



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 PM UTC

PDB ID : 2C13 / pdb_00002c13
Title : 5-hydroxy-levulinic acid bound to Porphobilinogen synthase from *Pseudomonas aeruginosa*
Authors : Frere, F.; Nentwich, M.; Gacond, S.; Heinz, D.W.; Neier, R.; Frankenberg-Dinkel, N.
Deposited on : 2005-09-11
Resolution : 2.15 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

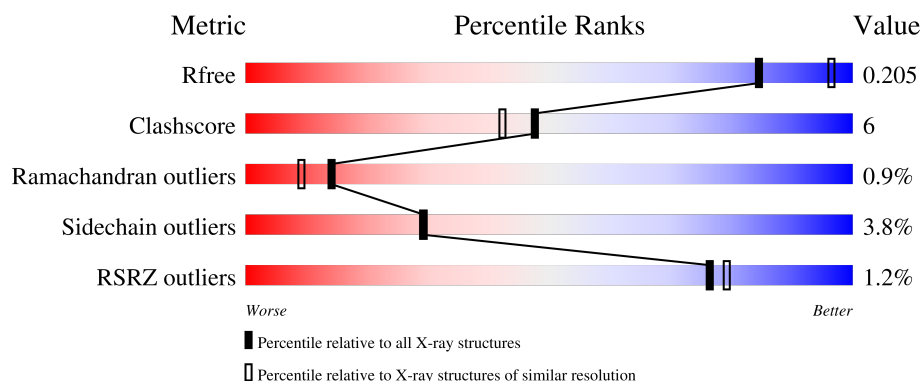
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. 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	337	% 82% 15% ...
1	B	337	% 85% 10% ...

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6020 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 DELTA-AMINOLEVULINIC ACID DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	21	1
			2777	1740	492	533	12			
1	B	331	Total	C	N	O	S	0	22	1
			2753	1723	482	536	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	VAL	ILE	engineered mutation	UNP Q59643
B	199	VAL	ILE	engineered mutation	UNP Q59643

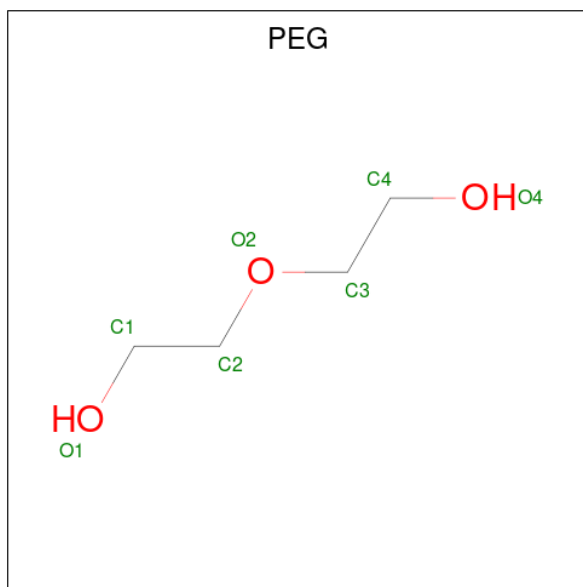
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

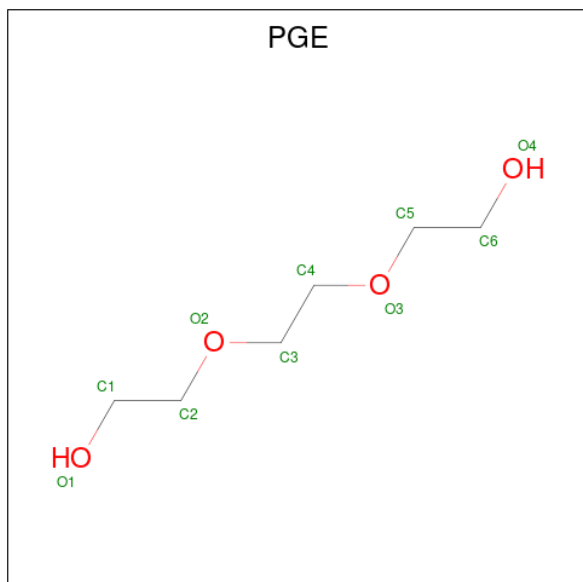


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 10	C 6	O 4	0	0
6	B	1	Total 10	C 6	O 4	0	0

