Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 12:17 PM EDT

PDB ID	:	4YWE
Title	:	Crystal Structure of a Putative Aldehyde Dehydrogenase from Burkholderia cenocepacia
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2015-03-20
Resolution	:	2.15 Å(reported)

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

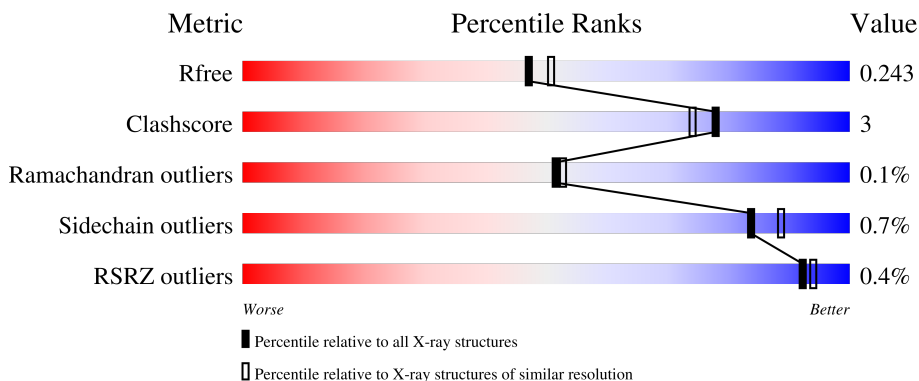|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.243
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		0.7%
RSRZ outliers		0.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 <=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	487	91% 6% •
1	B	487	91% 7% •
1	C	487	89% 9% •
1	D	487	90% 7% •
1	E	487	92% 6% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	487	90% 8% ·
1	G	487	% 87% 10% ·
1	H	487	90% 7% ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 31507 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 aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total 3506	C 2212	N 635	O 649	S 10	0	1	0
1	B	476	Total 3543	C 2234	N 645	O 654	S 10	0	4	0
1	C	476	Total 3517	C 2218	N 638	O 651	S 10	0	2	0
1	D	476	Total 3521	C 2221	N 639	O 651	S 10	0	3	0
1	E	476	Total 3524	C 2228	N 636	O 649	S 11	0	6	0
1	F	476	Total 3517	C 2219	N 637	O 650	S 11	0	4	0
1	G	476	Total 3544	C 2240	N 642	O 652	S 10	0	6	0
1	H	474	Total 3536	C 2230	N 645	O 651	S 10	0	3	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP B4E8B7
A	-6	ALA	-	expression tag	UNP B4E8B7
A	-5	HIS	-	expression tag	UNP B4E8B7
A	-4	HIS	-	expression tag	UNP B4E8B7
A	-3	HIS	-	expression tag	UNP B4E8B7
A	-2	HIS	-	expression tag	UNP B4E8B7
A	-1	HIS	-	expression tag	UNP B4E8B7
A	0	HIS	-	expression tag	UNP B4E8B7
B	-7	MET	-	expression tag	UNP B4E8B7
B	-6	ALA	-	expression tag	UNP B4E8B7
B	-5	HIS	-	expression tag	UNP B4E8B7
B	-4	HIS	-	expression tag	UNP B4E8B7
B	-3	HIS	-	expression tag	UNP B4E8B7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B4E8B7
B	-1	HIS	-	expression tag	UNP B4E8B7
B	0	HIS	-	expression tag	UNP B4E8B7
C	-7	MET	-	expression tag	UNP B4E8B7
C	-6	ALA	-	expression tag	UNP B4E8B7
C	-5	HIS	-	expression tag	UNP B4E8B7
C	-4	HIS	-	expression tag	UNP B4E8B7
C	-3	HIS	-	expression tag	UNP B4E8B7
C	-2	HIS	-	expression tag	UNP B4E8B7
C	-1	HIS	-	expression tag	UNP B4E8B7
C	0	HIS	-	expression tag	UNP B4E8B7
D	-7	MET	-	expression tag	UNP B4E8B7
D	-6	ALA	-	expression tag	UNP B4E8B7
D	-5	HIS	-	expression tag	UNP B4E8B7
D	-4	HIS	-	expression tag	UNP B4E8B7
D	-3	HIS	-	expression tag	UNP B4E8B7
D	-2	HIS	-	expression tag	UNP B4E8B7
D	-1	HIS	-	expression tag	UNP B4E8B7
D	0	HIS	-	expression tag	UNP B4E8B7
E	-7	MET	-	expression tag	UNP B4E8B7
E	-6	ALA	-	expression tag	UNP B4E8B7
E	-5	HIS	-	expression tag	UNP B4E8B7
E	-4	HIS	-	expression tag	UNP B4E8B7
E	-3	HIS	-	expression tag	UNP B4E8B7
E	-2	HIS	-	expression tag	UNP B4E8B7
E	-1	HIS	-	expression tag	UNP B4E8B7
E	0	HIS	-	expression tag	UNP B4E8B7
F	-7	MET	-	expression tag	UNP B4E8B7
F	-6	ALA	-	expression tag	UNP B4E8B7
F	-5	HIS	-	expression tag	UNP B4E8B7
F	-4	HIS	-	expression tag	UNP B4E8B7
F	-3	HIS	-	expression tag	UNP B4E8B7
F	-2	HIS	-	expression tag	UNP B4E8B7
F	-1	HIS	-	expression tag	UNP B4E8B7
F	0	HIS	-	expression tag	UNP B4E8B7
G	-7	MET	-	expression tag	UNP B4E8B7
G	-6	ALA	-	expression tag	UNP B4E8B7
G	-5	HIS	-	expression tag	UNP B4E8B7
G	-4	HIS	-	expression tag	UNP B4E8B7
G	-3	HIS	-	expression tag	UNP B4E8B7
G	-2	HIS	-	expression tag	UNP B4E8B7
G	-1	HIS	-	expression tag	UNP B4E8B7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP B4E8B7
H	-7	MET	-	expression tag	UNP B4E8B7
H	-6	ALA	-	expression tag	UNP B4E8B7
H	-5	HIS	-	expression tag	UNP B4E8B7
H	-4	HIS	-	expression tag	UNP B4E8B7
H	-3	HIS	-	expression tag	UNP B4E8B7
H	-2	HIS	-	expression tag	UNP B4E8B7
H	-1	HIS	-	expression tag	UNP B4E8B7
H	0	HIS	-	expression tag	UNP B4E8B7

