



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 05:58 AM EDT

PDB ID : 5EGE
Title : Structure of ENPP6, a choline-specific glycerophosphodiester-phosphodiesterase
Authors : Morita, J.; Kano, K.; Kato, K.; Takita, H.; Ishitani, R.; Nishimasu, H.; Nureki, O.; Aoki, J.
Deposited on : 2015-10-27
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

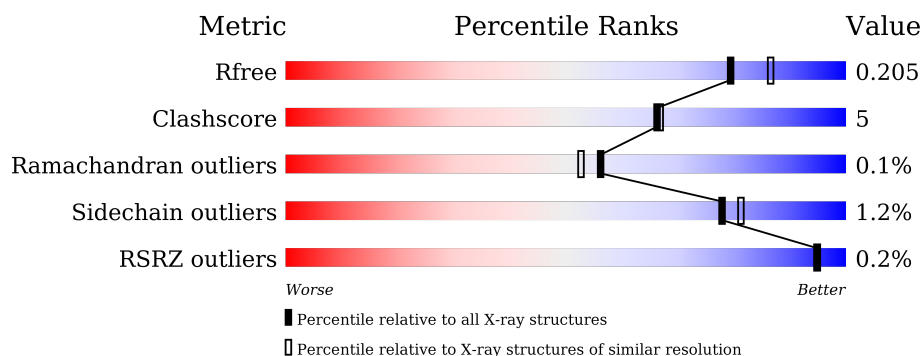
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	429	 84% 7% 9%
1	B	429	 80% 11% 9%
1	C	429	 81% 10% 9%
1	D	429	 81% 10% 9%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	510	-	-	-	X
5	EDO	C	511	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15249 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3201	2059	548	575	19			
1	B	392	Total	C	N	O	S	0	0	0
			3201	2059	548	575	19			
1	C	392	Total	C	N	O	S	0	1	0
			3204	2061	548	576	19			
1	D	392	Total	C	N	O	S	0	0	0
			3201	2059	548	575	19			

There are 40 discrepancies between the modelled and reference sequences:

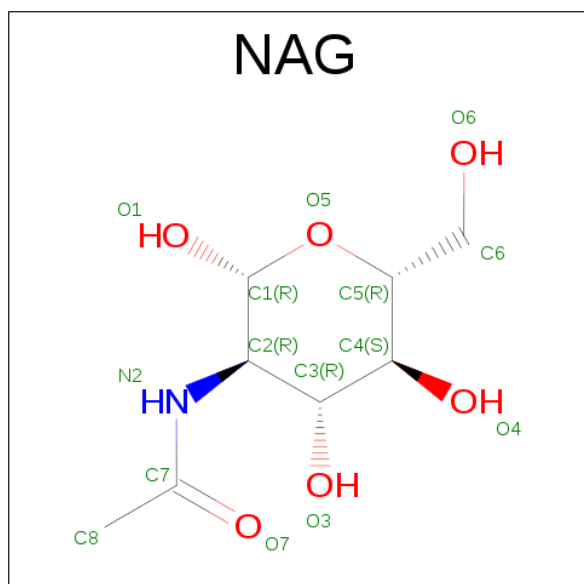
Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ALA	CYS	engineered mutation	UNP Q8BGN3
A	412	SER	CYS	engineered mutation	UNP Q8BGN3
A	422	SER	-	expression tag	UNP Q8BGN3
A	423	ARG	-	expression tag	UNP Q8BGN3
A	424	GLU	-	expression tag	UNP Q8BGN3
A	425	ASN	-	expression tag	UNP Q8BGN3
A	426	LEU	-	expression tag	UNP Q8BGN3
A	427	TYR	-	expression tag	UNP Q8BGN3
A	428	PHE	-	expression tag	UNP Q8BGN3
A	429	GLN	-	expression tag	UNP Q8BGN3
B	393	ALA	CYS	engineered mutation	UNP Q8BGN3
B	412	SER	CYS	engineered mutation	UNP Q8BGN3
B	422	SER	-	expression tag	UNP Q8BGN3
B	423	ARG	-	expression tag	UNP Q8BGN3
B	424	GLU	-	expression tag	UNP Q8BGN3
B	425	ASN	-	expression tag	UNP Q8BGN3
B	426	LEU	-	expression tag	UNP Q8BGN3
B	427	TYR	-	expression tag	UNP Q8BGN3
B	428	PHE	-	expression tag	UNP Q8BGN3
B	429	GLN	-	expression tag	UNP Q8BGN3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	393	ALA	CYS	engineered mutation	UNP Q8BGN3
C	412	SER	CYS	engineered mutation	UNP Q8BGN3
C	422	SER	-	expression tag	UNP Q8BGN3
C	423	ARG	-	expression tag	UNP Q8BGN3
C	424	GLU	-	expression tag	UNP Q8BGN3
C	425	ASN	-	expression tag	UNP Q8BGN3
C	426	LEU	-	expression tag	UNP Q8BGN3
C	427	TYR	-	expression tag	UNP Q8BGN3
C	428	PHE	-	expression tag	UNP Q8BGN3
C	429	GLN	-	expression tag	UNP Q8BGN3
D	393	ALA	CYS	engineered mutation	UNP Q8BGN3
D	412	SER	CYS	engineered mutation	UNP Q8BGN3
D	422	SER	-	expression tag	UNP Q8BGN3
D	423	ARG	-	expression tag	UNP Q8BGN3
D	424	GLU	-	expression tag	UNP Q8BGN3
D	425	ASN	-	expression tag	UNP Q8BGN3
D	426	LEU	-	expression tag	UNP Q8BGN3
D	427	TYR	-	expression tag	UNP Q8BGN3
D	428	PHE	-	expression tag	UNP Q8BGN3
D	429	GLN	-	expression tag	UNP Q8BGN3

