



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:55 PM UTC

PDB ID : 3C8V / pdb_00003c8v
Title : Crystal structure of putative acetyltransferase (YP_390128.1) from *Desulfovibrio desulfuricans* G20 at 2.28 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-02-13
Resolution : 2.28 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

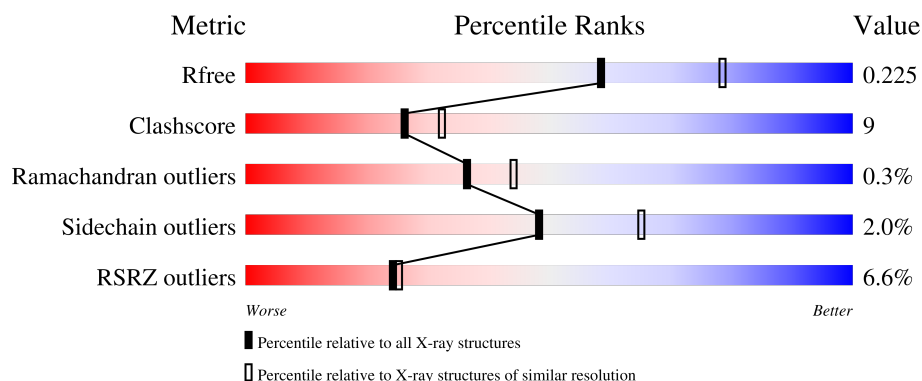
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	496	 7% 73% 18% • 9%
1	B	496	 3% 76% 16% • 7%
1	C	496	 9% 72% 21% • 6%
1	D	496	 5% 73% 19% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14949 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 Putative acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	Se	0	2	0
			3533	2249	606	662	6	10			
1	B	461	Total	C	N	O	S	Se	0	1	0
			3594	2281	615	683	5	10			
1	C	465	Total	C	N	O	S	Se	0	1	0
			3567	2269	611	672	5	10			
1	D	464	Total	C	N	O	S	Se	0	1	0
			3590	2287	616	671	6	10			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	expression tag	UNP Q30V63
A	-17	GLY	-	expression tag	UNP Q30V63
A	-16	SER	-	expression tag	UNP Q30V63
A	-15	ASP	-	expression tag	UNP Q30V63
A	-14	LYS	-	expression tag	UNP Q30V63
A	-13	ILE	-	expression tag	UNP Q30V63
A	-12	HIS	-	expression tag	UNP Q30V63
A	-11	HIS	-	expression tag	UNP Q30V63
A	-10	HIS	-	expression tag	UNP Q30V63
A	-9	HIS	-	expression tag	UNP Q30V63
A	-8	HIS	-	expression tag	UNP Q30V63
A	-7	HIS	-	expression tag	UNP Q30V63
A	-6	GLU	-	expression tag	UNP Q30V63
A	-5	ASN	-	expression tag	UNP Q30V63
A	-4	LEU	-	expression tag	UNP Q30V63
A	-3	TYR	-	expression tag	UNP Q30V63
A	-2	PHE	-	expression tag	UNP Q30V63
A	-1	GLN	-	expression tag	UNP Q30V63
A	0	GLY	-	expression tag	UNP Q30V63
B	-18	MSE	-	expression tag	UNP Q30V63
B	-17	GLY	-	expression tag	UNP Q30V63

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q30V63
B	-15	ASP	-	expression tag	UNP Q30V63
B	-14	LYS	-	expression tag	UNP Q30V63
B	-13	ILE	-	expression tag	UNP Q30V63
B	-12	HIS	-	expression tag	UNP Q30V63
B	-11	HIS	-	expression tag	UNP Q30V63
B	-10	HIS	-	expression tag	UNP Q30V63
B	-9	HIS	-	expression tag	UNP Q30V63
B	-8	HIS	-	expression tag	UNP Q30V63
B	-7	HIS	-	expression tag	UNP Q30V63
B	-6	GLU	-	expression tag	UNP Q30V63
B	-5	ASN	-	expression tag	UNP Q30V63
B	-4	LEU	-	expression tag	UNP Q30V63
B	-3	TYR	-	expression tag	UNP Q30V63
B	-2	PHE	-	expression tag	UNP Q30V63
B	-1	GLN	-	expression tag	UNP Q30V63
B	0	GLY	-	expression tag	UNP Q30V63
C	-18	MSE	-	expression tag	UNP Q30V63
C	-17	GLY	-	expression tag	UNP Q30V63
C	-16	SER	-	expression tag	UNP Q30V63
C	-15	ASP	-	expression tag	UNP Q30V63
C	-14	LYS	-	expression tag	UNP Q30V63
C	-13	ILE	-	expression tag	UNP Q30V63
C	-12	HIS	-	expression tag	UNP Q30V63
C	-11	HIS	-	expression tag	UNP Q30V63
C	-10	HIS	-	expression tag	UNP Q30V63
C	-9	HIS	-	expression tag	UNP Q30V63
C	-8	HIS	-	expression tag	UNP Q30V63
C	-7	HIS	-	expression tag	UNP Q30V63
C	-6	GLU	-	expression tag	UNP Q30V63
C	-5	ASN	-	expression tag	UNP Q30V63
C	-4	LEU	-	expression tag	UNP Q30V63
C	-3	TYR	-	expression tag	UNP Q30V63
C	-2	PHE	-	expression tag	UNP Q30V63
C	-1	GLN	-	expression tag	UNP Q30V63
C	0	GLY	-	expression tag	UNP Q30V63
D	-18	MSE	-	expression tag	UNP Q30V63
D	-17	GLY	-	expression tag	UNP Q30V63
D	-16	SER	-	expression tag	UNP Q30V63
D	-15	ASP	-	expression tag	UNP Q30V63
D	-14	LYS	-	expression tag	UNP Q30V63
D	-13	ILE	-	expression tag	UNP Q30V63

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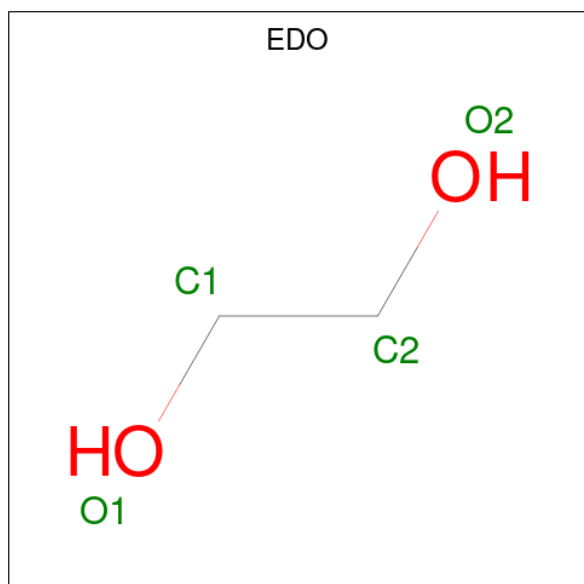
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q30V63
D	-11	HIS	-	expression tag	UNP Q30V63
D	-10	HIS	-	expression tag	UNP Q30V63
D	-9	HIS	-	expression tag	UNP Q30V63
D	-8	HIS	-	expression tag	UNP Q30V63
D	-7	HIS	-	expression tag	UNP Q30V63
D	-6	GLU	-	expression tag	UNP Q30V63
D	-5	ASN	-	expression tag	UNP Q30V63
D	-4	LEU	-	expression tag	UNP Q30V63
D	-3	TYR	-	expression tag	UNP Q30V63
D	-2	PHE	-	expression tag	UNP Q30V63
D	-1	GLN	-	expression tag	UNP Q30V63
D	0	GLY	-	expression tag	UNP Q30V63