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
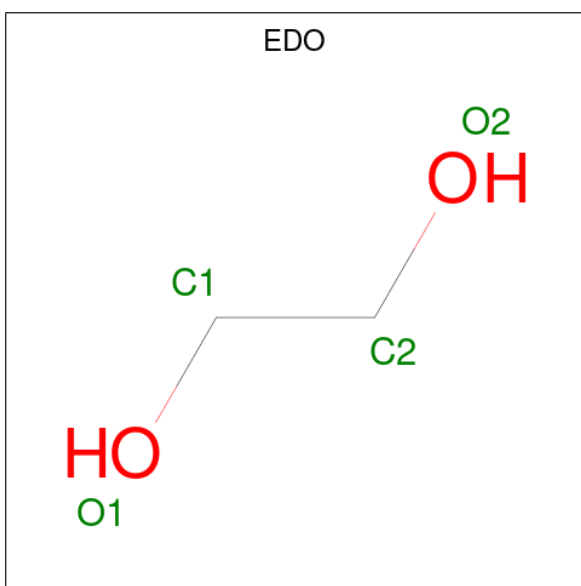
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0
2	F	1	Total 4	C 2	O 2	0	0

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	G	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0
2	H	1	Total 4	C 2	O 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0
3	C	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Ca 1	0	0
4	F	2	Total 2	Ca 2	0	0
4	G	2	Total 2	Ca 2	0	0
4	H	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	419	Total 419	O 419	0	0
5	B	445	Total 445	O 445	0	0
5	C	363	Total 363	O 363	0	0
5	D	429	Total 429	O 429	0	0
5	E	353	Total 353	O 353	0	0
5	F	411	Total 411	O 411	0	0
5	G	395	Total 395	O 395	0	0
5	H	401	Total 401	O 401	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.
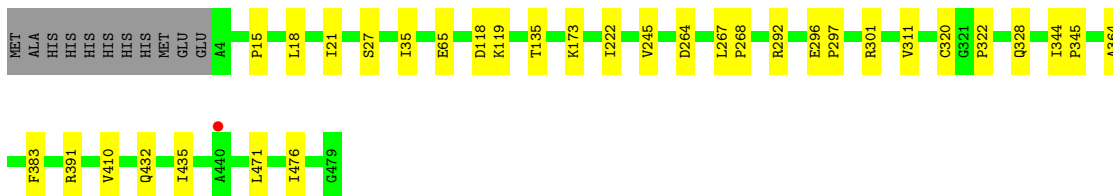
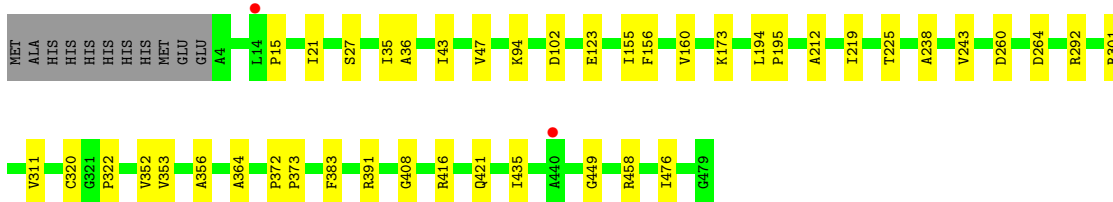• Molecule 1: Putative aldehyde dehydrogenase