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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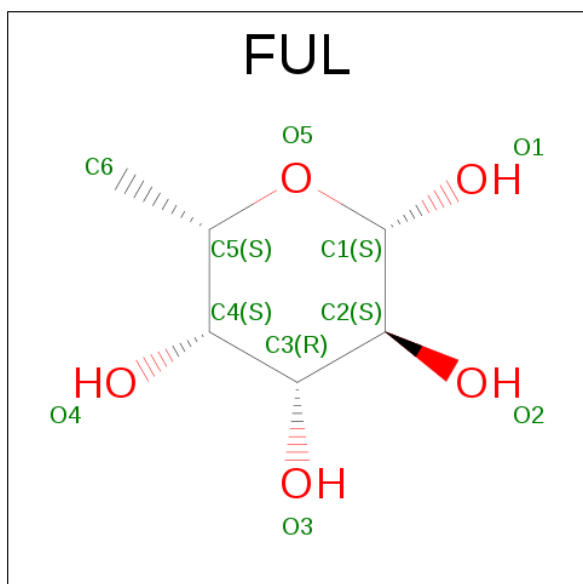
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-L-FUCOSE (three-letter code: FUL) (formula: $C_6H_{12}O_5$).

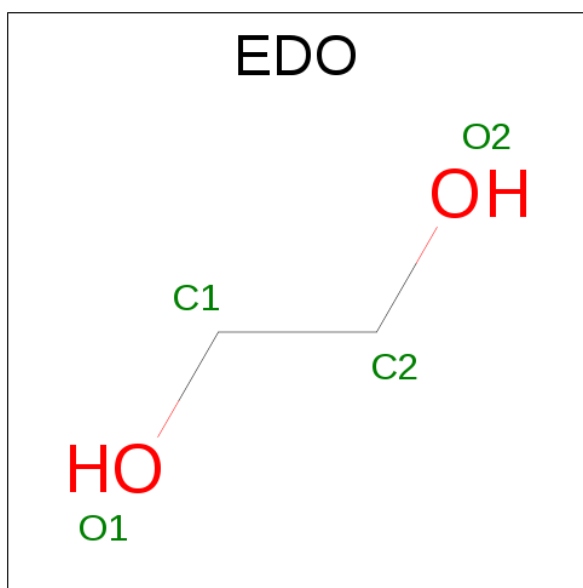


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

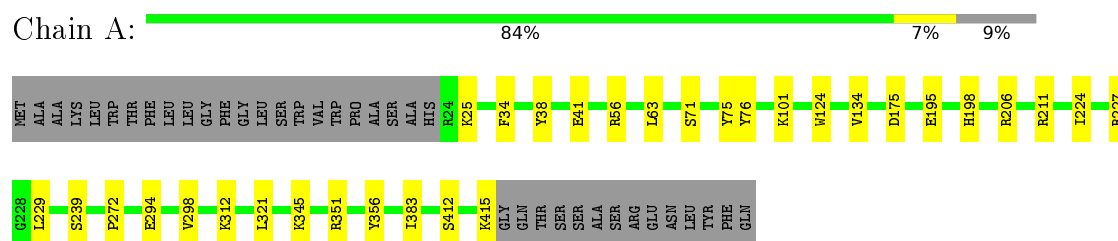
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	526	Total	O	0	0
			526	526		
6	B	551	Total	O	0	0
			551	551		
6	C	467	Total	O	0	0
			467	467		
6	D	504	Total	O	0	0
			504	504		