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	B	3	Total Cl 3 3	0	0
2	C	2	Total Cl 2 2	0	0
2	D	4	Total Cl 4 4	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0

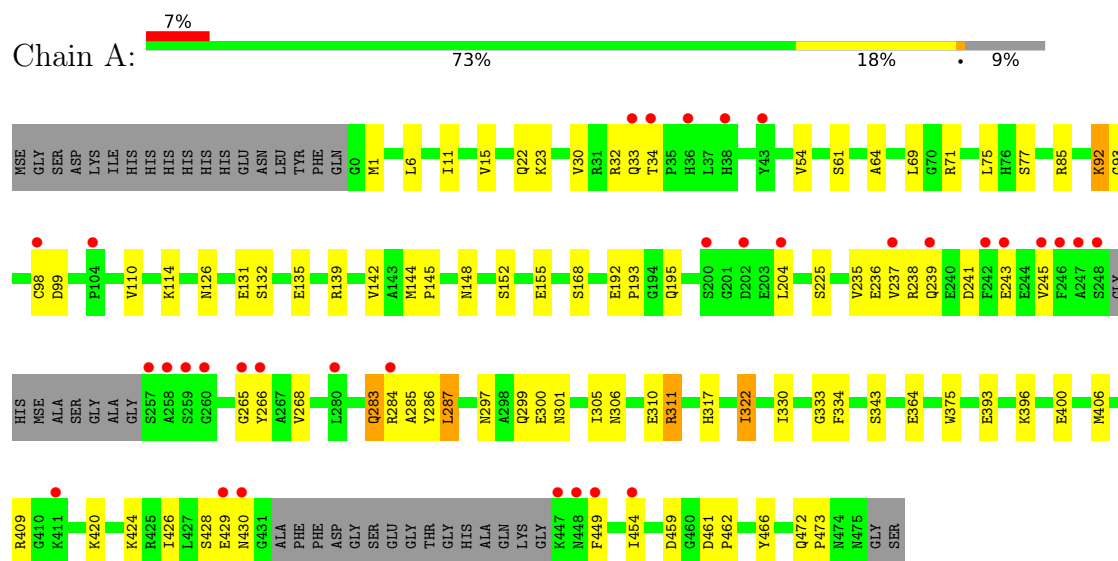
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	183	Total O 183 183	0	0
5	B	132	Total O 132 132	0	0
5	C	93	Total O 93 93	0	0
5	D	132	Total O 132 132	0	0

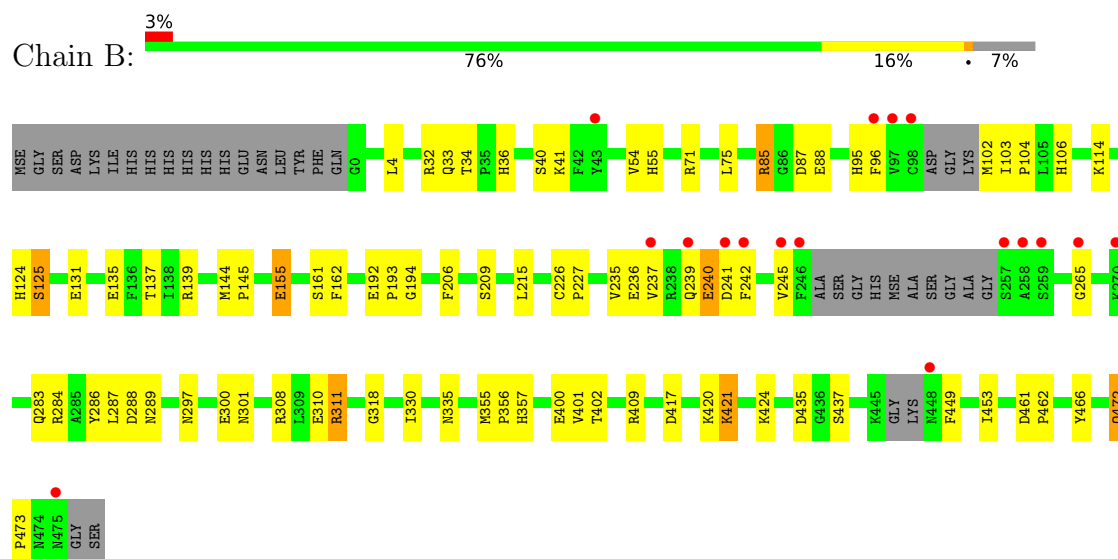
3 Residue-property plots [i](#)

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: Putative acetyltransferase

