Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:03 PM GMT

PDB ID	:	5EYU
Title	:	1.72 Angstrom resolution crystal structure of betaine aldehyde dehydrogenase (betB) P449M point mutant from Staphylococcus aureus in complex with NAD+ and BME-modified Cys289
Authors	:	Halavaty, A.S.; Minasov, G.; Chen, C.; Joo, J.C.; Yakunin, A.F.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2015-11-25
Resolution	:	1.72 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

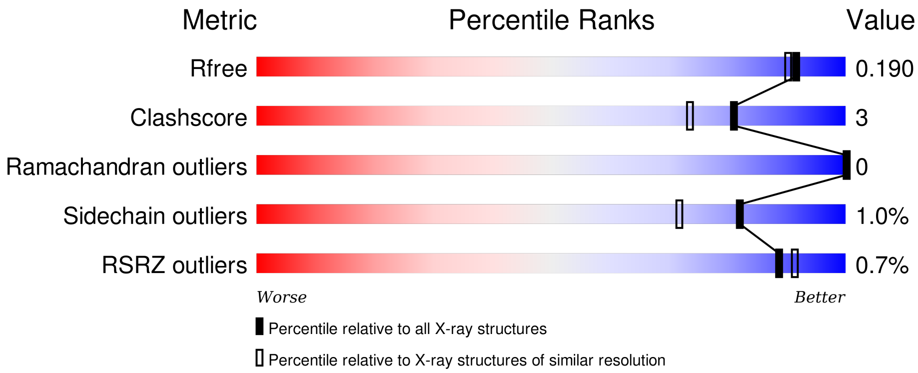
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	517	90% 5% 5%
1	B	517	% 90% 5% 5%
1	C	517	89% 6% 5%
1	D	517	% 90% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EPE	A	504[A]	-	-	-	X
4	EPE	A	504[B]	-	-	-	X
4	EPE	B	504[A]	-	-	-	X
4	EPE	B	504[B]	-	-	-	X
4	EPE	C	504	-	-	-	X
5	PGE	A	505	-	-	-	X
5	PGE	B	506	-	-	-	X
5	PGE	D	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18426 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 Betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total 3946	C 2480	N 671	O 778	S 17	0	17	0
1	B	491	Total 3945	C 2479	N 671	O 778	S 17	0	17	0
1	C	491	Total 3918	C 2466	N 662	O 771	S 19	0	15	0
1	D	491	Total 3939	C 2479	N 667	O 774	S 19	0	17	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9L4P8
A	-19	GLY	-	expression tag	UNP Q9L4P8
A	-18	SER	-	expression tag	UNP Q9L4P8
A	-17	SER	-	expression tag	UNP Q9L4P8
A	-16	HIS	-	expression tag	UNP Q9L4P8
A	-15	HIS	-	expression tag	UNP Q9L4P8
A	-14	HIS	-	expression tag	UNP Q9L4P8
A	-13	HIS	-	expression tag	UNP Q9L4P8
A	-12	HIS	-	expression tag	UNP Q9L4P8
A	-11	HIS	-	expression tag	UNP Q9L4P8
A	-10	SER	-	expression tag	UNP Q9L4P8
A	-9	SER	-	expression tag	UNP Q9L4P8
A	-8	GLY	-	expression tag	UNP Q9L4P8
A	-7	ARG	-	expression tag	UNP Q9L4P8
A	-6	GLU	-	expression tag	UNP Q9L4P8
A	-5	ASN	-	expression tag	UNP Q9L4P8
A	-4	LEU	-	expression tag	UNP Q9L4P8
A	-3	TYR	-	expression tag	UNP Q9L4P8
A	-2	PHE	-	expression tag	UNP Q9L4P8
A	-1	GLN	-	expression tag	UNP Q9L4P8
A	0	GLY	-	expression tag	UNP Q9L4P8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	449	MET	PRO	engineered mutation	UNP Q9L4P8
B	-20	MET	-	expression tag	UNP Q9L4P8
B	-19	GLY	-	expression tag	UNP Q9L4P8
B	-18	SER	-	expression tag	UNP Q9L4P8
B	-17	SER	-	expression tag	UNP Q9L4P8
B	-16	HIS	-	expression tag	UNP Q9L4P8
B	-15	HIS	-	expression tag	UNP Q9L4P8
B	-14	HIS	-	expression tag	UNP Q9L4P8
B	-13	HIS	-	expression tag	UNP Q9L4P8
B	-12	HIS	-	expression tag	UNP Q9L4P8
B	-11	HIS	-	expression tag	UNP Q9L4P8
B	-10	SER	-	expression tag	UNP Q9L4P8
B	-9	SER	-	expression tag	UNP Q9L4P8
B	-8	GLY	-	expression tag	UNP Q9L4P8
B	-7	ARG	-	expression tag	UNP Q9L4P8
B	-6	GLU	-	expression tag	UNP Q9L4P8
B	-5	ASN	-	expression tag	UNP Q9L4P8
B	-4	LEU	-	expression tag	UNP Q9L4P8
B	-3	TYR	-	expression tag	UNP Q9L4P8
B	-2	PHE	-	expression tag	UNP Q9L4P8
B	-1	GLN	-	expression tag	UNP Q9L4P8
B	0	GLY	-	expression tag	UNP Q9L4P8
B	449	MET	PRO	engineered mutation	UNP Q9L4P8
C	-20	MET	-	expression tag	UNP Q9L4P8
C	-19	GLY	-	expression tag	UNP Q9L4P8
C	-18	SER	-	expression tag	UNP Q9L4P8
C	-17	SER	-	expression tag	UNP Q9L4P8
C	-16	HIS	-	expression tag	UNP Q9L4P8
C	-15	HIS	-	expression tag	UNP Q9L4P8
C	-14	HIS	-	expression tag	UNP Q9L4P8
C	-13	HIS	-	expression tag	UNP Q9L4P8
C	-12	HIS	-	expression tag	UNP Q9L4P8
C	-11	HIS	-	expression tag	UNP Q9L4P8
C	-10	SER	-	expression tag	UNP Q9L4P8
C	-9	SER	-	expression tag	UNP Q9L4P8
C	-8	GLY	-	expression tag	UNP Q9L4P8
C	-7	ARG	-	expression tag	UNP Q9L4P8
C	-6	GLU	-	expression tag	UNP Q9L4P8
C	-5	ASN	-	expression tag	UNP Q9L4P8
C	-4	LEU	-	expression tag	UNP Q9L4P8
C	-3	TYR	-	expression tag	UNP Q9L4P8
C	-2	PHE	-	expression tag	UNP Q9L4P8