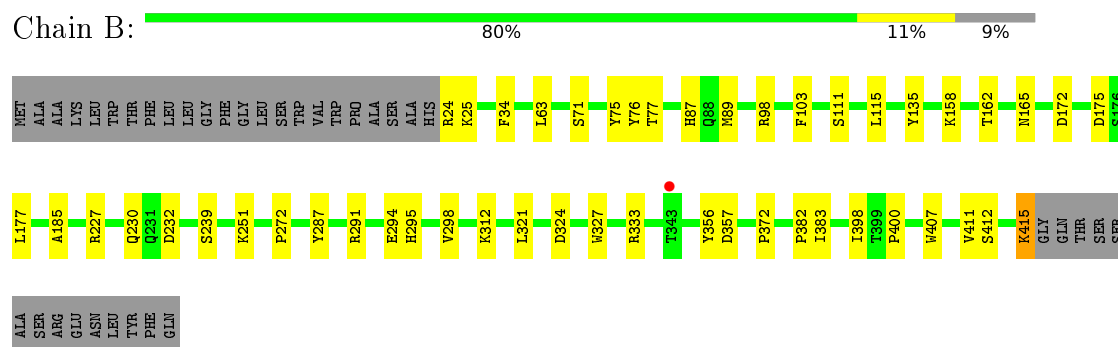
3 Residue-property plots

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.

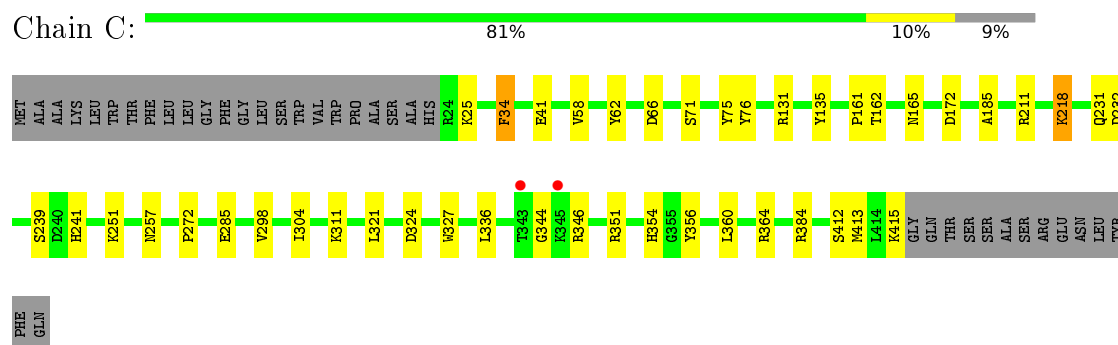
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6



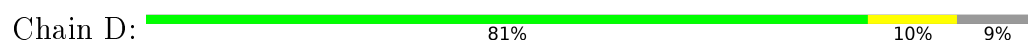
- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6

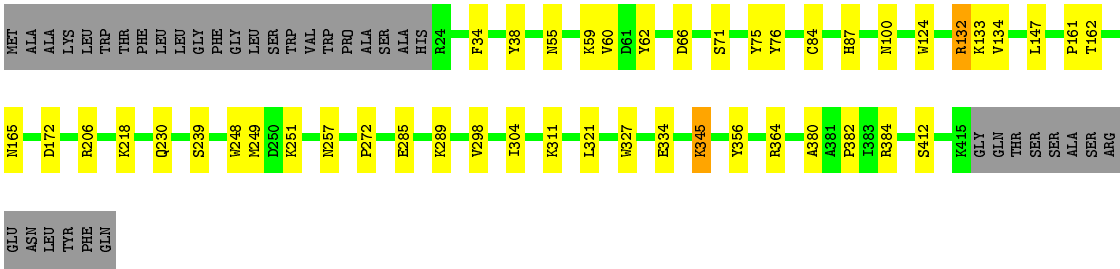


- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.29Å 78.24Å 103.64Å 90.04° 89.98° 114.61°	Depositor
Resolution (Å)	41.90 – 2.00 41.90 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.90-2.00) 96.5 (41.90-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.167 , 0.206 0.166 , 0.205	Depositor DCC
R_{free} test set	5992 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.5	EDS
Estimated twinning fraction	0.025 for h,-h-k,-l 0.437 for -h,-k,l 0.021 for -h,h+k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 120964 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15249	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, 0.375 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: ZN, EDO, FUL, NAG

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	0.37	0/3294	0.55	0/4473
1	B	0.38	0/3294	0.55	0/4473
1	C	0.39	1/3300 (0.0%)	0.54	0/4481
1	D	0.37	0/3294	0.53	0/4473
All	All	0.37	1/13182 (0.0%)	0.54	0/17900

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	336	LEU	C-N	6.51	1.46	1.34

There are no bond angle outliers.

