



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 08:08 AM EDT

PDB ID : 12UX / pdb_000012ux
Title : WT Human Aconitate Decarboxylase 1, apo
Authors : Runge, B.; Monteiro, D.C.F.
Deposited on : 2026-04-20
Resolution : 1.32 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

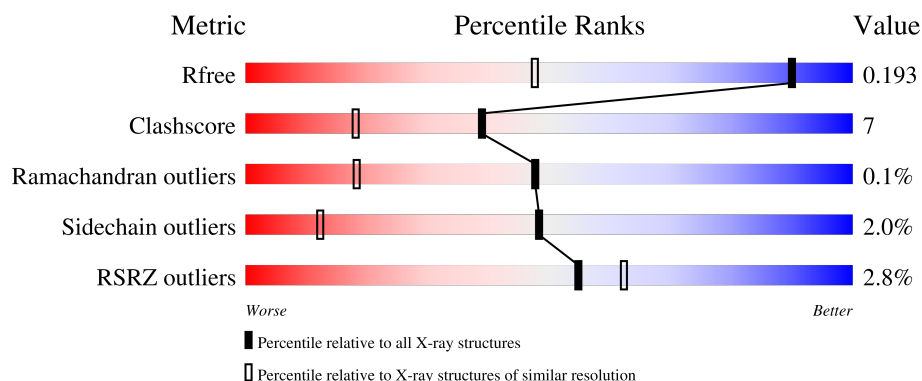
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

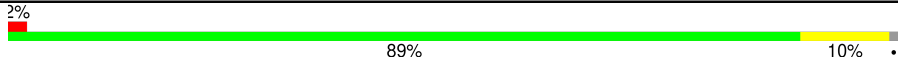
The reported resolution of this entry is 1.32 Å.

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	2531 (1.34-1.30)
Clashscore	190562	2585 (1.34-1.30)
Ramachandran outliers	187476	2528 (1.34-1.30)
Sidechain outliers	187428	2528 (1.34-1.30)
RSRZ outliers	180081	2528 (1.34-1.30)

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	462	
1	B	462	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15703 atoms, of which 7400 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 Cis-aconitate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	459	Total	C	H	N	O	S	122	26	0
			7395	2353	3723	633	674	12			
1	B	458	Total	C	H	N	O	S	120	11	0
			7260	2319	3654	618	656	13			

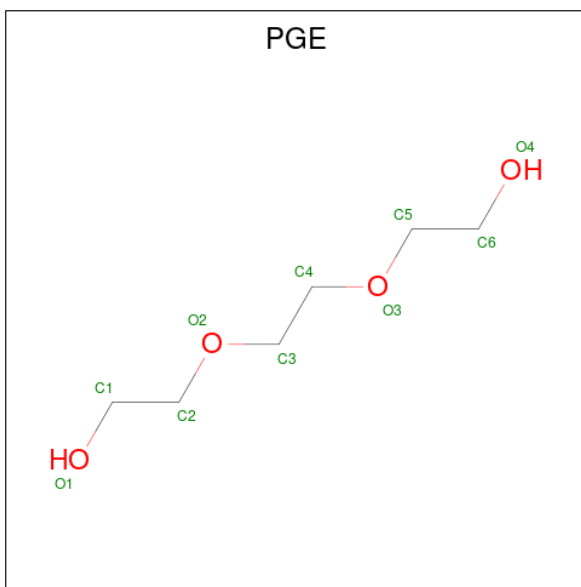
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A6NK06
A	1	GLY	-	expression tag	UNP A6NK06
A	2	GLY	-	expression tag	UNP A6NK06
A	3	ARG	-	expression tag	UNP A6NK06
B	0	GLY	-	expression tag	UNP A6NK06
B	1	GLY	-	expression tag	UNP A6NK06
B	2	GLY	-	expression tag	UNP A6NK06
B	3	ARG	-	expression tag	UNP A6NK06