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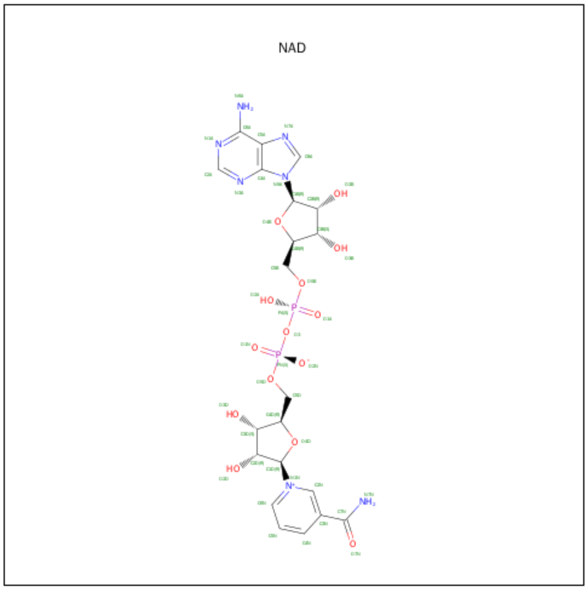
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLN	-	expression tag	UNP Q9L4P8
C	0	GLY	-	expression tag	UNP Q9L4P8
C	449	MET	PRO	engineered mutation	UNP Q9L4P8
D	-20	MET	-	expression tag	UNP Q9L4P8
D	-19	GLY	-	expression tag	UNP Q9L4P8
D	-18	SER	-	expression tag	UNP Q9L4P8
D	-17	SER	-	expression tag	UNP Q9L4P8
D	-16	HIS	-	expression tag	UNP Q9L4P8
D	-15	HIS	-	expression tag	UNP Q9L4P8
D	-14	HIS	-	expression tag	UNP Q9L4P8
D	-13	HIS	-	expression tag	UNP Q9L4P8
D	-12	HIS	-	expression tag	UNP Q9L4P8
D	-11	HIS	-	expression tag	UNP Q9L4P8
D	-10	SER	-	expression tag	UNP Q9L4P8
D	-9	SER	-	expression tag	UNP Q9L4P8
D	-8	GLY	-	expression tag	UNP Q9L4P8
D	-7	ARG	-	expression tag	UNP Q9L4P8
D	-6	GLU	-	expression tag	UNP Q9L4P8
D	-5	ASN	-	expression tag	UNP Q9L4P8
D	-4	LEU	-	expression tag	UNP Q9L4P8
D	-3	TYR	-	expression tag	UNP Q9L4P8
D	-2	PHE	-	expression tag	UNP Q9L4P8
D	-1	GLN	-	expression tag	UNP Q9L4P8
D	0	GLY	-	expression tag	UNP Q9L4P8
D	449	MET	PRO	engineered mutation	UNP Q9L4P8

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_{7}O_{14}P_{2}$).