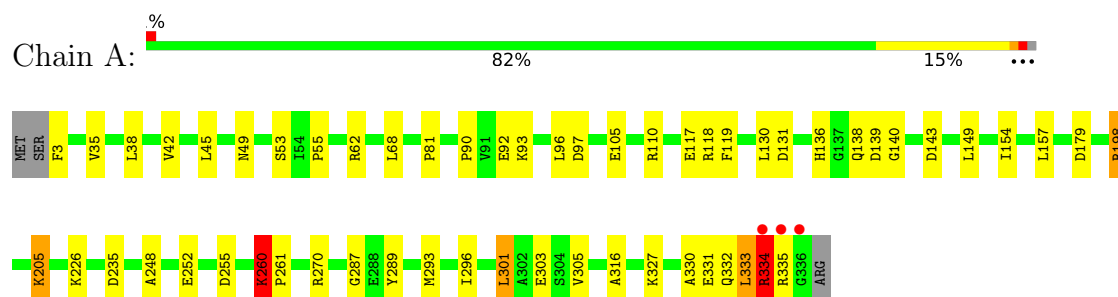
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	228	Total 228	O 228	0	0
7	B	229	Total 229	O 229	0	0

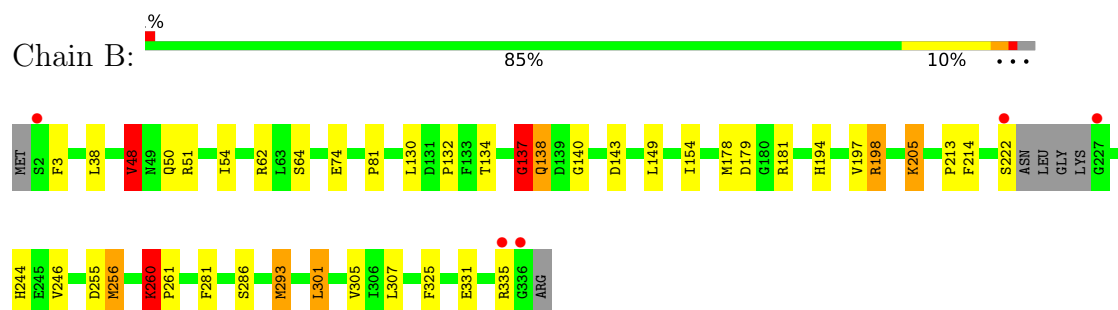
3 Residue-property plots

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: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



• Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.31Å 126.31Å 85.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.80 – 2.15 89.32 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (89.80-2.15) 99.2 (89.32-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.152 , 0.204 0.153 , 0.205	Depositor DCC
R_{free} test set	1931 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6020	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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, 0.333 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: PEG, MG, PGE, CL, K, FHL

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	0.96	0/2791	0.98	5/3782 (0.1%)
1	B	1.01	2/2766 (0.1%)	0.99	5/3749 (0.1%)
All	All	0.98	2/5557 (0.0%)	0.99	10/7531 (0.1%)

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	3
1	B	0	4
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	ILE	CA-CB	9.65	1.61	1.54
1	B	246	VAL	CA-CB	5.37	1.60	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	GLN	N-CA-C	7.45	126.67	110.80
1	A	333	LEU	N-CA-C	6.99	125.56	110.68
1	B	3	PHE	N-CA-C	6.34	118.40	107.93
1	B	64	SER	N-CA-C	-6.24	102.48	110.53
1	A	119	PHE	CA-C-N	5.20	124.99	119.28
1	A	119	PHE	C-N-CA	5.20	124.99	119.28
1	B	48	VAL	CB-CA-C	-5.07	102.59	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	GLY	N-CA-C	5.03	125.09	113.18
1	A	235	ASP	CA-C-N	5.01	125.28	119.47
1	A	235	ASP	C-N-CA	5.01	125.28	119.47