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

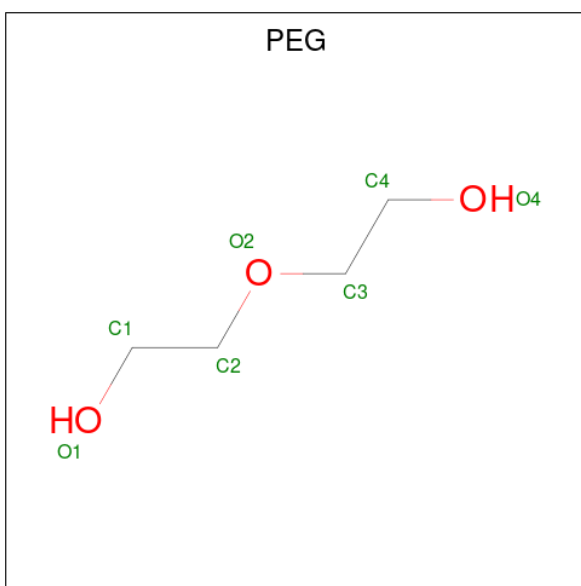


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	1	0
			23	6	13	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	2	0
			17	4	10	3		

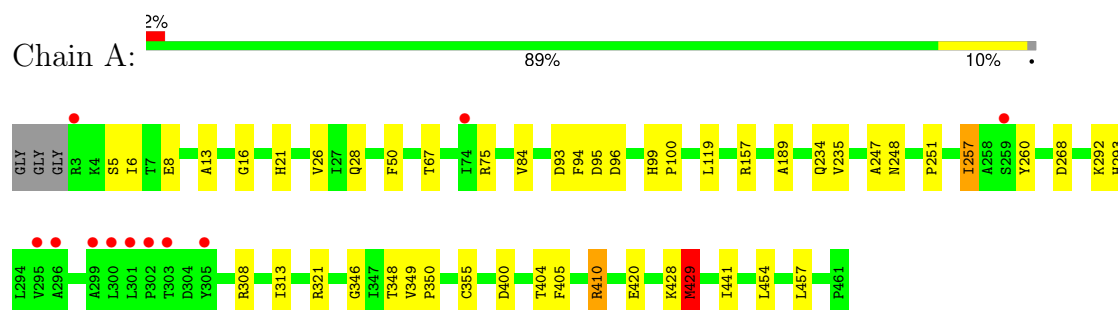
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	533	Total	O	0	2
			535	535		
6	B	471	Total	O	0	0
			471	471		

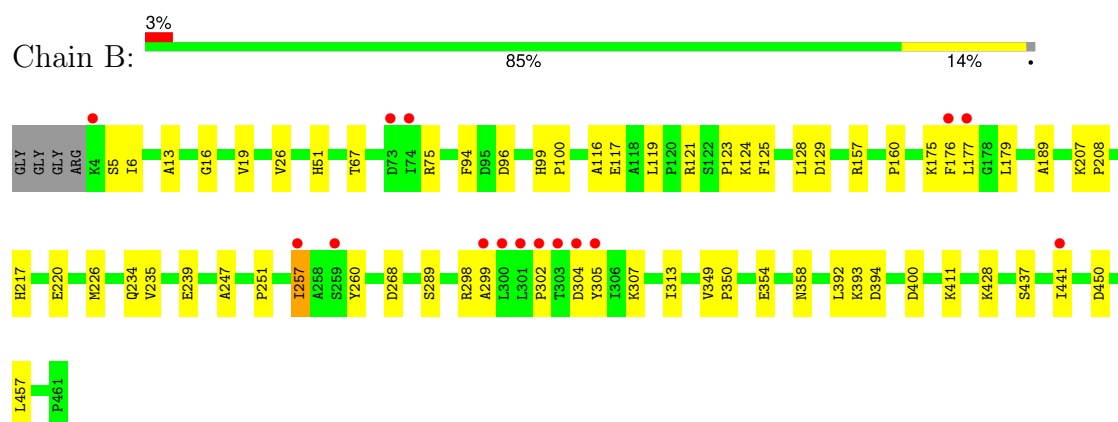
3 Residue-property plots [i](#)

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: Cis-aconitate decarboxylase



- Molecule 1: Cis-aconitate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.68Å 110.02Å 75.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.78 – 1.32 33.78 – 1.32	Depositor EDS
% Data completeness (in resolution range)	74.0 (33.78-1.32) 74.0 (33.78-1.32)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.158 , 0.193 0.158 , 0.193	Depositor DCC
R_{free} test set	7379 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15703	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 5.29% 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, PGE, NA, 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	0.74	0/3851	1.04	6/5237 (0.1%)
1	B	0.68	0/3738	1.07	9/5083 (0.2%)
All	All	0.71	0/7589	1.05	15/10320 (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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ASP	CA-CB-CG	8.47	121.07	112.60
1	B	260	TYR	N-CA-CB	7.04	121.89	110.42
1	B	268	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	96	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	354	GLU	CB-CG-CD	5.53	122.00	112.60
1	B	358	ASN	CB-CA-C	5.44	119.75	110.56
1	B	160	PRO	N-CA-C	5.42	117.31	110.70
1	A	429	MET	CG-SD-CE	-5.35	89.12	100.90
1	B	411	LYS	CB-CA-C	5.29	118.72	111.41
1	A	95	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	268	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	293	HIS	CB-CG-CD2	-5.26	124.37	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	119	LEU	O-C-N	-5.10	116.78	121.37
1	B	124	LYS	N-CA-CB	5.03	117.41	110.17