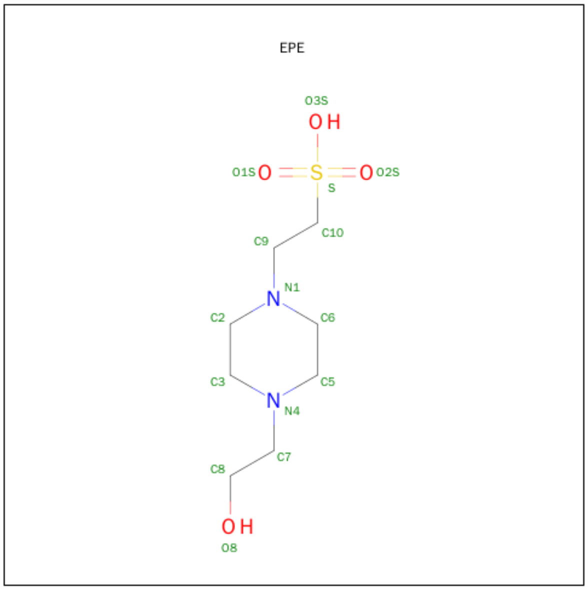


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 44 21 7 14 2	0	0
2	B	1	Total C N O P 44 21 7 14 2	0	0
2	C	1	Total C N O P 44 21 7 14 2	0	0
2	D	1	Total C N O P 44 21 7 14 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

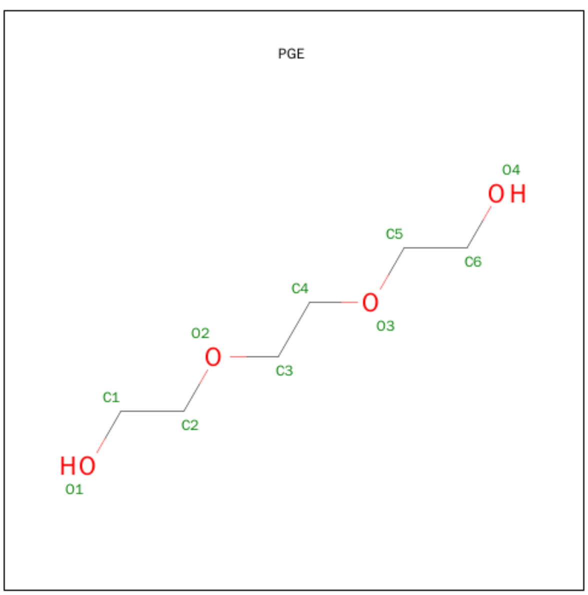
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0
3	A	2	Total Na 2 2	0	0
3	D	2	Total Na 2 2	0	0
3	C	2	Total Na 2 2	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 30 16 4 8 2	0	1
4	B	1	Total C N O S 30 16 4 8 2	0	1
4	B	1	Total C N O S 15 8 2 4 1	0	0
4	C	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

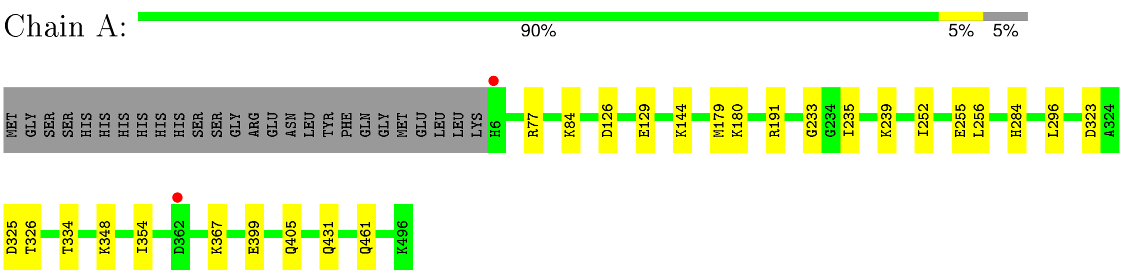
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	588	Total O 593 593	0	15
6	B	585	Total O 596 596	0	23
6	C	579	Total O 587 587	0	17
6	D	582	Total O 588 588	0	12

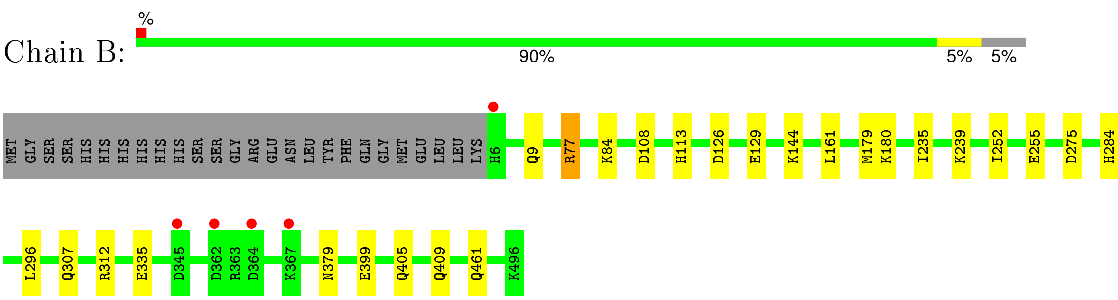
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