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	3201	0	3130	23	0
1	B	3201	0	3130	32	0
1	C	3204	0	3133	32	0
1	D	3201	0	3131	33	0
2	A	84	0	75	2	0
2	B	84	0	75	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	84	0	75	5	0
2	D	70	0	62	3	0
3	A	10	0	10	0	0
3	B	10	0	10	0	0
3	C	10	0	9	1	0
3	D	10	0	10	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	8	0	12	2	0
5	B	4	0	6	0	0
5	C	8	0	12	2	0
5	D	4	0	6	0	0
6	A	526	0	0	12	1
6	B	551	0	0	12	4
6	C	467	0	0	15	1
6	D	504	0	0	14	4
All	All	15249	0	12886	128	5

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 5.

All (128) 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:C:218:LYS:NZ	6:C:604:HOH:O	2.02	0.92
1:A:198:HIS:HE2	5:A:511:EDO:HO2	0.95	0.88
1:C:285:GLU:OE1	6:C:601:HOH:O	1.91	0.88
1:C:415:LYS:O	6:C:603:HOH:O	2.00	0.79
1:B:291:ARG:NH1	1:B:298:VAL:O	2.16	0.78
1:A:195:GLU:OE2	6:A:601:HOH:O	2.02	0.77
1:B:382:PRO:HG2	1:D:382:PRO:HG2	1.67	0.76
1:A:345:LYS:O	6:A:602:HOH:O	2.02	0.76
2:B:502:NAG:O3	6:B:602:HOH:O	2.02	0.75
1:D:257:ASN:OD1	6:D:602:HOH:O	2.04	0.75
1:B:312:LYS:NZ	6:B:605:HOH:O	2.18	0.71
1:B:87:HIS:HD2	1:B:89:MET:H	1.39	0.70
1:B:232:ASP:OD1	6:B:603:HOH:O	2.09	0.69
1:A:412:SER:HB3	1:C:412:SER:HB3	1.74	0.69
1:A:294:GLU:OE2	6:A:604:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASN:OD1	6:D:603:HOH:O	2.12	0.67
1:C:298:VAL:HG22	1:C:321:LEU:HD22	1.76	0.67
1:D:172:ASP:HB3	6:D:689:HOH:O	1.93	0.67
2:A:507:NAG:O4	6:A:605:HOH:O	2.14	0.64
1:D:59:LYS:NZ	6:D:609:HOH:O	2.28	0.64
1:D:345:LYS:NZ	6:D:612:HOH:O	2.31	0.63
1:D:162:THR:H	1:D:165:ASN:HD22	1.48	0.62
1:B:412:SER:HB3	1:D:412:SER:HB3	1.80	0.62
1:A:211:ARG:NH1	6:A:612:HOH:O	2.33	0.61
1:B:407:TRP:O	1:B:411:VAL:HG13	2.01	0.61
2:C:503:NAG:H83	2:C:503:NAG:H3	1.83	0.60
1:D:298:VAL:HG22	1:D:321:LEU:HD22	1.82	0.60
1:B:294:GLU:OE1	6:B:604:HOH:O	2.16	0.58
2:A:503:NAG:H3	2:A:503:NAG:H83	1.85	0.58
1:A:63:LEU:HD13	1:A:383:ILE:HG13	1.86	0.57
1:B:87:HIS:CD2	1:B:89:MET:H	2.22	0.57
1:C:257:ASN:OD1	6:C:607:HOH:O	2.17	0.57
1:A:101:LYS:NZ	6:A:611:HOH:O	2.31	0.57
1:C:324:ASP:HA	5:C:511:EDO:H11	1.86	0.56
1:D:272:PRO:HB3	1:D:356:TYR:CE1	2.40	0.56