Chain A:
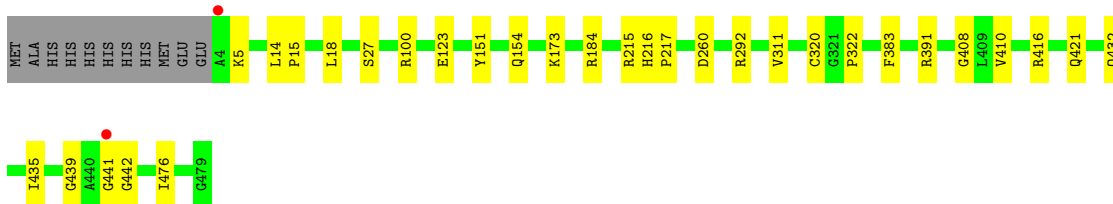
• Molecule 1: Putative aldehyde dehydrogenase

Chain B:

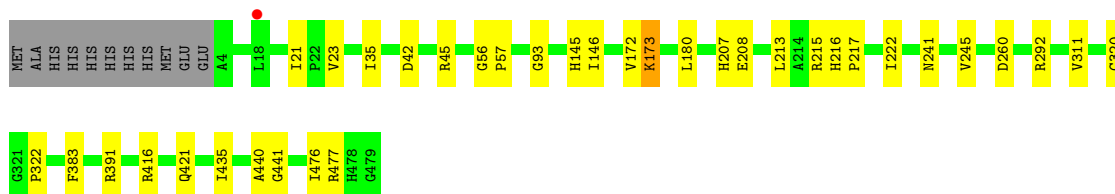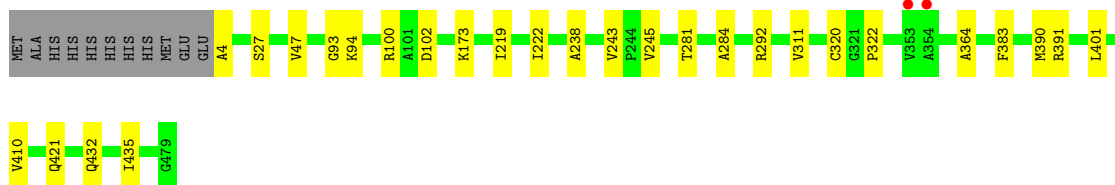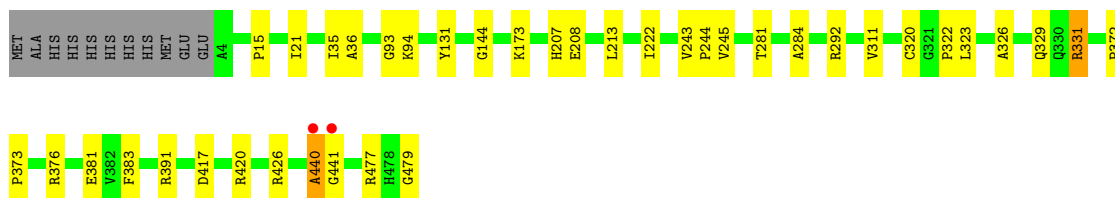• Molecule 1: Putative aldehyde dehydrogenase

Chain C:

• Molecule 1: Putative aldehyde dehydrogenase

Chain D:

MET ALA HIS HIS HIS HIS MET GLU GLU A4 L18 I21 P22 V23 I35 D42 R45 G56 P57 G93 H145 I146 V172 K173 L180 H207 E208 L213 A214 R215 H216 P217 I222 N241 V245 D260 R292 V311 C320

G321 P322 F383 R391 R416 Q421 I435 A440 G441 I476 R477 H478 G479

• Molecule 1: Putative aldehyde dehydrogenase

Chain E:

92%   6%   •

MET ALA HIS HIS HIS HIS MET GLU GLU A4 S27 V47 G93 K94 R100 A101 D102 K173 I219 I222 A238 V243 P244 V245 T281 A284 R292 V311 C320 G321 P322 V353 A354 A364 F383 M390 R391 L401

V410 Q421 Q432 I435 G479

• Molecule 1: Putative aldehyde dehydrogenase

Chain F:

90%   8%   •

MET ALA HIS HIS HIS HIS MET GLU GLU A4 P15 I21 I35 A36 G93 K94 Y131 G144 K173 H207 E208 L213 I222 V243 P244 V245 T281 A284 R292 V311 C320 G321 P322 L323 A326 Q329 Q330 R331 P372

P373 R376 E381 V382 F383 R391 D417 R420 R426 A440 G441 R477 H478 G479

• Molecule 1: Putative aldehyde dehydrogenase

Chain G:

%
87%   10%   •

MET ALA HIS HIS HIS HIS MET GLU GLU A4 S27 V47 A89 E123 Y131 R137 F156 V160 V172 K173 R184 E187 I201 R215 I219 I222 V245 L267 P268 T281 C282 S283 A284 R292 E296 V311

S314 C320 G321 P322 G350 A354 P365 R369 P372 P373 F383 R391 F392 V393 E397 N403 G408 L409 V410 D417 R420 Q421 R429 Q432 I435 M436 N437 Y438 G439 A440 G441 G442 I476 R477 H478 G479

• Molecule 1: Putative aldehyde dehydrogenase

Chain H:

90%   7%   •

MET ALA HIS HIS HIS HIS MET GLU GLU A4 L14 Q30 P31 V47 R68 T78 I81 A89 Q128 K173 V182 A186 I201 I219 D220 H221 I222 V243 P244 V245 D260 D264 R292 R301 R310 V311 S314

C320 A364 F383 R391 V410 R416 R429 Q432 I435 G439 ALA GLY G442 I476 G479

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.32Å 93.07Å 139.43Å 89.12° 78.55° 89.85°	Depositor
Resolution (Å)	19.95 – 2.15 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.95-2.15) 98.3 (19.95-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1932)	Depositor
R, R_{free}	0.198 , 0.243 0.198 , 0.243	Depositor DCC
R_{free} test set	11352 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.157 for -h,k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31507	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, EDO, MG

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	0.20	0/3589	0.35	0/4891
1	B	0.20	0/3626	0.36	0/4939
1	C	0.20	0/3603	0.35	0/4907
1	D	0.21	0/3610	0.37	0/4918
1	E	0.20	0/3618	0.35	0/4929
1	F	0.21	0/3609	0.38	1/4918 (0.0%)
1	G	0.20	0/3642	0.36	0/4961
1	H	0.21	0/3618	0.36	0/4924
All	All	0.20	0/28915	0.36	1/39387 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	440	ALA	CA-C-N	5.18	126.57	116.20

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	3506	0	3444	18	0
1	B	3543	0	3494	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3517	0	3462	22	0
1	D	3521	0	3468	21	0
1	E	3524	0	3473	16	0
1	F	3517	0	3458	22	0
1	G	3544	0	3511	29	0
1	H	3536	0	3494	22	0
2	A	4	0	6	0	0
2	B	8	0	12	1	0
2	C	8	0	12	0	0
2	F	12	0	18	1	0
2	G	20	0	30	1	0
2	H	16	0	24	2	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	419	0	0	4	0
5	B	445	0	0	1	0
5	C	363	0	0	0	0
5	D	429	0	0	1	0
5	E	353	0	0	2	0
5	F	411	0	0	2	0
5	G	395	0	0	1	0
5	H	401	0	0	3	0
All	All	31507	0	27906	161	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 3.