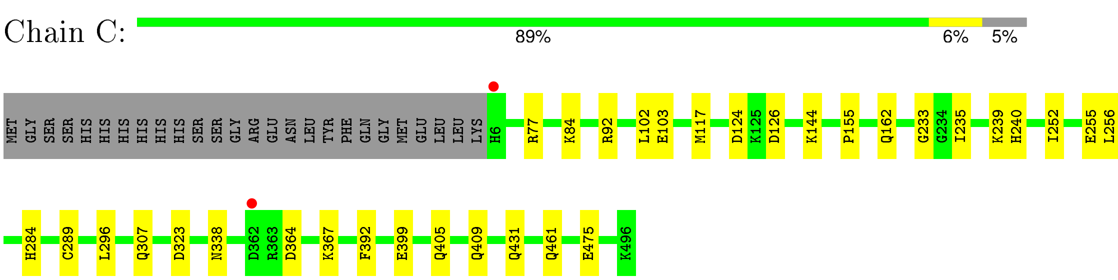
- Molecule 1: Betaine aldehyde dehydrogenase



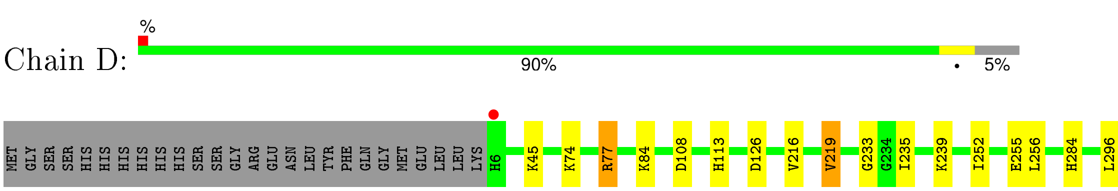
- Molecule 1: Betaine aldehyde dehydrogenase

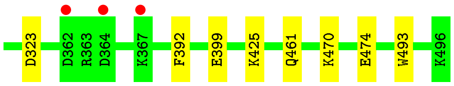


- Molecule 1: Betaine aldehyde dehydrogenase



- Molecule 1: Betaine aldehyde dehydrogenase




D323
D362
R363
D364
K367
F392
E399
K425
Q461
K470
E474
W493
K496

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	224.27Å 102.72Å 117.81Å 90.00° 104.75° 90.00°	Depositor
Resolution (Å)	29.66 – 1.72 29.66 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.66-1.72) 99.2 (29.66-1.72)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.164 , 0.183 0.174 , 0.190	Depositor DCC
R_{free} test set	13698 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| >$ = 0.46, $< L^2 >$ = 0.28	Xtriage
Outliers	0 of 271169 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18426	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, NA, CME, PGE, NAD