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	ARG	Sidechain
1	A	410[A]	ARG	Sidechain
1	B	157	ARG	Sidechain

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	3672	3723	3621	47	0
1	B	3606	3654	3615	52	0
2	A	1	0	0	0	0
3	A	10	13	14	3	0
4	B	1	0	0	0	1
5	B	7	10	10	1	0
6	A	535	0	0	13	1
6	B	471	0	0	5	1
All	All	8303	7400	7260	100	2

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 7.

All (100) 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:121[B]:ARG:NE	1:B:125[B]:PHE:CD2	2.31	0.99
1:B:121[B]:ARG:NE	1:B:125[B]:PHE:CE2	2.38	0.90
1:B:121[B]:ARG:CZ	1:B:125[B]:PHE:CD2	2.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121[B]:ARG:HG3	1:B:123:PRO:O	1.74	0.85
1:A:410[B]:ARG:NH1	6:A:602:HOH:O	2.11	0.83
1:A:410[A]:ARG:NH2	6:A:603:HOH:O	2.13	0.82
1:A:429:MET:N	1:A:429:MET:SD	2.55	0.79
1:B:121[B]:ARG:CZ	1:B:125[B]:PHE:HD2	1.95	0.78
1:A:428:LYS:HB2	1:A:429:MET:CE	2.14	0.78
1:B:239:GLU:OE2	6:B:601:HOH:O	2.02	0.76
1:A:428:LYS:HE3	6:A:950:HOH:O	1.88	0.73
1:B:121[B]:ARG:CZ	1:B:125[B]:PHE:CE2	2.73	0.71
1:B:299:ALA:HB1	1:B:392:LEU:HD11	1.73	0.71
1:B:119:LEU:O	1:B:125[B]:PHE:HZ	1.74	0.70
1:A:420:GLU:OE1	6:A:601:HOH:O	2.11	0.69
1:A:355:CYS:HB3	6:A:1003:HOH:O	1.94	0.67
1:A:410[A]:ARG:NH2	6:A:602:HOH:O	2.28	0.66
1:A:247[B]:ALA:O	1:A:248[B]:ASN:C	2.35	0.66
1:B:67:THR:CG2	1:B:75:ARG:NH1	2.59	0.66
1:B:437:SER:O	1:B:441:ILE:HG13	1.97	0.65
1:B:177:LEU:HD13	1:B:226[B]:MET:SD	2.37	0.65
1:B:13:ALA:HA	1:B:257:ILE:HD11	1.79	0.64
1:A:8:GLU:OE2	6:A:604:HOH:O	2.14	0.64
1:A:13:ALA:HA	1:A:257[A]:ILE:HD11	1.81	0.61
1:A:5:SER:CB	1:A:234:GLN:OE1	2.48	0.61
1:B:121[B]:ARG:CD	1:B:125[B]:PHE:CD2	2.83	0.61
1:B:247:ALA:O	6:B:602:HOH:O	2.16	0.61
1:A:67:THR:HB	6:A:617:HOH:O	2.00	0.61
1:B:121[B]:ARG:NH2	1:B:125[B]:PHE:HE2	1.98	0.61
1:A:67:THR:HG23	1:A:75:ARG:HH11	1.66	0.60
1:B:177:LEU:HD13	1:B:226[A]:MET:CE	2.33	0.59
1:A:50:PHE:CE1	1:A:84[B]:VAL:CG1	2.85	0.59
1:A:346:GLY:HA3	3:A:502:PGE:H6	1.84	0.58
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.69	0.57
1:B:121[B]:ARG:NH2	1:B:125[B]:PHE:CE2	2.72	0.57
1:B:121[B]:ARG:HH21	1:B:125[B]:PHE:HE2	1.53	0.57
1:B:441:ILE:HD12	1:B:457:LEU:HD12	1.87	0.57
1:B:67:THR:HG23	1:B:75:ARG:NH1	2.20	0.57
1:A:50:PHE:HE1	1:A:84[B]:VAL:HG12	1.70	0.56
1:A:428:LYS:HB2	1:A:429:MET:SD	2.44	0.56
1:B:428:LYS:HE2	6:B:635:HOH:O	2.05	0.56
1:A:67:THR:HG23	1:A:75:ARG:NH1	2.21	0.56
1:A:67:THR:CG2	1:A:75:ARG:HH11	2.18	0.56
1:A:308:ARG:NH2	6:A:614:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLY:HA3	3:A:502:PGE:C6	2.36	0.55