All (161) 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:D:440:ALA:HB1	1:D:441:GLY:HA3	1.63	0.81
1:F:440:ALA:HB3	1:F:441:GLY:HA3	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:VAL:HG22	1:F:320:CYS:HB3	1.71	0.72
1:B:410[B]:VAL:HG12	1:B:432:GLN:HB2	1.73	0.70
1:F:440:ALA:CB	1:F:441:GLY:HA3	2.23	0.69
1:G:410[A]:VAL:HG12	1:G:432:GLN:HB2	1.76	0.67
1:F:15:PRO:HG3	1:F:36:ALA:HB1	1.76	0.66
1:B:311:VAL:HG22	1:B:320:CYS:HB2	1.76	0.66
1:G:403:ASN:O	1:G:429[A]:ARG:NH2	2.29	0.66
1:F:477:ARG:HH11	1:F:479:GLY:HA2	1.62	0.65
1:A:476:ILE:HG12	1:B:435:ILE:HD12	1.78	0.65
1:G:311:VAL:HG22	1:G:320:CYS:HB3	1.78	0.64
1:C:15:PRO:HG3	1:C:36:ALA:HB1	1.80	0.64
1:G:292:ARG:HG2	1:G:391:ARG:HD2	1.80	0.63
1:H:222:ILE:HB	1:H:245:VAL:HG22	1.80	0.63
1:G:184:ARG:NH1	1:G:187:GLU:OE1	2.32	0.62
1:G:123[B]:GLU:OE2	1:G:137:ARG:NH2	2.33	0.62
1:H:68:ARG:HH12	2:H:503:EDO:H12	1.65	0.62
1:F:326:ALA:H	2:F:501:EDO:H12	1.64	0.62
1:E:421:GLN:HB3	1:E:435:ILE:HD13	1.83	0.61
1:D:311:VAL:HG22	1:D:320:CYS:HB3	1.82	0.60
1:H:4:ALA:N	5:H:610:HOH:O	2.34	0.60
1:H:429:ARG:NH1	5:H:608:HOH:O	2.34	0.60
1:F:331:ARG:NH2	1:F:381:GLU:O	2.36	0.58
1:G:410[B]:VAL:HG22	1:G:432:GLN:HB2	1.85	0.58
1:H:292:ARG:HG2	1:H:391:ARG:HD2	1.84	0.58
1:D:222:ILE:HB	1:D:245:VAL:HG22	1.85	0.58
1:E:222:ILE:HB	1:E:245:VAL:HG22	1.85	0.58
1:A:311:VAL:HG22	1:A:320:CYS:HB3	1.86	0.57
1:C:435:ILE:HD12	1:D:476:ILE:HG12	1.86	0.57
1:D:292:ARG:HG2	1:D:391:ARG:HD2	1.86	0.57
1:A:421:GLN:HB3	1:A:435:ILE:HD13	1.86	0.57
1:A:100:ARG:NH1	5:A:610:HOH:O	2.38	0.57
1:B:27:SER:HA	1:B:322:PRO:HG3	1.86	0.57
1:E:4:ALA:N	5:E:612:HOH:O	2.36	0.57
1:H:310:ARG:NH2	5:H:615:HOH:O	2.37	0.56
1:D:260:ASP:O	1:D:416:ARG:NH1	2.39	0.56
1:H:260:ASP:O	1:H:416[B]:ARG:NH2	2.35	0.55
1:G:282:CYS:SG	5:G:756:HOH:O	2.57	0.55
1:G:435:ILE:HD12	1:H:476:ILE:HG12	1.88	0.55
1:F:292:ARG:HG2	1:F:391:ARG:HD2	1.88	0.55
1:C:94:LYS:NZ	1:C:102:ASP:OD2	2.35	0.54
1:D:421:GLN:HB3	1:D:435:ILE:HD13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:VAL:HG21	1:E:364:ALA:HA	1.89	0.54
1:C:264:ASP:OD1	1:C:301:ARG:NH2	2.36	0.54
1:E:292:ARG:HG2	1:E:391:ARG:HD2	1.89	0.54
1:A:27:SER:HA	1:A:322:PRO:HG3	1.90	0.53
1:G:421:GLN:HB3	1:G:435:ILE:HD13	1.89	0.53
1:H:410:VAL:HG12	1:H:432:GLN:HB2	1.90	0.53
1:H:311:VAL:HG21	1:H:364:ALA:HA	1.91	0.53
1:A:184:ARG:NH2	5:A:607:HOH:O	2.36	0.52
1:E:311:VAL:HG22	1:E:320:CYS:HB2	1.89	0.52
1:A:5:LYS:HG2	1:A:14:LEU:HD23	1.90	0.52
1:F:376:ARG:NH2	5:F:609:HOH:O	2.36	0.52
1:D:477:ARG:NH1	5:D:614:HOH:O	2.40	0.52
1:G:222:ILE:HB	1:G:245:VAL:HG22	1.92	0.51
1:B:292:ARG:HG2	1:B:391:ARG:HD2	1.92	0.51
1:G:27:SER:HA	1:G:322:PRO:HG3	1.92	0.51
1:C:27:SER:HA	1:C:322:PRO:HG3	1.93	0.51
1:D:440:ALA:CB	1:D:441:GLY:HA3	2.38	0.51
1:E:27:SER:HA	1:E:322:PRO:HG3	1.92	0.51
1:H:47:VAL:HG22	1:H:219:ILE:HD11	1.92	0.51
1:H:182:VAL:HG12	1:H:201[B]:ILE:HD13	1.93	0.50
1:C:421:GLN:HB3	1:C:435:ILE:HD13	1.93	0.50
1:B:264:ASP:OD1	1:B:301:ARG:NH1	2.44	0.50
1:A:435:ILE:HD12	1:B:476:ILE:HG12	1.93	0.50
1:E:100:ARG:NH1	5:E:630:HOH:O	2.45	0.49
1:C:292:ARG:HG2	1:C:391:ARG:HD2	1.94	0.49
1:G:172:VAL:HB	1:G:201:ILE:HD13	1.94	0.49
1:B:328:GLN:NE2	5:B:618:HOH:O	2.43	0.49
1:C:155:ILE:HD13	1:C:225:THR:HG21	1.94	0.49