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	0.48	0/4005	0.67	0/5410
1	B	0.48	0/4004	0.67	0/5408
1	C	0.48	0/3977	0.66	0/5374
1	D	0.48	0/3998	0.68	1/5402 (0.0%)
All	All	0.48	0/15984	0.67	1/21594 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	108	ASP	CB-CG-OD2	-5.04	113.77	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3946	0	3870	24	0
1	B	3945	0	3873	28	0
1	C	3918	0	3853	33	0
1	D	3939	0	3873	20	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	30	0	36	2	0
4	B	45	0	54	2	0
4	C	15	0	18	0	0
5	A	10	0	14	0	0
5	B	10	0	14	0	0
5	C	10	0	14	0	0
5	D	10	0	14	0	0
6	A	593	0	0	19	0
6	B	596	0	0	20	0
6	C	587	0	0	22	0
6	D	588	0	0	11	0
All	All	18426	0	15737	106	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 (106) 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:474[A]:GLU:HG3	6:D:1087[A]:HOH:O	1.54	1.07
1:B:77[B]:ARG:HD3	1:C:77:ARG:HD3	1.53	0.89
1:B:126[A]:ASP:HB3	6:B:602[A]:HOH:O	1.71	0.88
1:B:235[A]:ILE:HD11	1:B:461:GLN:OE1	1.75	0.87
1:C:235[A]:ILE:HD11	1:C:461:GLN:OE1	1.76	0.86
1:A:235[A]:ILE:HD11	1:A:461:GLN:OE1	1.74	0.86
1:D:235[A]:ILE:HD11	1:D:461:GLN:OE1	1.76	0.83
1:C:126[B]:ASP:HB3	6:C:607[B]:HOH:O	1.83	0.79
1:C:289:CME:SD	6:C:624:HOH:O	2.41	0.78
1:B:161:LEU:HB2	6:B:690:HOH:O	1.85	0.75
1:A:326:THR:HA	6:A:1008:HOH:O	1.88	0.73
6:A:602:HOH:O	1:C:124:ASP:HB2	1.89	0.72
1:B:108:ASP:CG	6:B:690:HOH:O	2.31	0.68
1:B:307[B]:GLN:CD	6:B:609:HOH:O	2.31	0.68
1:B:409[A]:GLN:NE2	6:B:603:HOH:O	2.26	0.68
1:A:126[B]:ASP:HB3	6:A:601[B]:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379[A]:ASN:CB	6:B:753[A]:HOH:O	2.42	0.68
1:D:425:LYS:NZ	6:D:601:HOH:O	2.21	0.67
1:B:379[A]:ASN:HB2	6:B:753[A]:HOH:O	1.95	0.67
1:B:312:ARG:NH2	6:B:604:HOH:O	2.29	0.66
1:C:84:LYS:NZ	6:C:602:HOH:O	2.27	0.65
1:C:240:HIS:NE2	6:C:601:HOH:O	2.30	0.65
1:C:240:HIS:CE1	6:C:601:HOH:O	2.49	0.64
1:C:126[B]:ASP:CG	6:C:607[B]:HOH:O	2.36	0.64
1:A:431[B]:GLN:NE2	6:A:606:HOH:O	2.30	0.64
1:D:77[B]:ARG:NH1	6:D:603:HOH:O	2.30	0.63
1:D:126[B]:ASP:HB3	6:D:615[B]:HOH:O	1.98	0.63
1:B:312:ARG:NH1	6:B:604:HOH:O	2.32	0.63
1:C:126[B]:ASP:CB	6:C:607[B]:HOH:O	2.44	0.62
1:A:323:ASP:HB3	6:A:851:HOH:O	2.00	0.61
1:A:84:LYS:NZ	6:A:607:HOH:O	2.34	0.60
1:B:307[B]:GLN:NE2	6:B:609:HOH:O	2.35	0.60
1:A:144:LYS:NZ	6:A:603:HOH:O	2.25	0.59
1:D:126[B]:ASP:CG	6:D:615[B]:HOH:O	2.41	0.58
1:D:216:VAL:O	1:D:219[A]:VAL:HG13	2.04	0.58
1:B:108:ASP:CB	6:B:690:HOH:O	2.53	0.57
1:A:126[B]:ASP:CG	6:A:601[B]:HOH:O	2.43	0.56
1:A:126[B]:ASP:CB	6:A:601[B]:HOH:O	2.53	0.54
1:B:126[A]:ASP:CB	6:B:602[A]:HOH:O	2.44	0.54
1:C:162:GLN:CG	6:C:736:HOH:O	2.55	0.54
1:C:338[A]:ASN:HB3	6:C:1016[A]:HOH:O	2.07	0.54
1:C:92:ARG:HD3	6:C:1001:HOH:O	2.07	0.53
6:A:1160:HOH:O	1:B:129:GLU:HG2	2.08	0.53
1:B:312:ARG:CZ	6:B:604:HOH:O	2.55	0.53
1:D:470:LYS:O	1:D:474[B]:GLU:HG3	2.09	0.52
1:D:126[B]:ASP:CB	6:D:615[B]:HOH:O	2.57	0.52
1:A:367:LYS:HG2	6:A:1135:HOH:O	2.10	0.52
1:C:117[B]:MET:CE	6:C:1003:HOH:O	2.57	0.52
1:C:431:GLN:HG2	6:D:998:HOH:O	2.10	0.51
1:C:162:GLN:HG2	6:C:736:HOH:O	2.10	0.50
1:B:275:ASP:HA	6:B:604:HOH:O	2.10	0.50
1:A:191:ARG:NH1	4:A:504[B]:EPE:O8	2.42	0.49
1:B:379[A]:ASN:CG	6:B:753[A]:HOH:O	2.48	0.49
1:C:409:GLN:HG2	6:C:1135:HOH:O	2.13	0.49