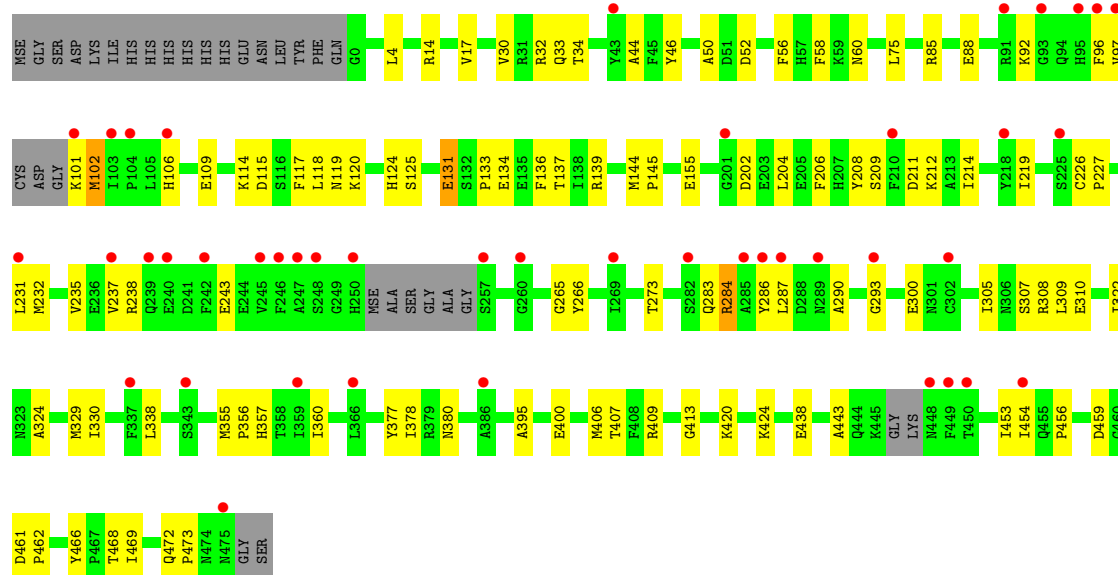


- Molecule 1: Putative acetyltransferase



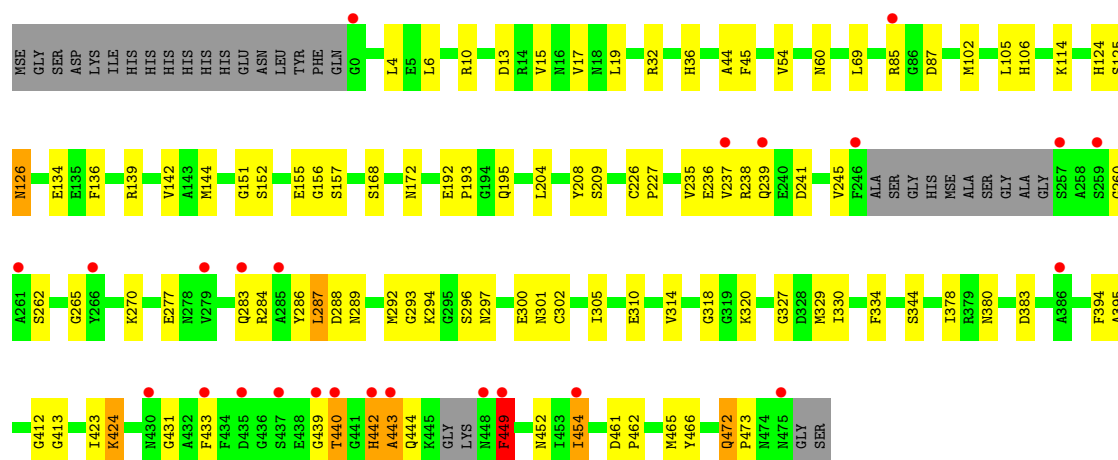
- Molecule 1: Putative acetyltransferase

Chain C: 



• Molecule 1: Putative acetyltransferase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	249.62Å 249.62Å 104.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.06 – 2.28 48.06 – 2.29	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.06-2.28) 95.1 (48.06-2.29)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.4.0067, PHENIX	Depositor
R, R_{free}	0.180 , 0.223 0.185 , 0.225	Depositor DCC
R_{free} test set	5271 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: EDO, MG, CL

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	0.91	0/3609	1.08	13/4865 (0.3%)
1	B	0.81	0/3670	1.07	9/4947 (0.2%)
1	C	0.71	0/3640	1.11	15/4910 (0.3%)
1	D	0.79	0/3667	1.09	15/4945 (0.3%)
All	All	0.81	0/14586	1.09	52/19667 (0.3%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	SER	N-CA-C	7.44	120.72	109.41
1	A	265	GLY	N-CA-C	-7.10	106.02	115.32
1	B	265	GLY	N-CA-C	-6.41	107.62	114.67
1	C	30	VAL	CB-CA-C	-6.38	106.29	111.71
1	D	239	GLN	N-CA-C	-6.18	105.70	113.18
1	D	443	ALA	N-CA-C	-6.18	105.60	113.01
1	A	32	ARG	N-CA-C	6.12	116.16	108.45
1	D	32	ARG	N-CA-C	6.03	117.06	108.74
1	B	466	TYR	CA-C-N	-5.97	112.38	119.84
1	B	466	TYR	C-N-CA	-5.97	112.38	119.84
1	A	239	GLN	N-CA-C	-5.96	105.27	112.54
1	B	32	ARG	N-CA-C	5.94	116.40	108.38
1	A	364	GLU	CA-C-N	-5.89	113.71	119.78
1	A	364	GLU	C-N-CA	-5.89	113.71	119.78
1	A	132	SER	CA-C-N	-5.88	113.70	119.64
1	A	132	SER	C-N-CA	-5.88	113.70	119.64
1	C	32	ARG	N-CA-C	5.86	116.29	108.38
1	D	245	VAL	N-CA-C	-5.84	105.67	112.98
1	C	413	GLY	CA-C-N	5.82	125.68	119.28
1	C	413	GLY	C-N-CA	5.82	125.68	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	GLY	N-CA-C	-5.81	107.70	115.32
1	A	459	ASP	N-CA-C	5.78	117.03	108.60
1	A	126	ASN	N-CA-C	5.75	116.67	108.74
1	B	239	GLN	N-CA-C	-5.67	106.20	113.01
1	C	395	ALA	N-CA-C	-5.66	106.33	113.18
1	C	265	GLY	N-CA-C	-5.63	107.94	115.32
1	C	443	ALA	N-CA-C	-5.57	106.44	113.18
1	C	102	MSE	N-CA-C	5.56	117.70	108.13
1	A	131	GLU	N-CA-C	-5.47	106.10	112.89
1	C	243	GLU	N-CA-C	-5.43	105.91	112.54
1	A	135	GLU	N-CA-C	5.42	117.46	108.13
1	D	126	ASN	N-CA-C	5.40	115.25	108.45
1	C	459	ASP	N-CA-C	5.36	116.42	108.60
1	D	449	PHE	N-CA-C	5.36	116.43	108.60
1	D	413	GLY	CA-C-N	5.29	125.11	119.28
1	D	413	GLY	C-N-CA	5.29	125.11	119.28
1	C	30	VAL	O-C-N	5.29	125.87	121.85
1	D	395	ALA	N-CA-C	-5.29	106.78	113.18
1	D	472	GLN	N-CA-C	5.29	114.22	108.14
1	D	380	ASN	N-CA-C	5.25	115.07	108.45
1	D	442	HIS	N-CA-C	-5.20	106.09	112.90
1	C	380	ASN	N-CA-C	5.15	114.94	108.45
1	C	50	ALA	N-CA-C	-5.14	106.27	112.54
1	B	453	ILE	CB-CA-C	-5.12	104.56	111.63
1	D	439	GLY	N-CA-C	-5.11	108.27	115.32
1	A	333	GLY	N-CA-C	5.11	119.08	112.54
1	B	40	SER	N-CA-C	-5.09	107.02	113.18
1	A	30	VAL	CB-CA-C	-5.08	106.61	111.44
1	B	125	SER	CB-CA-C	-5.07	109.20	115.89
1	B	472	GLN	N-CA-C	5.04	113.93	108.14
1	C	131	GLU	N-CA-C	-5.01	107.02	113.23
1	C	266	TYR	N-CA-C	-5.01	106.42	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3533	0	3415	61	0
1	B	3594	0	3437	58	0
1	C	3567	0	3400	75	0
1	D	3590	0	3435	70	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	4	0	0	0	0
3	A	40	0	60	3	0
3	B	28	0	42	0	0
3	C	8	0	12	0	0
3	D	36	0	54	4	0
4	C	1	0	0	0	0
5	A	183	0	0	3	0
5	B	132	0	0	2	0
5	C	93	0	0	3	0
5	D	132	0	0	1	0
All	All	14949	0	13855	265	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 9.