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	FHL	Peptide,Mainchain
1	A	333	LEU	Peptide
1	B	137	GLY	Peptide
1	B	205	FHL	Mainchain
1	B	260	FHL	Peptide,Mainchain

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	0	2718	32	0
1	B	2753	0	2670	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	7	0	10	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	20	0	28	1	0
7	A	228	0	0	5	0
7	B	229	0	0	1	0
All	All	6020	0	5426	62	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 6.

All (62) 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:330:ALA:O	1:A:334:ARG:HB2	1.83	0.78
1:B:293[B]:MET:CE	1:B:325:PHE:HE1	1.97	0.76
7:A:2002:HOH:O	1:B:244[B]:HIS:HD2	1.72	0.73
1:B:198:ARG:HD3	1:B:198:ARG:N	2.04	0.73
1:B:293[B]:MET:HE2	1:B:325:PHE:HE1	1.54	0.72
1:B:194:HIS:HB3	1:B:197[B]:VAL:CG1	2.24	0.67
1:B:154[B]:ILE:HD11	1:B:178:MET:HB3	1.78	0.66
1:B:154[B]:ILE:HD11	1:B:178:MET:CB	2.26	0.65
1:B:293[B]:MET:HE2	1:B:325:PHE:CE1	2.34	0.63
1:B:213:PRO:HB2	1:B:286:SER:HB2	1.81	0.62
1:A:136[A]:HIS:HD2	1:A:138:GLN:H	1.48	0.62
1:A:301:LEU:HG	1:A:305:VAL:HG11	1.83	0.60
1:B:143:ASP:HB3	1:B:149:LEU:HD21	1.84	0.59
1:A:252:GLU:HA	4:A:1338:PEG:H42	1.84	0.58
1:A:327:LYS:HE2	1:A:331:GLU:OE2	2.03	0.58
1:B:301:LEU:HG	1:B:305:VAL:HG11	1.87	0.56
1:A:252:GLU:HA	4:A:1338:PEG:C4	2.37	0.55
1:B:38:LEU:O	1:B:81:PRO:HD2	2.06	0.55
1:B:293[B]:MET:CE	1:B:325:PHE:CE1	2.86	0.55
1:A:289:TYR:CZ	1:A:293[A]:MET:HG3	2.42	0.54
1:A:45:LEU:HD21	1:A:62[A]:ARG:HD3	1.89	0.54
1:B:130:LEU:HD12	1:B:140:GLY:HA2	1.88	0.54
1:B:134:THR:OG1	1:B:137:GLY:HA2	2.06	0.54
1:A:35[A]:VAL:HG11	7:A:2074:HOH:O	2.09	0.53
1:B:48:VAL:O	1:B:50:GLN:HG2	2.09	0.52
1:A:136[A]:HIS:CD2	1:A:138:GLN:HB2	2.44	0.52
1:A:143:ASP:HB3	1:A:149:LEU:HD21	1.90	0.52