1:C:384:ARG:NH2	6:C:620:HOH:O	2.37	0.56
1:C:211:ARG:NH1	6:C:611:HOH:O	2.24	0.55
1:D:55:ASN:ND2	6:D:601:HOH:O	2.04	0.55
1:D:384:ARG:NH2	6:D:616:HOH:O	2.40	0.54
2:B:507:NAG:O4	6:B:606:HOH:O	2.19	0.54
1:D:84:CYS:HA	1:D:87:HIS:CE1	2.42	0.54
1:C:25:LYS:NZ	1:C:232:ASP:OD2	2.40	0.54
1:A:56:ARG:NH2	6:A:607:HOH:O	2.22	0.53
1:A:312:LYS:NZ	6:A:619:HOH:O	2.40	0.53
1:A:41:GLU:OE2	6:A:606:HOH:O	2.19	0.52
1:D:162:THR:H	1:D:165:ASN:ND2	2.06	0.52
1:B:415:LYS:NZ	6:B:627:HOH:O	2.42	0.52
1:C:71:SER:HB3	1:C:75:TYR:CZ	2.46	0.51
1:B:63:LEU:HD13	1:B:383:ILE:HG13	1.93	0.50
1:B:272:PRO:HB3	1:B:356:TYR:CE1	2.46	0.50
1:A:298:VAL:HG22	1:A:321:LEU:HD22	1.92	0.50
1:A:198:HIS:CD2	5:A:511:EDO:HO2	2.28	0.50
1:C:161:PRO:HA	1:C:165:ASN:HD22	1.77	0.49
1:B:98:ARG:NE	6:B:611:HOH:O	2.28	0.49
1:D:71:SER:HB3	1:D:75:TYR:CZ	2.48	0.48
1:A:124:TRP:HB2	1:A:134:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:ILE:HB	1:C:311:LYS:HB3	1.96	0.47
1:B:298:VAL:HG22	1:B:321:LEU:HD22	1.96	0.47
1:D:272:PRO:HB3	1:D:356:TYR:CD1	2.50	0.47
1:A:71:SER:HB3	1:A:75:TYR:CZ	2.50	0.47
1:D:34:PHE:HB3	1:D:239:SER:HB3	1.97	0.47
1:C:272:PRO:HB3	1:C:356:TYR:CD1	2.49	0.46
1:C:58:VAL:HG11	1:C:413:MET:HB2	1.97	0.46
1:A:175:ASP:OD1	1:A:227:ARG:NH1	2.48	0.46
1:C:354:HIS:HE1	6:C:744:HOH:O	1.99	0.46
1:B:172:ASP:OD1	6:B:607:HOH:O	2.21	0.46
1:C:415:LYS:HD2	6:C:692:HOH:O	2.15	0.46
2:D:503:NAG:O4	6:D:605:HOH:O	2.21	0.46
1:C:211:ARG:NH2	6:C:611:HOH:O	2.46	0.46
1:C:351:ARG:NE	3:C:505:FUL:O4	2.47	0.46
1:D:285:GLU:OE2	1:D:289:LYS:NZ	2.34	0.46
1:B:158:LYS:HE2	6:B:678:HOH:O	2.16	0.45
1:B:25:LYS:HB3	1:B:177:LEU:HD22	1.98	0.45
2:C:503:NAG:H3	2:C:503:NAG:C8	2.46	0.45
1:C:360:LEU:HD11	5:C:511:EDO:H12	1.97	0.45
1:D:100:ASN:O	6:D:604:HOH:O	2.20	0.45
1:C:251:LYS:HA	1:C:327:TRP:CZ3	2.52	0.45
1:C:131:ARG:NH2	6:C:632:HOH:O	2.50	0.44
1:C:162:THR:H	1:C:165:ASN:ND2	2.14	0.44
1:D:62:TYR:CG	1:D:364:ARG:HD3	2.52	0.44
1:D:345:LYS:HD3	1:D:345:LYS:HA	1.63	0.44
1:B:162:THR:H	1:B:165:ASN:ND2	2.15	0.44
1:A:272:PRO:HB3	1:A:356:TYR:CE1	2.52	0.44
1:B:24:ARG:HD3	1:B:372:PRO:HG2	1.99	0.44
1:C:272:PRO:HB3	1:C:356:TYR:CE1	2.52	0.44