All (265) 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)
5:A:564:HOH:O	3:D:490:EDO:H11	1.59	1.01
1:B:240:GLU:HG3	1:B:241:ASP:N	1.75	0.99
1:B:283:GLN:O	1:B:300:GLU:HG2	1.61	0.98
1:B:85:ARG:NH1	1:B:87:ASP:OD2	2.00	0.95
1:B:310:GLU:O	1:B:311:ARG:HB2	1.71	0.89
1:C:238:ARG:HG3	1:C:238:ARG:HH11	1.40	0.84
1:D:85:ARG:CZ	1:D:300:GLU:HG2	2.11	0.81
1:B:240:GLU:CG	1:B:241:ASP:N	2.48	0.75
1:A:449:PHE:CD1	1:A:449:PHE:C	2.66	0.73
1:C:284:ARG:HG3	1:C:284:ARG:HH11	1.53	0.71
1:C:92:LYS:HG3	1:C:106:HIS:O	1.91	0.71
1:D:286:TYR:C	1:D:287:LEU:HD23	2.16	0.70
1:D:237:VAL:CG1	1:D:237:VAL:O	2.41	0.69
1:C:238:ARG:HG3	1:C:238:ARG:NH1	2.07	0.68
1:A:472:GLN:HB2	1:A:473:PRO:HD2	1.76	0.68
1:C:44:ALA:HB3	1:C:454:ILE:HG22	1.76	0.67
1:C:472:GLN:HB2	1:C:473:PRO:CD	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HB2	1:A:473:PRO:CD	2.25	0.66
1:B:85:ARG:HH21	1:B:300:GLU:HG3	1.59	0.66
1:A:1:MSE:HE3	1:A:6:LEU:HD13	1.78	0.65
1:A:139:ARG:O	1:A:155:GLU:HA	1.96	0.64
1:B:472:GLN:HB2	1:B:473:PRO:CD	2.26	0.64
1:D:431:GLY:C	1:D:433:PHE:H	2.04	0.64
1:B:472:GLN:HB2	1:B:473:PRO:HD2	1.79	0.64
1:D:237:VAL:O	1:D:237:VAL:HG12	1.96	0.64
1:D:283:GLN:O	1:D:284:ARG:HB2	1.96	0.63
1:B:237:VAL:O	1:B:237:VAL:CG1	2.47	0.62
1:D:54:VAL:O	1:D:473:PRO:HD3	2.00	0.62
1:D:472:GLN:HB2	1:D:473:PRO:CD	2.30	0.62
1:D:85:ARG:NH2	1:D:300:GLU:HG2	2.15	0.61
1:B:85:ARG:NH2	1:B:300:GLU:HG3	2.15	0.61
1:C:85:ARG:CZ	1:C:300:GLU:HG2	2.30	0.61
1:D:204:LEU:C	1:D:204:LEU:HD23	2.25	0.61
1:C:226:CYS:HB2	1:C:227:PRO:CD	2.29	0.61
1:C:329:MSE:HE1	1:C:424:LYS:HZ3	1.66	0.61
1:D:260:GLY:O	1:D:444:GLN:NE2	2.32	0.61
1:D:238:ARG:HH21	1:D:305:ILE:HD13	1.66	0.60
1:D:235:VAL:HG23	1:D:236:GLU:N	2.17	0.60
1:B:237:VAL:O	1:B:237:VAL:HG12	2.01	0.60
1:D:262:SER:HB2	1:D:443:ALA:O	2.02	0.60
1:D:472:GLN:HB2	1:D:473:PRO:HD2	1.83	0.59
1:B:435:ASP:OD1	1:B:437:SER:N	2.36	0.59
1:C:101:LYS:C	1:C:102:MSE:HG3	2.26	0.59
1:A:237:VAL:CG1	1:A:237:VAL:O	2.51	0.58
1:C:226:CYS:HB2	1:C:227:PRO:HD2	1.85	0.58
1:C:284:ARG:HG3	1:C:284:ARG:NH1	2.19	0.58
1:A:426:ILE:HD11	3:A:490:EDO:H11	1.84	0.58
1:B:400:GLU:HG2	1:B:409:ARG:HG3	1.84	0.58
1:D:454:ILE:HG23	1:D:466:TYR:CE2	2.38	0.58
1:A:237:VAL:O	1:A:237:VAL:HG12	2.03	0.58
1:C:139:ARG:O	1:C:155:GLU:HA	2.04	0.57
1:C:44:ALA:HB3	1:C:454:ILE:CG2	2.33	0.57
1:D:330:ILE:N	1:D:330:ILE:HD12	2.19	0.57
1:A:69:LEU:HD11	1:A:449:PHE:CE2	2.40	0.56
1:C:202:ASP:O	1:C:409:ARG:NH2	2.36	0.56
1:C:400:GLU:HG2	1:C:409:ARG:HG3	1.87	0.56
1:D:13:ASP:O	1:D:17[B]:VAL:HG22	2.06	0.55
1:B:144:MSE:HB3	1:B:145:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HG	1:D:134:GLU:HG3	1.89	0.55
1:D:287:LEU:HD23	1:D:287:LEU:N	2.20	0.55
1:B:4:LEU:HD23	1:B:36:HIS:HA	1.88	0.55
1:A:54:VAL:O	1:A:473:PRO:HD3	2.07	0.54
1:B:242:PHE:CE1	1:B:284:ARG:HA	2.42	0.54
1:C:338:LEU:HD22	1:C:360:ILE:HD12	1.89	0.54
1:A:310:GLU:O	1:A:311:ARG:HB2	2.08	0.54
1:C:237:VAL:O	1:C:237:VAL:CG1	2.56	0.54
1:D:44:ALA:HB3	1:D:454:ILE:HG22	1.88	0.54
1:D:292:MSE:HE3	1:D:296:SER:HB3	1.89	0.54
1:C:308:ARG:HD3	1:C:310:GLU:OE2	2.09	0.53
1:A:449:PHE:C	1:A:449:PHE:HD1	2.14	0.53
1:D:156:GLY:O	1:D:172:ASN:HA	2.08	0.53
1:B:144:MSE:HB3	1:B:145:PRO:CD	2.39	0.53
1:C:238:ARG:HD3	1:C:286:TYR:CZ	2.44	0.53
1:B:308:ARG:HD3	1:B:310:GLU:OE2	2.09	0.52
1:B:96:PHE:CZ	1:B:103:ILE:CB	2.93	0.52
1:B:288:ASP:O	1:B:289:ASN:HB2	2.10	0.52
1:B:41:LYS:NZ	5:B:592:HOH:O	2.32	0.52
1:D:235:VAL:CG2	1:D:236:GLU:N	2.73	0.52
1:A:461:ASP:N	1:A:462:PRO:CD	2.73	0.52
1:A:33:GLN:O	1:A:34:THR:C	2.53	0.51
1:D:423:ILE:HG23	1:D:424:LYS:N	2.25	0.51
1:C:286:TYR:C	1:C:287:LEU:HD23	2.35	0.51
1:A:1:MSE:CE	1:A:6:LEU:HD13	2.39	0.51
1:C:438:GLU:CA	5:C:549:HOH:O	2.58	0.51
1:C:284:ARG:HH11	1:C:284:ARG:CG	2.21	0.51
1:D:139:ARG:O	1:D:155:GLU:HA	2.09	0.51
1:A:204:LEU:C	1:A:204:LEU:HD23	2.36	0.50