1:B:144:LYS:NZ	6:B:618:HOH:O	2.46	0.49
1:D:323:ASP:HB3	6:D:945:HOH:O	2.13	0.49
1:D:74[B]:LYS:HE3	6:D:644:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD23	1:A:399:GLU:HB2	1.93	0.49
1:B:296:LEU:HD23	1:B:399:GLU:HB2	1.95	0.48
1:D:45:LYS:HB2	1:D:219[B]:VAL:HG21	1.95	0.48
1:D:219[B]:VAL:HG23	6:D:810:HOH:O	2.13	0.48
2:C:501:NAD:H51A	6:C:1020:HOH:O	2.13	0.48
1:D:296:LEU:HD23	1:D:399:GLU:HB2	1.95	0.48
1:A:325:ASP:HB2	6:A:851:HOH:O	2.14	0.48
1:C:296:LEU:HD23	1:C:399:GLU:HB2	1.95	0.47
1:C:475:GLU:CD	6:C:683:HOH:O	2.51	0.47
1:B:77[B]:ARG:HD3	1:C:77:ARG:CD	2.36	0.47
1:A:405:GLN:HG3	6:A:1092:HOH:O	2.14	0.47
1:C:307:GLN:HB2	6:C:777:HOH:O	2.14	0.47
1:C:77:ARG:NH2	6:C:623:HOH:O	2.48	0.47
1:C:92:ARG:HA	1:C:102:LEU:HD21	1.97	0.46
1:D:474[A]:GLU:CB	6:D:1087[A]:HOH:O	2.64	0.46
1:A:77[A]:ARG:NH2	6:A:623[A]:HOH:O	2.49	0.46
4:B:504[B]:EPE:H51	4:B:504[B]:EPE:H81	1.61	0.46
1:C:405:GLN:HG3	6:C:1083[A]:HOH:O	2.16	0.46
1:A:144:LYS:HD2	6:A:890:HOH:O	2.15	0.45
1:D:84:LYS:HE3	1:D:113:HIS:CE1	2.50	0.45
1:A:129:GLU:HG2	6:A:1154:HOH:O	2.16	0.45
1:A:334[B]:THR:CG2	6:A:965:HOH:O	2.64	0.45
1:C:144:LYS:HE2	6:C:754:HOH:O	2.16	0.45
1:B:9[A]:GLN:NE2	6:B:614:HOH:O	2.42	0.45
1:B:405:GLN:HG3	6:B:1068:HOH:O	2.17	0.44
1:A:179[B]:MET:HG3	1:A:180:LYS:N	2.31	0.44
1:C:162:GLN:HG3	6:C:736:HOH:O	2.18	0.43
1:C:117[B]:MET:HA	1:C:117[B]:MET:HE3	2.00	0.43
1:A:348:LYS:HE2	1:A:354:ILE:HG13	2.00	0.43
1:A:235[A]:ILE:HG12	1:A:239:LYS:HE3	2.01	0.43
1:D:45:LYS:HB2	1:D:219[B]:VAL:CG2	2.49	0.43
1:C:364:ASP:O	1:C:367:LYS:HG2	2.19	0.42
1:B:335:GLU:HG3	6:B:1022:HOH:O	2.18	0.42
1:C:235[A]:ILE:HG12	1:C:239:LYS:HE3	2.01	0.42
1:A:334[B]:THR:HG22	6:A:965:HOH:O	2.19	0.42
4:A:504[B]:EPE:H81	4:A:504[B]:EPE:H31	1.60	0.42
4:B:504[A]:EPE:H51	4:B:504[A]:EPE:H81	1.75	0.42
1:C:323:ASP:HB3	6:C:1013:HOH:O	2.19	0.41
1:C:233:GLY:O	1:C:256:LEU:HA	2.21	0.41
1:B:179[B]:MET:HG3	1:B:180:LYS:N	2.36	0.41
1:C:103[B]:GLU:HB3	1:D:493:TRP:HH2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:GLY:O	1:D:256:LEU:HA	2.21	0.41
1:C:155:PRO:HG2	6:C:736:HOH:O	2.19	0.41
1:A:233:GLY:O	1:A:256:LEU:HA	2.21	0.41
1:B:84:LYS:HE3	1:B:113:HIS:CE1	2.55	0.41
1:B:235[A]:ILE:HG12	1:B:239:LYS:HE3	2.03	0.40
1:D:235[A]:ILE:HG12	1:D:239:LYS:HE3	2.03	0.40
1:A:431[A]:GLN:NE2	6:A:635:HOH:O	2.54	0.40
1:B:144:LYS:HD2	6:B:880:HOH:O	2.21	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	505/517 (98%)	496 (98%)	9 (2%)	0	100	100
1	B	505/517 (98%)	496 (98%)	9 (2%)	0	100	100
1	C	503/517 (97%)	492 (98%)	11 (2%)	0	100	100
1	D	505/517 (98%)	495 (98%)	10 (2%)	0	100	100
All	All	2018/2068 (98%)	1979 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	421/428 (98%)	418 (99%)	3 (1%)	88	82
1	B	421/428 (98%)	416 (99%)	5 (1%)	78	65
1	C	419/428 (98%)	415 (99%)	4 (1%)	82	72
1	D	421/428 (98%)	413 (98%)	8 (2%)	65	45
All	All	1682/1712 (98%)	1662 (99%)	20 (1%)	82	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ILE
1	A	255	GLU
1	A	284	HIS
1	B	77[A]	ARG
1	B	77[B]	ARG
1	B	252	ILE
1	B	255	GLU
1	B	284	HIS
1	C	252	ILE
1	C	255	GLU
1	C	284	HIS
1	C	392	PHE
1	D	77[A]	ARG
1	D	77[B]	ARG
1	D	219[A]	VAL
1	D	219[B]	VAL
1	D	252	ILE
1	D	255	GLU
1	D	284	HIS
1	D	392	PHE