1:B:132:PRO:HB3	7:B:2084:HOH:O	2.10	0.52
1:A:130:LEU:HD12	1:A:140:GLY:HA2	1.92	0.51
1:A:105:GLU:O	1:A:110[A]:ARG:HD3	2.10	0.51
1:B:154[A]:ILE:HD11	1:B:179:ASP:O	2.11	0.50
1:A:332[B]:GLN:HG2	1:A:335:ARG:NH2	2.26	0.50
1:A:136[A]:HIS:CD2	1:A:138:GLN:H	2.30	0.49
1:B:198:ARG:HA	1:B:255:ASP:OD2	2.12	0.49
1:A:38:LEU:O	1:A:81:PRO:HD2	2.12	0.49
1:A:45:LEU:HG	1:A:62[A]:ARG:HB3	1.95	0.48
1:A:55:PRO:HB3	6:B:1338:PGE:H52	1.96	0.48
1:B:154[B]:ILE:HD11	1:B:178:MET:HB2	1.95	0.47
1:A:198:ARG:HA	1:A:255:ASP:OD2	2.15	0.47
1:A:131:ASP:HB3	1:A:139:ASP:OD1	2.16	0.46
1:A:136[A]:HIS:HE1	7:A:2084:HOH:O	1.98	0.46
1:A:90:PRO:HD2	1:A:93:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PHE:CG	1:B:260:FHL:H2C1	2.52	0.45
1:A:42[B]:VAL:HG21	1:A:68:LEU:HD13	1.99	0.45
1:B:260:FHL:H3C1	1:B:260:FHL:HEC2	1.81	0.45
1:A:97:ASP:HB3	7:A:2088:HOH:O	2.16	0.44
1:B:154[B]:ILE:CD1	1:B:178:MET:CB	2.93	0.44
1:B:256[A]:MET:HB2	1:B:281:PHE:CD1	2.53	0.43
1:A:42[B]:VAL:HG21	1:A:68:LEU:CD1	2.48	0.43
1:B:198:ARG:N	1:B:198:ARG:CD	2.79	0.42
1:A:205:FHL:H3C2	1:A:260:FHL:NZ	2.35	0.42
1:A:154:ILE:HD11	1:A:179:ASP:O	2.19	0.41
1:B:154[B]:ILE:HD12	1:B:181:ARG:CB	2.50	0.41
1:A:296:ILE:HG21	1:A:303[B]:GLU:HG2	2.01	0.41
1:A:92[A]:GLU:HG3	7:A:2081:HOH:O	2.20	0.41
1:A:248:ALA:O	1:A:252:GLU:HG3	2.21	0.41
1:A:270:ARG:HA	1:A:316:ALA:O	2.19	0.41
1:A:287:GLY:HA3	1:B:301:LEU:HD11	2.03	0.41
1:B:154[B]:ILE:CD1	1:B:178:MET:HB2	2.51	0.41
1:B:51:ARG:HA	1:B:62:ARG:O	2.21	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	351/337 (104%)	340 (97%)	9 (3%)	2 (1%)	21	15
1	B	346/337 (103%)	331 (96%)	11 (3%)	4 (1%)	10	5
All	All	697/674 (103%)	671 (96%)	20 (3%)	6 (1%)	14	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	PRO
1	B	137	GLY
1	B	261	PRO
1	A	334	ARG
1	B	138	GLN
1	B	335	ARG