1:A:400:GLU:HG2	1:A:409:ARG:HG3	1.94	0.50
1:C:453:ILE:CG2	1:C:454:ILE:N	2.74	0.50
1:A:85:ARG:CZ	1:A:300:GLU:HG2	2.41	0.50
1:B:283:GLN:O	1:B:284:ARG:HB2	2.11	0.50
1:A:11:ILE:O	1:A:15:VAL:HG23	2.11	0.50
1:A:142:VAL:CG1	1:A:144:MSE:HE3	2.42	0.50
1:C:237:VAL:O	1:C:237:VAL:HG12	2.10	0.50
1:C:293:GLY:HA3	1:C:310:GLU:O	2.10	0.50
1:D:69:LEU:HD21	1:D:87:ASP:HB3	1.92	0.50
1:D:318:GLY:O	1:D:320:LYS:NZ	2.44	0.50
1:B:449:PHE:CD1	1:B:449:PHE:C	2.89	0.50
1:D:114:LYS:HD3	3:D:490:EDO:H21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ASP:OD2	1:D:270:LYS:NZ	2.45	0.50
1:A:322:ILE:HD12	1:A:322:ILE:N	2.27	0.49
1:B:96:PHE:CE1	1:B:103:ILE:CB	2.95	0.49
1:D:461:ASP:N	1:D:462:PRO:CD	2.75	0.49
1:B:300:GLU:O	1:B:301:ASN:HB2	2.12	0.49
1:D:431:GLY:C	1:D:433:PHE:N	2.69	0.49
1:C:14:ARG:NH1	1:C:115:ASP:OD2	2.46	0.48
1:C:137[A]:THR:CG2	1:C:139:ARG:HD3	2.44	0.48
1:D:310:GLU:HB2	1:D:327:GLY:O	2.13	0.48
1:A:61:SER:HB3	1:A:77:SER:O	2.12	0.48
1:A:144:MSE:HB3	1:A:145:PRO:CD	2.44	0.48
1:C:211:ASP:OD2	1:C:214:ILE:HG13	2.12	0.48
1:C:322:ILE:HD12	1:C:322:ILE:N	2.28	0.48
1:B:75:LEU:O	1:B:114:LYS:HA	2.14	0.48
1:B:54:VAL:O	1:B:473:PRO:HD3	2.14	0.48
1:C:85:ARG:NH2	1:C:300:GLU:HG2	2.27	0.48
1:A:235:VAL:HG23	1:A:236:GLU:N	2.29	0.48
1:C:33:GLN:O	1:C:34:THR:C	2.56	0.48
1:D:300:GLU:O	1:D:301:ASN:HB2	2.12	0.48
1:A:192:GLU:HB3	1:A:193:PRO:CD	2.43	0.48
1:A:148:ASN:HB3	5:A:565:HOH:O	2.13	0.47
1:A:454:ILE:HG23	1:A:466:TYR:CE2	2.49	0.47
1:A:286:TYR:C	1:A:287:LEU:HD23	2.39	0.47
1:C:137[A]:THR:HG21	1:C:139:ARG:HD3	1.94	0.47
1:C:355:MSE:HB3	1:C:356:PRO:HD2	1.96	0.47
1:C:85:ARG:NH1	1:C:283:GLN:OE1	2.47	0.47
1:C:88:GLU:OE2	1:C:124:HIS:CE1	2.68	0.47
1:C:117:PHE:O	1:C:118:LEU:HD23	2.14	0.47
1:C:453:ILE:HG22	1:C:454:ILE:N	2.28	0.47
1:A:299:GLN:O	1:A:300:GLU:C	2.58	0.47
1:A:375:TRP:CH2	1:A:406:MSE:HE3	2.49	0.47
1:B:139:ARG:O	1:B:155:GLU:HA	2.15	0.47
1:B:161:SER:O	1:B:162:PHE:HB2	2.15	0.47
1:B:297:ASN:C	1:B:297:ASN:ND2	2.72	0.47
1:C:472:GLN:HB2	1:C:473:PRO:HD2	1.96	0.47
1:B:33:GLN:O	1:B:34:THR:C	2.57	0.47
1:C:356:PRO:O	1:C:357:HIS:HB2	2.15	0.47
1:B:417:ASP:O	1:B:421:LYS:HB2	2.15	0.46
1:C:330:ILE:HD12	1:C:330:ILE:N	2.30	0.46
1:D:394:PHE:O	1:D:412:GLY:HA3	2.15	0.46
1:B:355:MSE:HB3	1:B:356:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASP:HB3	1:B:462:PRO:HD3	1.97	0.46
1:C:136:PHE:CD1	1:C:136:PHE:C	2.93	0.46
1:C:461:ASP:N	1:C:462:PRO:CD	2.79	0.46
1:D:262:SER:CB	1:D:443:ALA:O	2.63	0.46
1:D:4:LEU:HD23	1:D:36:HIS:HA	1.97	0.46
1:B:435:ASP:OD1	1:B:435:ASP:C	2.58	0.46
1:C:329:MSE:CE	1:C:424:LYS:HZ3	2.29	0.46
1:C:208:TYR:CG	1:C:209:SER:N	2.83	0.46
1:B:209:SER:HB3	5:B:577:HOH:O	2.16	0.46
1:A:92:LYS:HG2	1:A:93:GLY:N	2.30	0.46
1:B:88:GLU:OE1	1:B:125:SER:HA	2.16	0.45
1:C:308:ARG:C	1:C:309:LEU:HD12	2.41	0.45
1:C:101:LYS:O	1:C:102:MSE:HG3	2.17	0.45
1:C:456:PRO:HB3	1:C:466:TYR:CE1	2.51	0.45
1:A:297:ASN:C	1:A:297:ASN:OD1	2.59	0.45
1:A:428:SER:C	1:A:430:ASN:N	2.72	0.45
1:B:124:HIS:CD2	1:B:125:SER:H	2.35	0.45
1:B:318:GLY:HA3	1:B:335:ASN:OD1	2.17	0.45
1:C:117:PHE:C	1:C:118:LEU:HD23	2.42	0.45
1:D:288:ASP:O	1:D:289:ASN:HB2	2.16	0.45
1:C:377:TYR:C	1:C:378:ILE:HG13	2.42	0.45
1:D:442:HIS:C	1:D:444:GLN:H	2.23	0.45
1:B:194:GLY:HA3	1:B:215:LEU:HD22	1.98	0.45
1:D:6:LEU:O	1:D:10:ARG:HG2	2.17	0.45
1:C:96:PHE:CB	5:C:541:HOH:O	2.65	0.45
1:D:152:SER:HB3	1:D:168:SER:O	2.17	0.45
1:A:241:ASP:O	1:A:245:VAL:HG23	2.17	0.45
1:A:300:GLU:HB2	1:A:317:HIS:CE1	2.51	0.45
1:C:124:HIS:CG	1:C:125:SER:H	2.33	0.45
1:D:106:HIS:ND1	3:D:488:EDO:H12	2.32	0.45
1:A:22:GLN:O	1:A:23:LYS:C	2.60	0.44
1:C:206:PHE:CD1	1:C:206:PHE:C	2.95	0.44
1:D:292:MSE:HE3	1:D:296:SER:CB	2.47	0.44
1:A:85:ARG:NE	1:A:300:GLU:HG2	2.32	0.44
1:A:393:GLU:OE1	1:A:396:LYS:NZ	2.39	0.44
1:B:114:LYS:O	1:B:139:ARG:HA	2.16	0.44
1:C:307:SER:HB3	1:C:324:ALA:O	2.18	0.44