Some 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 (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CME	A	289	1	7,9,10	0.63	0	6,9,11	1.20	1 (16%)
1	CME	B	289	1	7,9,10	0.63	0	6,9,11	1.23	1 (16%)
1	CME	C	289	1	7,9,10	0.71	0	6,9,11	1.18	0
1	CME	D	289	1	7,9,10	0.62	0	6,9,11	1.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	289	1	-	0/5/8/10	0/0/0/0
1	CME	B	289	1	-	0/5/8/10	0/0/0/0
1	CME	C	289	1	-	0/5/8/10	0/0/0/0
1	CME	D	289	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	CME	O-C-CA	-2.18	119.86	125.72
1	B	289	CME	O-C-CA	-2.03	120.28	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	289	CME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	NAD	A	501	-	42,48,48	0.99	3 (7%)	46,73,73	1.91	6 (13%)
4	EPE	A	504[A]	-	15,15,15	2.06	1 (6%)	19,20,20	1.46	4 (21%)
4	EPE	A	504[B]	-	15,15,15	1.90	1 (6%)	19,20,20	1.54	3 (15%)
5	PGE	A	505	-	9,9,9	0.44	0	8,8,8	0.29	0
2	NAD	B	501	-	42,48,48	0.96	1 (2%)	46,73,73	1.69	5 (10%)
4	EPE	B	504[A]	-	15,15,15	1.85	1 (6%)	19,20,20	1.54	3 (15%)
4	EPE	B	504[B]	-	15,15,15	1.94	1 (6%)	19,20,20	1.95	4 (21%)
4	EPE	B	505	-	15,15,15	1.91	1 (6%)	19,20,20	1.44	3 (15%)
5	PGE	B	506	-	9,9,9	0.50	0	8,8,8	0.33	0
2	NAD	C	501	-	42,48,48	0.83	1 (2%)	46,73,73	1.72	6 (13%)
4	EPE	C	504	-	15,15,15	1.84	1 (6%)	19,20,20	1.57	3 (15%)
5	PGE	C	505	-	9,9,9	0.53	0	8,8,8	0.27	0
2	NAD	D	501	-	42,48,48	1.05	2 (4%)	46,73,73	1.78	4 (8%)
5	PGE	D	504	-	9,9,9	0.47	0	8,8,8	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	501	-	-	0/22/62/62	0/5/5/5
4	EPE	A	504[A]	-	-	0/9/19/19	0/1/1/1
4	EPE	A	504[B]	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	A	505	-	-	0/7/7/7	0/0/0/0
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
4	EPE	B	504[A]	-	-	0/9/19/19	0/1/1/1
4	EPE	B	504[B]	-	-	0/9/19/19	0/1/1/1
4	EPE	B	505	-	-	0/9/19/19	0/1/1/1
5	PGE	B	506	-	-	0/7/7/7	0/0/0/0
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
4	EPE	C	504	-	-	0/9/19/19	0/1/1/1
5	PGE	C	505	-	-	0/7/7/7	0/0/0/0
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5
5	PGE	D	504	-	-	0/7/7/7	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504[A]	EPE	C10-S	-7.71	1.66	1.77
4	B	504[B]	EPE	C10-S	-7.22	1.66	1.77
4	B	505	EPE	C10-S	-7.12	1.66	1.77
4	A	504[B]	EPE	C10-S	-7.06	1.66	1.77
4	B	504[A]	EPE	C10-S	-6.86	1.67	1.77
4	C	504	EPE	C10-S	-6.79	1.67	1.77
2	A	501	NAD	O4B-C1B	2.10	1.44	1.41
2	D	501	NAD	O4B-C1B	2.22	1.44	1.41
2	A	501	NAD	C2A-N3A	2.24	1.36	1.32
2	C	501	NAD	O7N-C7N	3.48	1.31	1.24
2	A	501	NAD	O7N-C7N	4.27	1.33	1.24
2	B	501	NAD	O7N-C7N	4.62	1.34	1.24
2	D	501	NAD	O7N-C7N	5.09	1.35	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	NAD	N3A-C2A-N1A	-9.08	121.73	128.87
2	A	501	NAD	N3A-C2A-N1A	-9.00	121.80	128.87
2	C	501	NAD	N3A-C2A-N1A	-8.03	122.56	128.87
2	B	501	NAD	N3A-C2A-N1A	-7.73	122.80	128.87
2	B	501	NAD	C1B-N9A-C4A	-4.39	121.90	126.81
2	A	501	NAD	C1B-N9A-C4A	-2.91	123.56	126.81
4	A	504[A]	EPE	C3-C2-N1	-2.82	105.15	110.65
2	C	501	NAD	C1B-N9A-C4A	-2.68	123.81	126.81
2	C	501	NAD	C5B-C4B-C3B	-2.20	106.67	115.20
2	D	501	NAD	C5B-C4B-C3B	-2.17	106.79	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	C5B-C4B-C3B	-2.15	106.87	115.20
2	C	501	NAD	O7N-C7N-C3N	-2.15	117.21	119.60
2	B	501	NAD	C5B-C4B-C3B	-2.15	106.89	115.20
4	A	504[A]	EPE	C5-C6-N1	-2.01	106.73	110.65