1:B:305:TYR:HA	1:B:393:LYS:HD2	1.88	0.55
1:A:50:PHE:HE1	1:A:84[B]:VAL:CG1	2.20	0.54
1:B:67:THR:HG23	1:B:117:GLU:OE1	2.08	0.53
1:A:428:LYS:HB2	1:A:429:MET:HE1	1.89	0.53
1:A:441[B]:ILE:HD11	1:A:454:LEU:CD1	2.38	0.53
1:A:348:THR:CG2	3:A:502:PGE:H5	2.39	0.52
1:B:67:THR:HG23	1:B:75:ARG:HH12	1.75	0.52
1:B:177:LEU:HD13	1:B:226[A]:MET:HE2	1.90	0.52
1:B:428:LYS:CE	6:B:635:HOH:O	2.58	0.52
1:B:289[B]:SER:OG	1:B:400:ASP:CG	2.53	0.51
1:A:16:GLY:HA3	1:A:257[A]:ILE:HD13	1.93	0.51
1:A:404:THR:HG21	1:A:410[B]:ARG:HB2	1.92	0.50
1:A:67:THR:HG22	1:A:75:ARG:HG2	1.94	0.50
1:A:410[A]:ARG:CZ	6:A:602:HOH:O	2.59	0.50
1:B:5:SER:CB	1:B:234:GLN:OE1	2.60	0.50
1:B:441:ILE:HD12	1:B:457:LEU:CD1	2.41	0.49
1:A:441[B]:ILE:HD11	1:A:454:LEU:HD13	1.96	0.47
1:A:404:THR:HG23	6:A:603:HOH:O	2.15	0.47
1:B:177:LEU:HD13	1:B:226[A]:MET:HE1	1.97	0.47
1:B:177:LEU:HB2	1:B:179[B]:LEU:CD1	2.45	0.46
1:A:441[B]:ILE:CD1	1:A:454:LEU:HD13	2.45	0.46
1:B:189:ALA:HA	1:B:235:VAL:HG11	1.98	0.46
1:B:6:ILE:HD13	1:B:251:PRO:HB2	1.99	0.45
1:B:299:ALA:HA	5:B:502:PEG:H42	1.97	0.45
1:B:119:LEU:O	1:B:125[B]:PHE:CZ	2.62	0.44
1:A:404:THR:HG22	1:A:405:PHE:N	2.33	0.44
1:B:305:TYR:HH	1:B:394:ASP:HB3	1.83	0.44
1:A:6:ILE:HD13	1:A:251:PRO:HB2	2.00	0.44
1:B:302:PRO:C	1:B:304:ASP:N	2.76	0.43
1:A:5:SER:HB2	1:A:234:GLN:OE1	2.19	0.43
1:B:176[A]:PHE:HD2	1:B:177:LEU:HG	1.83	0.42
1:B:16:GLY:HA3	1:B:257:ILE:HD13	2.01	0.42
1:A:349:VAL:HB	1:A:350:PRO:HD3	2.01	0.42
1:A:441[A]:ILE:CD1	1:A:457:LEU:CD1	2.97	0.42
1:B:51:HIS:HD2	6:B:973:HOH:O	2.02	0.42
1:B:125[A]:PHE:CE1	1:B:129:ASP:HB3	2.55	0.42
1:B:217:HIS:HD2	1:B:220:GLU:OE1	2.02	0.42
1:B:305:TYR:OH	1:B:394:ASP:HB3	2.19	0.42
1:B:99:HIS:HA	1:B:100:PRO:C	2.44	0.41
1:B:226[B]:MET:HE3	1:B:226[B]:MET:HB3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PHE:CE1	1:A:84[B]:VAL:HG13	2.54	0.41
1:B:67:THR:CG2	1:B:75:ARG:HH12	2.30	0.41
1:A:21:HIS:NE2	1:A:257[A]:ILE:HG23	2.34	0.41
1:B:349:VAL:HB	1:B:350:PRO:HD3	2.02	0.41
1:A:28:GLN:NE2	6:A:634:HOH:O	2.53	0.41
1:B:177:LEU:HD22	1:B:226[A]:MET:HE1	2.02	0.41
1:A:189:ALA:HA	1:A:235:VAL:HG11	2.03	0.40
1:A:404:THR:HG22	1:A:405:PHE:H	1.86	0.40
1:B:19[A]:VAL:HG11	1:B:128:LEU:HD13	2.03	0.40
1:B:116:ALA:HA	1:B:125[B]:PHE:CE1	2.57	0.40
1:B:207:LYS:HB3	1:B:208:PRO:HD3	2.02	0.40
1:A:99:HIS:HA	1:A:100:PRO:C	2.47	0.40
1:A:441[A]:ILE:HD12	1:A:457:LEU:CD1	2.51	0.40
1:A:441[B]:ILE:HD11	1:A:454:LEU:HD12	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:501:CA:CA	6:A:615:HOH:O[4_544]	1.66	0.54
6:B:602:HOH:O	6:B:612:HOH:O[4_444]	2.11	0.09