1:C:454:ILE:HG23	1:C:466:TYR:CE2	2.52	0.44
1:D:15:VAL:HG21	1:D:142:VAL:HG23	1.99	0.44
1:A:152:SER:HB3	1:A:168:SER:O	2.17	0.44
1:A:461:ASP:N	1:A:462:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASP:N	1:B:462:PRO:HD2	2.32	0.44
1:C:4:LEU:HD12	1:C:4:LEU:O	2.18	0.44
1:C:109:GLU:HA	1:C:134:GLU:O	2.17	0.44
1:C:232:MSE:O	1:C:235:VAL:HG22	2.18	0.44
1:C:420:LYS:O	1:C:424:LYS:HB2	2.18	0.44
1:D:208:TYR:CG	1:D:209:SER:N	2.86	0.44
1:A:75:LEU:O	1:A:114:LYS:HA	2.18	0.44
1:C:284:ARG:HD2	1:C:284:ARG:HA	1.80	0.44
1:B:135:GLU:HG2	1:B:137:THR:HG23	1.99	0.44
1:D:114:LYS:HZ1	3:D:490:EDO:H22	1.82	0.44
1:C:206:PHE:CE2	1:C:406:MSE:HE2	2.53	0.43
1:D:124:HIS:CG	1:D:125:SER:H	2.36	0.43
1:A:98:CYS:O	1:A:99:ASP:C	2.61	0.43
1:B:330:ILE:N	1:B:330:ILE:HD12	2.32	0.43
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.83	0.43
1:A:204:LEU:HD12	5:A:606:HOH:O	2.18	0.43
1:D:114:LYS:O	1:D:139:ARG:HA	2.17	0.43
1:B:85:ARG:NE	1:B:300:GLU:OE2	2.51	0.43
1:B:286:TYR:C	1:B:287:LEU:HD23	2.43	0.43
1:D:192:GLU:O	1:D:195:GLN:HG2	2.19	0.43
1:B:226:CYS:HB2	1:B:227:PRO:HD2	2.01	0.43
1:D:126:ASN:O	1:D:151:GLY:HA2	2.19	0.43
1:A:69:LEU:HD11	1:A:449:PHE:CZ	2.54	0.43
1:A:283:GLN:C	1:A:285:ALA:H	2.27	0.43
1:A:426:ILE:HD11	3:A:490:EDO:C1	2.47	0.43
1:C:305:ILE:C	1:C:307:SER:N	2.73	0.43
1:B:235:VAL:HG23	1:B:236:GLU:N	2.35	0.42
1:C:273:THR:HG23	1:C:290:ALA:O	2.19	0.42
1:D:192:GLU:HB3	1:D:193:PRO:CD	2.49	0.42
1:D:330:ILE:N	1:D:330:ILE:CD1	2.82	0.42
1:A:144:MSE:HB3	1:A:145:PRO:HD2	2.00	0.42
1:A:192:GLU:O	1:A:195:GLN:HG2	2.19	0.42
1:A:236:GLU:C	1:A:238:ARG:H	2.26	0.42
1:D:297:ASN:HB3	1:D:314:VAL:HG22	2.00	0.42
1:D:442:HIS:C	1:D:444:GLN:N	2.75	0.42
1:D:449:PHE:C	1:D:449:PHE:CD1	2.97	0.42
1:A:420:LYS:O	1:A:424:LYS:HB2	2.19	0.42
1:A:454:ILE:HG23	1:A:466:TYR:HE2	1.85	0.42
1:A:71:ARG:HB3	1:A:110:VAL:HG12	2.01	0.42
1:A:283:GLN:O	1:A:284:ARG:HB2	2.19	0.42
1:A:330:ILE:HD12	1:A:330:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:GLY:HA3	1:D:310:GLU:O	2.20	0.42
1:A:245:VAL:HG12	1:A:245:VAL:O	2.18	0.42
1:C:454:ILE:HD11	1:C:469:ILE:HD13	2.01	0.42
1:D:378:ILE:HA	1:D:383:ASP:HB3	2.02	0.42
1:B:95:HIS:HB3	1:B:102:MSE:HG3	2.01	0.41
1:B:401:VAL:HG12	1:B:402:THR:N	2.35	0.41
1:D:226:CYS:HB2	1:D:227:PRO:CD	2.49	0.41
1:A:266:TYR:HB2	1:A:283:GLN:HB3	2.01	0.41
1:C:75:LEU:O	1:C:114:LYS:HA	2.20	0.41
1:C:204:LEU:C	1:C:204:LEU:HD23	2.44	0.41
1:D:454:ILE:HG23	1:D:466:TYR:HE2	1.84	0.41
1:A:426:ILE:O	1:A:430:ASN:CB	2.69	0.41
1:B:420:LYS:O	1:B:424:LYS:HB2	2.20	0.41
1:D:440:THR:O	1:D:440:THR:HG22	2.20	0.41
1:B:104:PRO:HG2	1:B:106:HIS:CE1	2.55	0.41
1:C:97:VAL:HG22	1:C:102:MSE:HG2	2.02	0.41
1:C:119:ASN:O	1:C:120:LYS:C	2.64	0.41
1:D:136:PHE:CD1	1:D:136:PHE:C	2.96	0.41
1:C:136:PHE:C	1:C:136:PHE:HD1	2.28	0.41
1:B:206:PHE:CD1	1:B:206:PHE:C	2.99	0.41
1:C:46:TYR:HB2	1:C:56:PHE:CE2	2.55	0.41
1:C:226:CYS:CB	1:C:227:PRO:CD	2.96	0.41
1:D:45:PHE:HA	1:D:452:ASN:O	2.21	0.41
1:B:192:GLU:HB3	1:B:193:PRO:CD	2.51	0.41
1:B:356:PRO:O	1:B:357:HIS:HB2	2.20	0.41
1:A:334:PHE:CZ	3:A:490:EDO:H21	2.56	0.41
1:C:144:MSE:HB3	1:C:145:PRO:CD	2.51	0.41
1:D:277:GLU:O	1:D:294:LYS:HA	2.21	0.41
1:C:58:PHE:O	1:C:468:THR:HA	2.21	0.40
1:D:284:ARG:NH2	5:D:613:HOH:O	2.53	0.40
1:B:55:HIS:HB3	1:B:71:ARG:HG2	2.02	0.40
1:A:245:VAL:HG21	1:A:268:VAL:HG22	2.02	0.40
1:A:300:GLU:O	1:A:301:ASN:HB2	2.21	0.40
1:B:355:MSE:HB3	1:B:355:MSE:HE2	1.99	0.40
1:D:142:VAL:CG1	1:D:144:MSE:HE3	2.51	0.40
1:D:423:ILE:CG2	1:D:424:LYS:N	2.83	0.40
1:D:461:ASP:N	1:D:462:PRO:HD2	2.35	0.40
1:D:465:MSE:HE3	1:D:465:MSE:HB3	2.00	0.40
1:A:305:ILE:O	1:A:306:ASN:C	2.64	0.40
1:B:287:LEU:HD23	1:B:287:LEU:N	2.37	0.40
1:D:19:LEU:HA	1:D:19:LEU:HD23	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:PRO:HD2	5:C:503:HOH:O	2.20	0.40
1:D:69:LEU:C	1:D:69:LEU:HD23	2.46	0.40