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	285/267 (107%)	274 (96%)	11 (4%)	28	28
1	B	284/267 (106%)	270 (95%)	14 (5%)	22	19
All	All	569/534 (107%)	544 (96%)	25 (4%)	29	23

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	49	ASN
1	A	53	SER
1	A	96	LEU
1	A	117	GLU
1	A	118	ARG
1	A	157	LEU
1	A	198	ARG
1	A	226	LYS
1	A	301	LEU
1	A	334	ARG
1	B	48	VAL
1	B	74[A]	GLU
1	B	74[B]	GLU
1	B	198	ARG
1	B	222[A]	SER
1	B	222[B]	SER
1	B	256[A]	MET

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Mol	Chain	Res	Type
1	B	256[B]	MET
1	B	293[A]	MET
1	B	293[B]	MET
1	B	301	LEU
1	B	307	LEU
1	B	331[A]	GLU
1	B	331[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	50	GLN
1	A	297	GLN
1	B	7	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	FHL	B	260	1	14,16,17	0.99	0	11,18,20	1.54	1 (9%)
1	FHL	A	260	1	14,16,17	0.93	0	11,18,20	2.56	5 (45%)
1	FHL	B	205	1	14,16,17	0.95	0	11,18,20	1.29	1 (9%)
1	FHL	A	205	1	14,16,17	0.89	1 (7%)	11,18,20	0.96	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	FHL	B	260	1	-	0/15/17/19	-
1	FHL	A	260	1	-	0/15/17/19	-
1	FHL	B	205	1	-	3/15/17/19	-
1	FHL	A	205	1	-	2/15/17/19	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	FHL	O2-C1	-2.05	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	FHL	O3-C5-C4	5.22	122.46	111.84
1	A	260	FHL	C2-C3-C4	-4.93	109.99	115.17
1	B	260	FHL	O3-C5-C4	4.14	120.25	111.84
1	A	260	FHL	CD-CE-NZ	-2.75	105.80	110.67
1	A	260	FHL	CE-NZ-C4	2.25	128.72	122.33
1	B	205	FHL	O3-C5-C4	2.07	116.05	111.84
1	A	260	FHL	C3-C4-C5	2.01	123.67	118.79

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	205	FHL	C1-C2-C3-C4
1	A	205	FHL	C2-C3-C4-NZ
1	B	205	FHL	C2-C3-C4-C5
1	B	205	FHL	C2-C3-C4-NZ
1	A	205	FHL	C2-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	260	FHL	2	0
1	A	260	FHL	1	0
1	A	205	FHL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
6	PGE	B	1338	-	9,9,9	0.64	0	8,8,8	0.46	0
6	PGE	B	1339	-	9,9,9	0.68	0	8,8,8	0.33	0
4	PEG	A	1338	-	6,6,6	0.46	0	5,5,5	0.80	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
6	PGE	B	1338	-	-	5/7/7/7	-
6	PGE	B	1339	-	-	5/7/7/7	-
4	PEG	A	1338	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1338	PGE	O2-C3-C4-O3
6	B	1338	PGE	O1-C1-C2-O2
6	B	1339	PGE	O3-C5-C6-O4
6	B	1339	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	B	1339	PGE	O1-C1-C2-O2
4	A	1338	PEG	C1-C2-O2-C3
6	B	1338	PGE	C3-C4-O3-C5
6	B	1339	PGE	C1-C2-O2-C3
6	B	1338	PGE	O3-C5-C6-O4
4	A	1338	PEG	C4-C3-O2-C2
6	B	1338	PGE	C4-C3-O2-C2
6	B	1339	PGE	C6-C5-O3-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1338	PGE	1	0
4	A	1338	PEG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	205:FHL	C	206:TYR	N	1.62

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	332/337 (98%)	-0.65	3 (0%) 81 83	6, 15, 26, 58	21 (6%)
1	B	329/337 (97%)	-0.56	5 (1%) 72 76	6, 15, 27, 50	25 (7%)
All	All	661/674 (98%)	-0.61	8 (1%) 76 79	6, 15, 27, 58	46 (6%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	ARG	5.9
1	B	336	GLY	4.7
1	B	2	SER	3.5
1	A	336	GLY	2.7
1	B	222[A]	SER	2.5
1	A	334	ARG	2.3
1	B	227	GLY	2.2
1	A	335	ARG	2.0

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

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
1	FHL	B	205	17/18	0.95	0.07	15,20,29,33	0
1	FHL	A	205	17/18	0.96	0.06	10,13,19,22	0
1	FHL	B	260	17/18	0.96	0.06	5,12,14,16	0
1	FHL	A	260	17/18	0.97	0.05	2,12,14,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
6	PGE	B	1339	10/10	0.78	0.14	36,43,47,47	0
6	PGE	B	1338	10/10	0.86	0.17	23,30,33,34	10
4	PEG	A	1338	7/7	0.91	0.11	29,31,35,36	0
5	K	B	1340	1/1	0.98	0.06	22,22,22,22	0
3	CL	A	1337	1/1	0.98	0.08	23,23,23,23	0
2	MG	B	1336	1/1	0.98	0.04	10,10,10,10	0
2	MG	A	1336	1/1	0.99	0.01	10,10,10,10	0
3	CL	B	1337	1/1	0.99	0.09	23,23,23,23	0
5	K	A	1339	1/1	1.00	0.06	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.