1:C:194:LEU:HD12	1:C:195:PRO:HD2	1.95	0.49
1:E:410[A]:VAL:HG12	1:E:432:GLN:HB2	1.94	0.49
1:G:215:ARG:HB2	2:G:504:EDO:H21	1.94	0.48
1:G:435:ILE:O	1:G:437:ASN:ND2	2.46	0.48
1:E:390[A]:MET:HE1	1:E:401:LEU:HD22	1.95	0.48
1:F:144:GLY:HA3	1:F:213:LEU:HD21	1.96	0.47
1:B:222:ILE:HB	1:B:245:VAL:HG22	1.96	0.47
1:C:476:ILE:HG12	1:D:435:ILE:HD12	1.95	0.47
1:D:146:ILE:HD11	1:D:213:LEU:HD22	1.96	0.47
1:F:222:ILE:HB	1:F:245:VAL:HG22	1.97	0.47
1:D:42:ASP:OD1	1:D:45:ARG:NH2	2.47	0.47
1:B:65:GLU:HG2	2:B:501:EDO:H22	1.96	0.47
1:C:43:ILE:HG13	1:C:212:ALA:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:VAL:HG23	1:C:364:ALA:HB2	1.97	0.46
1:E:47:VAL:HG22	1:E:219:ILE:HD11	1.98	0.46
1:B:21:ILE:HB	1:B:35:ILE:HG13	1.99	0.45
1:F:21:ILE:HB	1:F:35:ILE:HG13	1.98	0.45
1:G:131:TYR:CZ	1:G:477:ARG:HD3	2.51	0.45
1:A:215:ARG:NH1	5:A:630:HOH:O	2.50	0.45
1:C:372:PRO:HA	1:C:373:PRO:HD3	1.87	0.45
1:D:215:ARG:O	1:D:241:ASN:ND2	2.49	0.45
1:F:93:GLY:O	1:F:322:PRO:HD2	2.16	0.45
1:G:47:VAL:HG22	1:G:219[A]:ILE:HD11	1.98	0.45
1:A:441:GLY:HA2	1:A:442:GLY:HA2	1.64	0.45
1:F:417:ASP:HB3	1:F:420:ARG:HB3	1.99	0.45
1:H:14:LEU:HD13	2:H:502:EDO:H12	1.98	0.45
1:D:173:LYS:HB2	1:D:213:LEU:HD13	1.98	0.45
1:D:216:HIS:HA	1:D:217:PRO:HD3	1.79	0.44
1:G:372:PRO:HA	1:G:373:PRO:HD3	1.92	0.44
1:C:260:ASP:O	1:C:416:ARG:NH1	2.49	0.44
1:D:93:GLY:O	1:D:322:PRO:HD2	2.17	0.44
1:D:207:HIS:ND1	1:D:208:GLU:HG3	2.33	0.44
1:F:131:TYR:CZ	1:F:477:ARG:HD2	2.53	0.44
1:D:21:ILE:HB	1:D:35:ILE:HG13	1.98	0.44
1:H:89:ALA:HB1	1:H:314:SER:OG	2.18	0.44
1:H:186:ALA:HB2	1:H:201[B]:ILE:HD12	2.00	0.44
1:G:476:ILE:HA	1:H:435:ILE:HB	1.98	0.44
1:H:264:ASP:OD1	1:H:301:ARG:NH1	2.51	0.43
1:A:216:HIS:HA	1:A:217:PRO:HD3	1.75	0.43
1:D:23:VAL:HG11	1:D:180:LEU:HD11	1.99	0.43
1:H:30:GLN:HA	1:H:31:PRO:HD3	1.84	0.43
1:A:410:VAL:HG22	1:A:432:GLN:HB2	2.00	0.43
1:G:441:GLY:O	1:H:128:GLN:NE2	2.52	0.43
1:C:238:ALA:HB1	1:C:243:VAL:HB	2.00	0.43
1:B:118:ASP:OD1	1:B:119:LYS:NZ	2.45	0.43
1:B:410[A]:VAL:HG22	1:B:432:GLN:HB2	1.99	0.43
1:G:441:GLY:HA2	1:G:442:GLY:HA2	1.68	0.43
1:A:184:ARG:NH2	5:A:608:HOH:O	2.38	0.42
1:B:267:LEU:HB3	1:B:268:PRO:HD3	2.01	0.42
1:C:47:VAL:HG22	1:C:219:ILE:HD11	2.01	0.42
1:C:353:VAL:HG23	1:C:356:ALA:HB2	2.00	0.42
1:C:311:VAL:HG22	1:C:320:CYS:HB3	2.01	0.42
1:C:449:GLY:HA3	1:C:458:ARG:HD3	2.01	0.42
1:G:89:ALA:HB1	1:G:314:SER:OG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:THR:O	1:H:81:ILE:HG12	2.20	0.42
1:B:344:ILE:HA	1:B:345:PRO:HD3	1.90	0.42
1:A:260:ASP:O	1:A:416:ARG:NH1	2.50	0.42
1:F:243:VAL:HA	1:F:244:PRO:HD3	1.92	0.42
1:F:207:HIS:CD2	1:F:208:GLU:HG3	2.54	0.42
1:F:426:ARG:NH2	5:F:638:HOH:O	2.53	0.42
1:A:15:PRO:HG2	1:A:18:LEU:HA	2.02	0.42
1:A:292:ARG:HG2	1:A:391:ARG:HD2	2.00	0.42
1:F:372:PRO:HA	1:F:373:PRO:HD3	1.92	0.42
1:H:243:VAL:HA	1:H:244:PRO:HD2	1.94	0.42
1:E:93:GLY:O	1:E:322:PRO:HD2	2.20	0.41
1:F:323:LEU:HD12	1:F:329:GLN:HA	2.02	0.41
1:G:296:GLU:OE2	1:G:369:ARG:NH2	2.46	0.41
1:E:94:LYS:NZ	1:E:102:ASP:OD2	2.43	0.41
1:E:238:ALA:HB1	1:E:243:VAL:HB	2.02	0.41
1:A:123:GLU:HA	1:C:123:GLU:HA	2.02	0.41
1:G:281:THR:HB	1:G:284:ALA:HB2	2.03	0.41
1:G:393:VAL:HG12	1:G:397:GLU:OE1	2.19	0.41
1:A:151:TYR:HB3	1:A:154:GLN:HB2	2.03	0.41