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	449/496 (90%)	433 (96%)	13 (3%)	3 (1%)	18	21
1	B	454/496 (92%)	436 (96%)	17 (4%)	1 (0%)	43	53
1	C	458/496 (92%)	437 (95%)	20 (4%)	1 (0%)	43	53
1	D	459/496 (92%)	440 (96%)	18 (4%)	1 (0%)	43	53
All	All	1820/1984 (92%)	1746 (96%)	68 (4%)	6 (0%)	36	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	ARG
1	A	311	ARG
1	A	429	GLU
1	C	219	ILE
1	A	64	ALA
1	D	334	PHE

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	376/408 (92%)	369 (98%)	7 (2%)	50	66
1	B	382/408 (94%)	376 (98%)	6 (2%)	55	71
1	C	372/408 (91%)	365 (98%)	7 (2%)	50	66
1	D	377/408 (92%)	367 (97%)	10 (3%)	39	55
All	All	1507/1632 (92%)	1477 (98%)	30 (2%)	48	65

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LYS
1	A	225	SER
1	A	243	GLU
1	A	283	GLN
1	A	287	LEU
1	A	322	ILE
1	A	343	SER
1	B	85	ARG
1	B	131	GLU
1	B	155	GLU
1	B	240	GLU
1	B	245	VAL
1	B	421	LYS
1	C	17	VAL
1	C	52	ASP
1	C	60	ASN
1	C	131	GLU
1	C	212	LYS
1	C	284	ARG
1	C	407	THR
1	D	60	ASN
1	D	102	MSE
1	D	287	LEU
1	D	302	CYS
1	D	329	MSE
1	D	344	SER
1	D	424	LYS
1	D	440	THR
1	D	449	PHE
1	D	454	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	182	GLN
1	A	239	GLN
1	A	312	ASN
1	A	475	ASN
1	B	57	HIS
1	B	60	ASN
1	B	106	HIS
1	B	475	ASN
1	C	221	GLN
1	D	57	HIS
1	D	182	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 13 are monoatomic - leaving 28 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	$\# Z > 2$
3	EDO	A	488	-	3,3,3	0.36	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	487	-	3,3,3	0.63	0	2,2,2	0.37	0
3	EDO	B	486	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	D	485	-	3,3,3	0.53	0	2,2,2	0.25	0
3	EDO	D	487	-	3,3,3	0.42	0	2,2,2	0.36	0
3	EDO	B	484	-	3,3,3	0.43	0	2,2,2	0.44	0
3	EDO	B	485	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	A	486	-	3,3,3	0.51	0	2,2,2	0.23	0
3	EDO	B	483	-	3,3,3	0.45	0	2,2,2	0.19	0
3	EDO	A	482	-	3,3,3	0.43	0	2,2,2	0.25	0
3	EDO	A	485	-	3,3,3	0.53	0	2,2,2	0.21	0
3	EDO	B	482	-	3,3,3	0.82	0	2,2,2	0.23	0
3	EDO	D	489	-	3,3,3	0.48	0	2,2,2	0.11	0
3	EDO	B	481	-	3,3,3	0.48	0	2,2,2	0.26	0
3	EDO	D	482	-	3,3,3	0.61	0	2,2,2	0.06	0
3	EDO	A	483	-	3,3,3	0.51	0	2,2,2	0.04	0
3	EDO	D	488	-	3,3,3	0.53	0	2,2,2	0.40	0
3	EDO	A	481	-	3,3,3	0.55	0	2,2,2	0.19	0
3	EDO	D	483	-	3,3,3	0.48	0	2,2,2	0.32	0
3	EDO	A	490	-	3,3,3	0.46	0	2,2,2	0.18	0
3	EDO	A	489	-	3,3,3	0.38	0	2,2,2	0.42	0
3	EDO	C	481	-	3,3,3	0.43	0	2,2,2	0.21	0
3	EDO	D	490	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	A	484	-	3,3,3	0.48	0	2,2,2	0.59	0
3	EDO	C	482	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	B	487	-	3,3,3	0.52	0	2,2,2	0.25	0
3	EDO	D	484	-	3,3,3	0.62	0	2,2,2	0.06	0
3	EDO	D	486	-	3,3,3	0.51	0	2,2,2	0.13	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
3	EDO	A	488	-	-	0/1/1/1	-
3	EDO	A	487	-	-	1/1/1/1	-
3	EDO	B	486	-	-	1/1/1/1	-
3	EDO	D	485	-	-	1/1/1/1	-
3	EDO	D	487	-	-	1/1/1/1	-
3	EDO	B	484	-	-	0/1/1/1	-
3	EDO	B	485	-	-	1/1/1/1	-
3	EDO	A	486	-	-	1/1/1/1	-
3	EDO	B	483	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	482	-	-	0/1/1/1	-
3	EDO	A	485	-	-	1/1/1/1	-
3	EDO	B	482	-	-	1/1/1/1	-
3	EDO	D	489	-	-	1/1/1/1	-
3	EDO	B	481	-	-	1/1/1/1	-
3	EDO	D	482	-	-	0/1/1/1	-
3	EDO	A	483	-	-	0/1/1/1	-
3	EDO	D	488	-	-	1/1/1/1	-
3	EDO	A	481	-	-	1/1/1/1	-
3	EDO	D	483	-	-	0/1/1/1	-
3	EDO	A	490	-	-	1/1/1/1	-
3	EDO	A	489	-	-	1/1/1/1	-
3	EDO	C	481	-	-	0/1/1/1	-
3	EDO	D	490	-	-	1/1/1/1	-
3	EDO	A	484	-	-	1/1/1/1	-
3	EDO	C	482	-	-	1/1/1/1	-
3	EDO	B	487	-	-	1/1/1/1	-
3	EDO	D	484	-	-	1/1/1/1	-
3	EDO	D	486	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	487	EDO	O1-C1-C2-O2
3	D	488	EDO	O1-C1-C2-O2
3	D	490	EDO	O1-C1-C2-O2
3	A	486	EDO	O1-C1-C2-O2
3	A	490	EDO	O1-C1-C2-O2
3	B	482	EDO	O1-C1-C2-O2
3	B	485	EDO	O1-C1-C2-O2
3	A	489	EDO	O1-C1-C2-O2
3	B	481	EDO	O1-C1-C2-O2
3	A	481	EDO	O1-C1-C2-O2
3	D	485	EDO	O1-C1-C2-O2
3	A	485	EDO	O1-C1-C2-O2
3	A	487	EDO	O1-C1-C2-O2
3	B	486	EDO	O1-C1-C2-O2
3	D	489	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	484	EDO	O1-C1-C2-O2
3	C	482	EDO	O1-C1-C2-O2
3	D	484	EDO	O1-C1-C2-O2
3	D	486	EDO	O1-C1-C2-O2
3	D	487	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	488	EDO	1	0
3	A	490	EDO	3	0
3	D	490	EDO	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	443/496 (89%)	0.68	33 (7%)	20	21	26, 46, 68, 94	2 (0%)