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	483/462 (104%)	473 (98%)	9 (2%)	1 (0%)	43 17
1	B	468/462 (101%)	461 (98%)	7 (2%)	0	100 100
All	All	951/924 (103%)	934 (98%)	16 (2%)	1 (0%)	48 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	TYR

5.3.2 Protein sidechains [i](#)

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	406/383 (106%)	397 (98%)	9 (2%)	45	10
1	B	394/383 (103%)	387 (98%)	7 (2%)	51	15
All	All	800/766 (104%)	784 (98%)	16 (2%)	48	12

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	93	ASP
1	A	94	PHE
1	A	257[A]	ILE
1	A	257[B]	ILE
1	A	292	LYS
1	A	313	ILE
1	A	400	ASP
1	A	429	MET
1	B	26	VAL
1	B	94	PHE
1	B	175	LYS
1	B	257	ILE
1	B	298	ARG
1	B	307	LYS
1	B	313	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	281	HIS

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Mol	Chain	Res	Type
1	A	356	GLN
1	A	444	ASN
1	B	51	HIS
1	B	217	HIS
1	B	266	GLN
1	B	353	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
5	PEG	B	502	-	6,6,6	0.31	0	5,5,5	0.24	0
3	PGE	A	502	-	9,9,9	0.45	0	8,8,8	0.37	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
5	PEG	B	502	-	-	3/4/4/4	-
3	PGE	A	502	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PGE	O2-C3-C4-O3
5	B	502	PEG	O1-C1-C2-O2
3	A	502	PGE	C1-C2-O2-C3
5	B	502	PEG	C4-C3-O2-C2
3	A	502	PGE	C4-C3-O2-C2
5	B	502	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	PEG	1	0
3	A	502	PGE	3	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	459/462 (99%)	-0.42	11 (2%) 59 66	5, 12, 33, 75	17 (3%)
1	B	458/462 (99%)	-0.26	15 (3%) 49 57	5, 15, 35, 64	9 (1%)
All	All	917/924 (99%)	-0.34	26 (2%) 55 62	5, 13, 34, 75	26 (2%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	ALA	4.3
1	A	301	LEU	4.0
1	B	305	TYR	4.0
1	A	296	ALA	3.6
1	A	295	VAL	3.6
1	A	300	LEU	3.3
1	A	302	PRO	3.1
1	B	301	LEU	2.8
1	A	74	ILE	2.8
1	A	305	TYR	2.7
1	B	257	ILE	2.7
1	B	304	ASP	2.7
1	B	74	ILE	2.6
1	B	176[A]	PHE	2.4
1	B	259	SER	2.4
1	A	3	ARG	2.4
1	A	259	SER	2.3
1	B	300	LEU	2.3
1	B	302	PRO	2.2
1	B	4	LYS	2.2
1	B	441	ILE	2.2
1	B	177	LEU	2.1
1	A	303	THR	2.1
1	A	299	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	303	THR	2.1
1	B	73	ASP	2.0

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

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

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
5	PEG	B	502	7/7	0.66	0.19	53,60,64,66	2
3	PGE	A	502	10/10	0.82	0.12	27,37,39,40	1
4	CA	B	501	1/1	0.97	0.12	41,41,41,41	0
2	NA	A	501	1/1	0.99	0.02	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.