4	B	505	EPE	O3S-S-C10	2.01	109.17	104.99
4	B	504[A]	EPE	O3S-S-C10	2.03	109.20	104.99
4	B	504[B]	EPE	O3S-S-C10	2.06	109.28	104.99
4	B	504[B]	EPE	C6-N1-C2	2.20	113.79	108.87
4	A	504[B]	EPE	O3S-S-C10	2.32	109.82	104.99
2	D	501	NAD	O4B-C1B-N9A	2.48	112.79	108.11
2	B	501	NAD	O4B-C1B-N9A	2.55	112.92	108.11
4	A	504[A]	EPE	O3S-S-C10	2.55	110.29	104.99
2	A	501	NAD	O2A-PA-O3	2.56	116.22	105.27
4	B	504[A]	EPE	O1S-S-C10	2.57	108.69	106.87
2	B	501	NAD	O4D-C1D-N1N	2.64	110.96	108.10
2	A	501	NAD	O4B-C1B-N9A	2.75	113.31	108.11
4	C	504	EPE	O3S-S-C10	2.86	110.93	104.99
4	A	504[A]	EPE	O1S-S-C10	2.88	108.91	106.87
4	C	504	EPE	O2S-S-C10	2.89	108.91	106.87
2	C	501	NAD	O4D-C1D-N1N	2.91	111.24	108.10
2	C	501	NAD	C3N-C7N-N7N	2.99	121.20	117.82
4	B	505	EPE	O1S-S-C10	3.21	109.14	106.87
4	B	505	EPE	O2S-S-C10	3.64	109.44	106.87
4	C	504	EPE	O1S-S-C10	3.69	109.47	106.87
4	A	504[B]	EPE	O2S-S-C10	3.69	109.48	106.87
4	B	504[B]	EPE	O1S-S-C10	3.74	109.51	106.87
2	D	501	NAD	O4D-C1D-N1N	3.84	112.25	108.10
4	A	504[B]	EPE	O1S-S-C10	3.94	109.65	106.87
4	B	504[A]	EPE	O2S-S-C10	4.93	110.36	106.87
2	A	501	NAD	O4D-C1D-N1N	5.28	113.81	108.10
4	B	504[B]	EPE	O2S-S-C10	6.15	111.21	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504[B]	EPE	2	0
4	B	504[A]	EPE	1	0
4	B	504[B]	EPE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	490/517 (94%)	-0.38	2 (0%)	93	94	8, 14, 28, 52	0
1	B	490/517 (94%)	-0.32	5 (1%)	84	87	8, 15, 30, 49	0
1	C	490/517 (94%)	-0.38	2 (0%)	93	94	9, 15, 28, 46	0
1	D	490/517 (94%)	-0.36	4 (0%)	87	90	8, 15, 28, 53	0
All	All	1960/2068 (94%)	-0.36	13 (0%)	89	91	8, 15, 29, 53	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	HIS	4.3
1	C	6	HIS	4.3
1	B	345	ASP	4.1
1	A	362	ASP	3.5
1	B	6	HIS	3.4
1	D	367	LYS	3.3
1	D	362	ASP	3.2
1	D	364	ASP	3.1
1	B	367	LYS	2.9
1	B	362	ASP	2.9
1	A	6	HIS	2.7
1	C	362	ASP	2.7
1	B	364	ASP	2.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	CME	C	289	10/11	0.95	0.12	-	13,15,35,42	0
1	CME	D	289	10/11	0.91	0.11	-	13,17,32,41	0
1	CME	A	289	10/11	0.95	0.09	-	13,16,32,42	0
1	CME	B	289	10/11	0.95	0.10	-	14,16,35,43	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	EPE	A	504[B]	15/15	0.78	0.21	8.28	38,44,58,59	15
5	PGE	A	505	10/10	0.88	0.19	7.54	36,44,47,48	0
4	EPE	B	504[A]	15/15	0.82	0.18	6.56	28,33,46,47	15
5	PGE	D	504	10/10	0.78	0.13	6.01	40,42,49,50	0
5	PGE	B	506	10/10	0.83	0.16	5.42	32,40,42,49	0
4	EPE	B	504[B]	15/15	0.82	0.18	5.39	29,34,36,38	15
4	EPE	C	504	15/15	0.67	0.27	2.49	50,56,98,102	0
4	EPE	A	504[A]	15/15	0.78	0.21	2.45	30,34,39,39	15
4	EPE	B	505	15/15	0.67	0.21	1.92	36,44,63,64	15
5	PGE	C	505	10/10	0.77	0.14	1.01	36,42,53,53	0
2	NAD	A	501	44/44	0.94	0.09	0.39	16,22,29,30	0
2	NAD	B	501	44/44	0.94	0.09	0.22	16,23,29,33	0
2	NAD	D	501	44/44	0.95	0.08	-0.05	12,20,26,28	0
2	NAD	C	501	44/44	0.96	0.07	-0.32	13,20,22,25	0
3	NA	B	503	1/1	0.97	0.07	-0.78	21,21,21,21	0
3	NA	D	502	1/1	0.99	0.05	-0.93	12,12,12,12	0
3	NA	A	502	1/1	1.00	0.06	-1.14	12,12,12,12	0
3	NA	D	503	1/1	0.98	0.05	-1.37	18,18,18,18	0
3	NA	A	503	1/1	0.99	0.02	-2.32	17,17,17,17	0
3	NA	C	502	1/1	0.99	0.04	-2.39	10,10,10,10	0
3	NA	C	503	1/1	0.97	0.04	-3.25	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	NA	B	502	1/1	0.99	0.03	-3.78	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.