1	B	451/496 (90%)	0.46	17 (3%)	44	46	29, 47, 68, 91	1 (0%)
1	C	455/496 (91%)	0.84	44 (9%)	13	14	24, 47, 66, 96	1 (0%)
1	D	454/496 (91%)	0.67	25 (5%)	30	31	26, 47, 74, 94	1 (0%)
All	All	1803/1984 (90%)	0.66	119 (6%)	24	25	24, 47, 69, 96	5 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	448	ASN	5.1
1	B	246	PHE	4.8
1	B	98	CYS	4.8
1	C	448	ASN	4.7
1	D	246	PHE	4.5
1	B	245	VAL	4.4
1	C	250	HIS	4.3
1	A	266	TYR	4.0
1	C	101	LYS	4.0
1	A	429	GLU	3.9
1	C	257	SER	3.8
1	C	97	VAL	3.8
1	A	448	ASN	3.8
1	B	96	PHE	3.7
1	B	257	SER	3.6
1	B	97	VAL	3.6
1	C	104	PRO	3.4
1	A	257	SER	3.4
1	A	43	TYR	3.4
1	C	246	PHE	3.3
1	C	96	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	259	SER	3.3
1	C	247	ALA	3.2
1	A	36	HIS	3.2
1	C	103	ILE	3.2
1	A	248	SER	3.2
1	A	247	ALA	3.1
1	B	265	GLY	3.1
1	C	95	HIS	3.1
1	D	257	SER	3.1
1	D	437	SER	3.1
1	C	475	ASN	3.1
1	C	237	VAL	3.0
1	C	218	TYR	3.0
1	C	449	PHE	3.0
1	C	91	ARG	3.0
1	A	34	THR	2.9
1	C	260	GLY	2.9
1	C	285	ALA	2.9
1	C	225	SER	2.9
1	A	33	GLN	2.8
1	C	43	TYR	2.8
1	D	433	PHE	2.8
1	A	200	SER	2.8
1	C	242	PHE	2.8
1	C	343	SER	2.7
1	C	240	GLU	2.7
1	A	258	ALA	2.7
1	D	0	GLY	2.7
1	C	106	HIS	2.6
1	D	442	HIS	2.6
1	A	239	GLN	2.6
1	D	475	ASN	2.6
1	A	454	ILE	2.6
1	C	201	GLY	2.6
1	C	337	PHE	2.6
1	B	43	TYR	2.6
1	A	447	LYS	2.6
1	D	440	THR	2.6
1	B	237	VAL	2.6
1	A	259	SER	2.6
1	D	443	ALA	2.5
1	C	293	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	239	GLN	2.5
1	D	283	GLN	2.5
1	A	204	LEU	2.5
1	A	280	LEU	2.5
1	D	430	ASN	2.5
1	B	258	ALA	2.5
1	D	261	ALA	2.5
1	C	231	LEU	2.4
1	A	38	HIS	2.4
1	B	475	ASN	2.4
1	D	279	VAL	2.4
1	D	449	PHE	2.4
1	A	202	ASP	2.4
1	B	259	SER	2.4
1	B	241	ASP	2.3
1	D	266	TYR	2.3
1	A	237	VAL	2.3
1	A	242	PHE	2.3
1	A	246	PHE	2.3
1	A	449	PHE	2.3
1	C	248	SER	2.3
1	B	242	PHE	2.3
1	C	302	CYS	2.3
1	A	243	GLU	2.3
1	A	430	ASN	2.2
1	D	386	ALA	2.2
1	C	239	GLN	2.2
1	A	245	VAL	2.2
1	C	366	LEU	2.2
1	D	285	ALA	2.2
1	D	454	ILE	2.2
1	B	239	GLN	2.2
1	C	386	ALA	2.2
1	A	284	ARG	2.2
1	D	237	VAL	2.2
1	A	98	CYS	2.2
1	C	450	THR	2.1
1	A	411	LYS	2.1
1	B	448	ASN	2.1
1	C	245	VAL	2.1
1	A	260	GLY	2.1
1	A	265	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	439	GLY	2.1
1	C	289	ASN	2.1
1	C	210	PHE	2.1
1	D	85	ARG	2.1
1	C	287	LEU	2.1
1	C	359	ILE	2.1
1	C	93	GLY	2.1
1	C	282	SER	2.0
1	C	454	ILE	2.0
1	A	104	PRO	2.0
1	C	286	TYR	2.0
1	D	435	ASP	2.0
1	C	269	ILE	2.0
1	B	270	LYS	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(Å ²)	Q<0.9
3	EDO	B	486	4/4	0.71	0.19	80,82,87,87	0
3	EDO	D	484	4/4	0.72	0.23	71,76,76,77	0
2	CL	C	479	1/1	0.77	0.18	94,94,94,94	0
3	EDO	A	485	4/4	0.80	0.30	45,56,59,61	0
3	EDO	A	481	4/4	0.83	0.24	66,74,75,77	0
3	EDO	A	486	4/4	0.83	0.21	65,67,72,73	0
3	EDO	D	487	4/4	0.83	0.21	77,78,79,79	0
3	EDO	A	489	4/4	0.84	0.19	66,71,72,72	0
3	EDO	B	487	4/4	0.84	0.19	65,71,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	482	4/4	0.86	0.20	50,51,53,61	0
3	EDO	B	485	4/4	0.86	0.21	64,65,67,68	0
3	EDO	C	482	4/4	0.86	0.17	58,59,61,61	0
3	EDO	D	490	4/4	0.87	0.24	37,46,49,55	0
3	EDO	A	487	4/4	0.88	0.22	58,58,60,62	0
3	EDO	D	488	4/4	0.88	0.19	47,52,52,54	0
3	EDO	D	485	4/4	0.88	0.17	60,60,63,64	0
3	EDO	A	490	4/4	0.89	0.19	55,58,59,63	0
3	EDO	B	482	4/4	0.90	0.18	45,51,52,58	0
2	CL	D	481	1/1	0.91	0.15	72,72,72,72	0
2	CL	B	480	1/1	0.91	0.13	74,74,74,74	0
3	EDO	B	481	4/4	0.92	0.13	44,46,46,49	0
2	CL	B	479	1/1	0.92	0.15	67,67,67,67	0
2	CL	D	478	1/1	0.93	0.14	61,61,61,61	0
2	CL	D	480	1/1	0.93	0.13	59,59,59,59	0
3	EDO	B	484	4/4	0.93	0.13	58,58,58,62	0
2	CL	A	480	1/1	0.93	0.16	67,67,67,67	0
2	CL	A	478	1/1	0.93	0.14	71,71,71,71	0
3	EDO	A	483	4/4	0.93	0.26	40,43,44,49	0
3	EDO	C	481	4/4	0.93	0.22	49,50,51,51	0
3	EDO	A	488	4/4	0.94	0.18	42,46,50,51	0
3	EDO	A	482	4/4	0.94	0.14	43,45,46,54	0
3	EDO	D	489	4/4	0.94	0.18	68,69,69,73	0
3	EDO	D	486	4/4	0.94	0.13	52,54,54,55	0
3	EDO	D	483	4/4	0.95	0.12	44,49,51,56	0
2	CL	C	478	1/1	0.95	0.13	76,76,76,76	0
3	EDO	B	483	4/4	0.96	0.12	41,47,51,56	0
3	EDO	A	484	4/4	0.96	0.14	33,34,42,44	0
4	MG	C	480	1/1	0.96	0.12	44,44,44,44	0
2	CL	D	479	1/1	0.97	0.12	40,40,40,40	0
2	CL	B	478	1/1	0.97	0.19	43,43,43,43	0
2	CL	A	479	1/1	0.99	0.16	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.