	EDO	B	1003	-	3,3,3	1.06	0	2,2,2	0.80	0
5	EDO	B	1004	-	3,3,3	0.48	0	2,2,2	1.22	0
5	EDO	B	1005	-	3,3,3	0.53	0	2,2,2	1.21	0
5	EDO	B	550	-	3,3,3	0.27	0	2,2,2	0.84	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	SFE	A	1000[A]	1	-	0/8/8/8	0/1/1/1
3	PHE	A	1001[B]	1	-	0/8/8/8	0/1/1/1
4	GOL	A	1002	-	-	0/4/4/4	0/0/0/0
5	EDO	A	1004	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1005	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1006	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1007	-	-	0/1/1/1	0/0/0/0
6	PO4	A	1008	-	-	0/0/0/0	0/0/0/0
6	PO4	A	550	-	-	0/0/0/0	0/0/0/0
2	SFE	B	1000	1	-	0/8/8/8	0/1/1/1
4	GOL	B	1001	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1002	-	-	0/4/4/4	0/0/0/0
5	EDO	B	1003	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1004	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1005	-	-	0/1/1/1	0/0/0/0
5	EDO	B	550	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000[A]	SFE	CG-CB	-3.82	1.46	1.52
2	B	1000	SFE	CG-CB	-2.63	1.48	1.52
6	A	550	PO4	P-O3	-2.03	1.44	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000[A]	SFE	CA-CB-CG	-4.11	104.94	111.79
2	A	1000[A]	SFE	CG-CB-N	-3.16	105.09	112.74
2	A	1000[A]	SFE	CD1-CG-CD2	2.73	121.96	118.33
2	B	1000	SFE	CE2-CD2-CG	-2.59	117.18	120.61
2	B	1000	SFE	CA-CB-CG	-2.57	107.51	111.79
3	A	1001[B]	PHE	CG-CB-CA	-2.56	108.31	114.34
2	A	1000[A]	SFE	CD1-CG-CB	-2.40	117.30	120.70
3	A	1001[B]	PHE	C-CA-N	2.26	113.11	109.36
2	B	1000	SFE	CD1-CG-CD2	2.01	121.01	118.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	514/547 (93%)	-0.08	11 (2%) 60 65	12, 19, 33, 42	1 (0%)
1	B	514/547 (93%)	-0.07	9 (1%) 65 71	12, 20, 33, 44	2 (0%)
All	All	1028/1094 (93%)	-0.07	20 (1%) 64 69	12, 20, 33, 44	3 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	ILE	10.9
1	B	541	ILE	9.5
1	B	54	ASP	5.4
1	B	32	GLY	3.9
1	A	191	GLY	3.3
1	B	55	GLU	3.1
1	B	191	GLY	2.9
1	A	216	LEU	2.5
1	B	28	HIS	2.5
1	A	539	SER	2.4
1	A	54	ASP	2.4
1	B	216	LEU	2.4
1	A	33	LYS	2.4
1	A	31	SER	2.3
1	A	308	LEU	2.3
1	B	190	GLN	2.3
1	A	53	HIS	2.3
1	A	295	HIS	2.2
1	B	198	MET	2.1
1	A	219	ILE	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	KWS	A	168[B]	15/16	0.11	0.75	19,20,23,27	15
1	KWS	A	168[A]	15/16	0.11	0.75	7,13,19,22	15
1	KWS	B	168	15/16	0.08	0.12	16,20,24,31	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	PO4	A	550	5/5	0.24	25.79	8,10,15,20	5
6	PO4	A	1008	5/5	0.24	9.16	53,54,56,56	0
5	EDO	B	1003	4/4	0.16	8.33	29,31,32,32	0
5	EDO	A	1007	4/4	0.16	5.64	48,53,54,56	0
5	EDO	B	1005	4/4	0.21	2.05	58,59,60,60	0
4	GOL	B	1002	6/6	0.11	1.96	26,32,33,37	0
5	EDO	B	1004	4/4	0.13	1.47	31,37,39,45	0
4	GOL	B	1001	6/6	0.10	1.23	22,27,29,29	0
2	SFE	B	1000	12/12	0.12	1.15	24,32,37,38	0
3	PHE	A	1001[B]	12/12	0.11	0.74	24,35,38,38	12
5	EDO	A	1006	4/4	0.11	0.73	29,30,31,33	0
2	SFE	A	1000[A]	12/12	0.11	0.68	23,26,27,27	12
4	GOL	A	1002	6/6	0.10	0.67	18,24,27,28	0
5	EDO	B	550	4/4	0.10	0.57	25,28,30,32	0
5	EDO	A	1004	4/4	0.08	0.46	24,25,27,28	0
5	EDO	A	1005	4/4	0.10	-0.60	41,42,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.