1:D:145:HIS:HB2	1:D:172:VAL:HG22	2.02	0.41
1:B:135:THR:HB	1:B:471:LEU:HD11	2.03	0.41
1:F:281:THR:HB	1:F:284:ALA:HB2	2.03	0.41
1:H:311:VAL:HG22	1:H:320:CYS:HB3	2.02	0.41
1:G:417:ASP:HB3	1:G:420:ARG:HB3	2.03	0.41
1:B:296:GLU:HB2	1:B:297:PRO:HD3	2.03	0.40
1:G:156:PHE:CE1	1:G:160:VAL:HG21	2.56	0.40
1:C:21:ILE:HB	1:C:35:ILE:HG13	2.02	0.40
1:D:56:GLY:HA3	1:D:57:PRO:HD3	1.89	0.40
1:E:281:THR:HB	1:E:284:ALA:HB2	2.03	0.40
1:E:410[B]:VAL:HG22	1:E:432:GLN:HB2	2.02	0.40
1:F:94:LYS:HB3	1:F:94:LYS:HE2	1.95	0.40
1:G:350:GLY:HA3	1:G:365:PRO:HD2	2.03	0.40
1:B:311:VAL:HG21	1:B:364:ALA:HA	2.02	0.40
1:G:267:LEU:HB3	1:G:268:PRO:HD3	2.04	0.40
1:B:15:PRO:HG2	1:B:18:LEU:HA	2.04	0.40
1:C:156:PHE:CE1	1:C:160:VAL:HG21	2.57	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	475/487 (98%)	461 (97%)	12 (2%)	2 (0%)	34	29
1	B	478/487 (98%)	461 (96%)	17 (4%)	0	100	100
1	C	476/487 (98%)	458 (96%)	17 (4%)	1 (0%)	47	46
1	D	477/487 (98%)	462 (97%)	15 (3%)	0	100	100
1	E	480/487 (99%)	462 (96%)	18 (4%)	0	100	100
1	F	478/487 (98%)	459 (96%)	19 (4%)	0	100	100
1	G	480/487 (99%)	462 (96%)	16 (3%)	2 (0%)	34	29
1	H	473/487 (97%)	458 (97%)	15 (3%)	0	100	100
All	All	3817/3896 (98%)	3683 (96%)	129 (3%)	5 (0%)	51	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	GLY
1	C	408	GLY
1	A	408	GLY
1	G	408	GLY
1	G	439	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	337/352 (96%)	335 (99%)	2 (1%)	86	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	343/352 (97%)	341 (99%)	2 (1%)	86	90
1	C	339/352 (96%)	337 (99%)	2 (1%)	86	90
1	D	340/352 (97%)	338 (99%)	2 (1%)	86	90
1	E	338/352 (96%)	336 (99%)	2 (1%)	86	90
1	F	339/352 (96%)	336 (99%)	3 (1%)	78	83
1	G	344/352 (98%)	341 (99%)	3 (1%)	78	83
1	H	343/352 (97%)	341 (99%)	2 (1%)	86	90
All	All	2723/2816 (97%)	2705 (99%)	18 (1%)	84	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LYS
1	A	383	PHE
1	B	173	LYS
1	B	383	PHE
1	C	173	LYS
1	C	383	PHE
1	D	173	LYS
1	D	383	PHE
1	E	173	LYS
1	E	383	PHE
1	F	173	LYS
1	F	331	ARG
1	F	383	PHE
1	G	173	LYS
1	G	383	PHE
1	G	437	ASN
1	H	173	LYS
1	H	383	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 15 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	EDO	H	502	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	B	502	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	G	503	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	H	504	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	F	501	-	3,3,3	0.47	0	2,2,2	0.25	0
2	EDO	H	501	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	501	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	H	503	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	F	502	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	F	503	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	G	504	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	G	505	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	C	501	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	G	501	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	G	502	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	B	501	-	3,3,3	0.46	0	2,2,2	0.33	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.