1:B:103:PHE:CD2	1:B:111:SER:HB2	2.52	0.44
1:B:400:PRO:HG3	6:B:803:HOH:O	2.18	0.44
1:B:407:TRP:NE1	1:B:411:VAL:HG12	2.32	0.44
1:D:133:LYS:HD3	6:D:768:HOH:O	2.17	0.43
1:B:34:PHE:HB3	1:B:239:SER:HB3	1.99	0.43
1:D:132:ARG:HD3	6:D:848:HOH:O	2.18	0.43
1:C:172:ASP:HB3	6:C:760:HOH:O	2.19	0.43
2:C:504:NAG:O3	6:C:608:HOH:O	2.18	0.43
1:C:34:PHE:HB3	1:C:239:SER:HB3	2.01	0.43
1:D:124:TRP:HB2	1:D:134:VAL:HG11	2.00	0.43
1:A:34:PHE:HB3	1:A:239:SER:HB3	2.01	0.42
1:D:304:ILE:HB	1:D:311:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:507:NAG:O4	6:C:610:HOH:O	2.21	0.42
1:A:224:ILE:HG23	1:A:229:LEU:HB2	2.01	0.42
1:B:295:HIS:HA	1:B:324:ASP:OD2	2.19	0.42
1:D:230:GLN:HG2	6:D:648:HOH:O	2.18	0.42
1:B:115:LEU:HD12	6:B:777:HOH:O	2.18	0.42
1:B:71:SER:HB3	1:B:75:TYR:CZ	2.54	0.42
1:B:251:LYS:HA	1:B:327:TRP:CZ3	2.54	0.42
1:D:147:LEU:HD22	2:D:501:NAG:H82	2.02	0.42
1:C:135:TYR:O	1:C:185:ALA:HA	2.20	0.42
1:D:218:LYS:HE2	6:D:766:HOH:O	2.20	0.42
1:D:60:VAL:HG12	1:D:380:ALA:HB3	2.02	0.42
1:A:351:ARG:NE	6:A:632:HOH:O	2.52	0.41
1:B:333:ARG:NE	6:B:625:HOH:O	2.41	0.41
1:B:287:TYR:CE1	1:B:291:ARG:HD3	2.55	0.41
1:A:25:LYS:NZ	6:A:620:HOH:O	2.40	0.41
1:D:248:TRP:HA	1:D:249:MET:HA	1.85	0.41
2:D:503:NAG:N2	6:D:607:HOH:O	2.21	0.41
1:A:38:TYR:CE2	1:A:206:ARG:HD3	2.55	0.41
1:B:175:ASP:OD1	1:B:227:ARG:NH1	2.53	0.41
1:C:135:TYR:OH	6:C:606:HOH:O	2.17	0.41
1:B:135:TYR:O	1:B:185:ALA:HA	2.20	0.41
1:B:77:THR:OG1	1:B:87:HIS:HE1	2.04	0.41
1:C:41:GLU:HG2	6:C:695:HOH:O	2.21	0.41
1:D:161:PRO:HA	1:D:165:ASN:HD22	1.86	0.40
1:D:38:TYR:CE2	1:D:206:ARG:HD3	2.56	0.40
1:D:251:LYS:HA	1:D:327:TRP:CZ3	2.55	0.40
1:C:162:THR:H	1:C:165:ASN:HD22	1.70	0.40
1:A:345:LYS:NZ	6:A:608:HOH:O	2.23	0.40
1:C:241:HIS:CE1	1:C:354:HIS:CE1	3.10	0.40
1:C:62:TYR:CG	1:C:364:ARG:HD3	2.57	0.40
2:C:503:NAG:H83	2:C:503:NAG:C3	2.49	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:646:HOH:O	6:D:819:HOH:O[1_545]	2.05	0.15
6:B:1021:HOH:O	6:D:897:HOH:O[1_445]	2.09	0.11
6:A:929:HOH:O	6:B:1023:HOH:O[1_556]	2.14	0.06
6:C:991:HOH:O	6:D:960:HOH:O[1_546]	2.16	0.04
6:B:982:HOH:O	6:D:740:HOH:O[1_655]	2.19	0.01

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	390/429 (91%)	375 (96%)	15 (4%)	0	100	100
1	B	390/429 (91%)	376 (96%)	13 (3%)	1 (0%)	46	41
1	C	391/429 (91%)	375 (96%)	15 (4%)	1 (0%)	46	41
1	D	390/429 (91%)	376 (96%)	14 (4%)	0	100	100
All	All	1561/1716 (91%)	1502 (96%)	57 (4%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	ASP
1	C	344	GLY

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	348/377 (92%)	346 (99%)	2 (1%)	90	93
1	B	348/377 (92%)	344 (99%)	4 (1%)	80	83
1	C	349/377 (93%)	343 (98%)	6 (2%)	68	71
1	D	348/377 (92%)	343 (99%)	5 (1%)	74	77
All	All	1393/1508 (92%)	1376 (99%)	17 (1%)	78	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	415	LYS
1	B	76	TYR
1	B	230	GLN
1	B	398	ILE
1	B	415	LYS
1	C	34	PHE
1	C	66	ASP
1	C	76	TYR
1	C	218	LYS
1	C	231	GLN
1	C	346	ARG
1	D	66	ASP
1	D	76	TYR
1	D	132	ARG
1	D	334	GLU
1	D	345	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	HIS
1	B	165	ASN
1	B	225	GLN
1	C	165	ASN
1	C	288	HIS
1	D	165	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 8 are monoatomic - leaving 33 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	NAG	A	501	1	14,14,15	0.36	0	15,19,21	0.41	0
2	NAG	A	502	1	14,14,15	0.19	0	15,19,21	0.64	1 (6%)
2	NAG	A	503	1,3,2	14,14,15	0.44	0	15,19,21	1.35	1 (6%)
2	NAG	A	504	2	14,14,15	0.24	0	15,19,21	0.32	0
3	FUL	A	505	2	10,10,11	1.34	2 (20%)	13,14,16	1.91	2 (15%)
2	NAG	A	506	1,2	14,14,15	0.85	1 (7%)	15,19,21	1.17	1 (6%)
2	NAG	A	507	2	14,14,15	0.21	0	15,19,21	0.43	0
5	EDO	A	510	-	3,3,3	0.49	0	2,2,2	0.33	0
5	EDO	A	511	-	3,3,3	0.43	0	2,2,2	0.57	0
2	NAG	B	501	1	14,14,15	0.35	0	15,19,21	0.44	0
2	NAG	B	502	1	14,14,15	0.28	0	15,19,21	0.49	0
2	NAG	B	503	1,3,2	14,14,15	0.51	0	15,19,21	0.73	0
2	NAG	B	504	2	14,14,15	0.19	0	15,19,21	0.47	0
3	FUL	B	505	2	10,10,11	1.54	2 (20%)	13,14,16	1.77	2 (15%)
2	NAG	B	506	1,2	14,14,15	0.43	0	15,19,21	0.52	0
2	NAG	B	507	2	14,14,15	0.33	0	15,19,21	0.54	0
5	EDO	B	510	-	3,3,3	0.48	0	2,2,2	0.42	0
2	NAG	C	501	1	14,14,15	0.19	0	15,19,21	0.45	0
2	NAG	C	502	1	14,14,15	0.32	0	15,19,21	0.80	1 (6%)
2	NAG	C	503	1,3,2	14,14,15	0.49	0	15,19,21	1.67	1 (6%)
2	NAG	C	504	2	14,14,15	0.17	0	15,19,21	0.29	0
3	FUL	C	505	1,2	10,10,11	1.29	2 (20%)	13,14,16	1.83	4 (30%)
2	NAG	C	506	1,2	14,14,15	0.52	0	15,19,21	0.56	0
2	NAG	C	507	2	14,14,15	0.33	0	15,19,21	0.44	0
5	EDO	C	510	-	3,3,3	0.53	0	2,2,2	0.32	0
5	EDO	C	511	-	3,3,3	0.49	0	2,2,2	0.31	0
2	NAG	D	501	1	14,14,15	0.33	0	15,19,21	0.74	1 (6%)
2	NAG	D	502	1,3,2	14,14,15	0.40	0	15,19,21	0.65	0
2	NAG	D	503	2	14,14,15	0.20	0	15,19,21	0.22	0
3	FUL	D	504	2	10,10,11	1.49	3 (30%)	13,14,16	1.81	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	505	1,2	14,14,15	0.40	0	15,19,21	0.51	0
2	NAG	D	506	2	14,14,15	0.24	0	15,19,21	0.39	0
5	EDO	D	509	-	3,3,3	0.47	0	2,2,2	0.31	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	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	503	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	504	2	-	0/6/23/26	0/1/1/1
3	FUL	A	505	2	-	0/0/17/20	0/1/1/1
2	NAG	A	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	507	2	-	0/6/23/26	0/1/1/1
5	EDO	A	510	-	-	0/1/1/1	0/0/0/0
5	EDO	A	511	-	-	0/1/1/1	0/0/0/0
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	504	2	-	0/6/23/26	0/1/1/1