Full wwPDB X-ray Structure Validation Report

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	H	502	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	G	503	-	-	0/1/1/1	-
2	EDO	H	504	-	-	0/1/1/1	-
2	EDO	F	501	-	-	0/1/1/1	-
2	EDO	H	501	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	H	503	-	-	0/1/1/1	-
2	EDO	F	502	-	-	0/1/1/1	-
2	EDO	F	503	-	-	0/1/1/1	-
2	EDO	G	504	-	-	1/1/1/1	-
2	EDO	G	505	-	-	0/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	G	501	-	-	0/1/1/1	-
2	EDO	G	502	-	-	0/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	504	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	502	EDO	1	0
2	F	501	EDO	1	0
2	H	503	EDO	1	0
2	G	504	EDO	1	0
2	B	501	EDO	1	0

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(Å²)	Q<0.9
1	A	476/487 (97%)	-0.37	2 (0%)	92	94	11, 21, 37, 73	0
1	B	476/487 (97%)	-0.33	1 (0%)	95	96	12, 21, 35, 85	0
1	C	476/487 (97%)	-0.24	2 (0%)	92	94	13, 27, 41, 64	0
1	D	476/487 (97%)	-0.35	1 (0%)	95	96	14, 22, 37, 82	0
1	E	476/487 (97%)	-0.23	2 (0%)	92	94	12, 27, 46, 62	0
1	F	476/487 (97%)	-0.32	2 (0%)	92	94	13, 22, 39, 73	0
1	G	476/487 (97%)	-0.31	4 (0%)	86	89	11, 21, 37, 71	0
1	H	474/487 (97%)	-0.27	1 (0%)	95	96	11, 22, 38, 67	0
All	All	3806/3896 (97%)	-0.30	15 (0%)	92	94	11, 23, 40, 85	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	ALA	4.5
1	F	440	ALA	4.4
1	H	221	HIS	4.2
1	G	439	GLY	3.3
1	G	441	GLY	2.6
1	A	441	GLY	2.5
1	E	354	ALA	2.5
1	C	440	ALA	2.3
1	A	4	ALA	2.2
1	D	18	LEU	2.2
1	E	353	VAL	2.2
1	G	354	ALA	2.2
1	G	440	ALA	2.1
1	C	14	LEU	2.0
1	F	441	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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
2	EDO	F	503	4/4	0.73	0.32	55,55,55,55	0
2	EDO	A	501	4/4	0.78	0.27	45,45,46,46	0
2	EDO	G	505	4/4	0.78	0.27	46,48,48,49	0
2	EDO	H	502	4/4	0.83	0.22	37,37,37,38	0
2	EDO	F	502	4/4	0.86	0.21	40,41,42,43	0
2	EDO	F	501	4/4	0.86	0.23	25,26,26,27	0
2	EDO	B	502	4/4	0.87	0.21	33,37,37,39	0
2	EDO	G	503	4/4	0.89	0.16	29,36,43,48	0
2	EDO	H	504	4/4	0.89	0.14	23,29,31,32	0
2	EDO	G	504	4/4	0.90	0.22	28,31,33,34	0
2	EDO	G	502	4/4	0.90	0.16	31,34,39,42	0
2	EDO	B	501	4/4	0.91	0.16	39,41,43,43	0
2	EDO	H	503	4/4	0.92	0.19	32,35,39,42	0
3	MG	C	503	1/1	0.92	0.14	45,45,45,45	0
4	CA	A	503	1/1	0.92	0.07	57,57,57,57	0
2	EDO	H	501	4/4	0.93	0.13	32,32,34,35	0
4	CA	F	505	1/1	0.93	0.26	61,61,61,61	0
4	CA	G	506	1/1	0.93	0.08	39,39,39,39	0
4	CA	G	507	1/1	0.94	0.10	70,70,70,70	0
4	CA	H	505	1/1	0.94	0.13	44,44,44,44	0
2	EDO	C	502	4/4	0.95	0.14	33,34,36,36	0
2	EDO	C	501	4/4	0.95	0.10	26,27,27,29	0
4	CA	C	504	1/1	0.96	0.08	54,54,54,54	0
4	CA	D	501	1/1	0.97	0.05	36,36,36,36	0
4	CA	F	504	1/1	0.97	0.06	40,40,40,40	0
4	CA	B	503	1/1	0.98	0.10	46,46,46,46	0
2	EDO	G	501	4/4	0.98	0.08	19,21,22,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	MG	E	501	1/1	0.98	0.12	41,41,41,41	0
3	MG	A	504	1/1	0.98	0.08	44,44,44,44	0
4	CA	E	502	1/1	0.99	0.07	46,46,46,46	0
3	MG	A	502	1/1	0.99	0.04	32,32,32,32	0
4	CA	D	502	1/1	0.99	0.12	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.