3	FUL	B	505	2	-	0/0/17/20	0/1/1/1
2	NAG	B	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	507	2	-	0/6/23/26	0/1/1/1
5	EDO	B	510	-	-	0/1/1/1	0/0/0/0
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
2	NAG	C	503	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	C	504	2	-	0/6/23/26	0/1/1/1
3	FUL	C	505	1,2	-	0/0/17/20	0/1/1/1
2	NAG	C	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	507	2	-	0/6/23/26	0/1/1/1
5	EDO	C	510	-	-	0/1/1/1	0/0/0/0
5	EDO	C	511	-	-	0/1/1/1	0/0/0/0
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	502	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	D	503	2	-	0/6/23/26	0/1/1/1
3	FUL	D	504	2	-	0/0/17/20	0/1/1/1
2	NAG	D	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	506	2	-	0/6/23/26	0/1/1/1
5	EDO	D	509	-	-	0/1/1/1	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	506	NAG	O5-C1	-3.00	1.38	1.43
3	B	505	FUL	O5-C1	-2.81	1.39	1.43
3	D	504	FUL	O5-C1	-2.59	1.39	1.43
3	C	505	FUL	O5-C1	-2.45	1.39	1.43
3	A	505	FUL	C4-C5	2.01	1.56	1.53
3	D	504	FUL	C4-C3	2.01	1.57	1.52
3	C	505	FUL	C4-C5	2.20	1.57	1.53
3	A	505	FUL	C4-C3	2.90	1.60	1.52
3	B	505	FUL	C4-C3	3.01	1.60	1.52
3	D	504	FUL	C4-C5	3.27	1.59	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	FUL	C1-C2-C3	-5.36	103.06	109.55
3	B	505	FUL	C1-C2-C3	-5.04	103.45	109.55
3	C	505	FUL	C1-C2-C3	-4.66	103.90	109.55
3	D	504	FUL	C1-C2-C3	-4.17	104.50	109.55
3	C	505	FUL	O2-C2-C1	2.10	113.44	109.23
2	A	502	NAG	C1-O5-C5	2.10	115.23	112.14
3	D	504	FUL	C3-C4-C5	2.37	113.20	109.66
3	B	505	FUL	O2-C2-C1	2.38	114.00	109.23
2	D	501	NAG	C1-O5-C5	2.40	115.66	112.14
3	D	504	FUL	O5-C5-C4	2.45	113.83	109.58
3	C	505	FUL	C3-C4-C5	2.57	113.50	109.66
3	C	505	FUL	O5-C5-C4	2.60	114.08	109.58
3	D	504	FUL	O2-C2-C1	2.60	114.45	109.23
2	C	502	NAG	C1-O5-C5	2.83	116.30	112.14
3	A	505	FUL	O2-C2-C1	2.98	115.20	109.23
2	A	506	NAG	C1-O5-C5	3.65	117.51	112.14
2	A	503	NAG	C2-N2-C7	4.48	128.93	123.11
2	C	503	NAG	C2-N2-C7	5.36	130.08	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	NAG	1	0
5	A	511	EDO	2	0
2	B	502	NAG	1	0
2	B	507	NAG	1	0
2	C	503	NAG	3	0
2	C	504	NAG	1	0
3	C	505	FUL	1	0
2	C	507	NAG	1	0
5	C	511	EDO	2	0
2	D	501	NAG	1	0
2	D	503	NAG	2	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	392/429 (91%)	-0.85	0 100 100	10, 17, 32, 62	0
1	B	392/429 (91%)	-0.84	1 (0%) 94 94	9, 17, 31, 64	0
1	C	392/429 (91%)	-0.80	2 (0%) 91 92	12, 20, 35, 68	0
1	D	392/429 (91%)	-0.83	0 100 100	12, 20, 36, 68	0
All	All	1568/1716 (91%)	-0.83	3 (0%) 95 95	9, 18, 33, 68	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	THR	4.4
1	C	345	LYS	2.9
1	C	343	THR	2.7

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 carbohydrates 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. 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(\AA^2)	Q<0.9
5	EDO	C	511	4/4	0.96	0.12	10.10	22,25,26,37	0
5	EDO	B	510	4/4	0.98	0.12	3.39	14,19,21,22	0
2	NAG	B	506	14/15	0.96	0.09	1.42	20,24,30,34	0
5	EDO	D	509	4/4	0.93	0.09	1.03	19,21,22,23	0
3	FUL	D	504	10/11	0.90	0.14	0.60	37,40,43,43	0
3	FUL	A	505	10/11	0.91	0.11	0.52	25,28,33,33	0
2	NAG	A	506	14/15	0.96	0.07	0.36	20,25,28,35	0
3	FUL	C	505	10/11	0.90	0.11	0.09	40,44,45,49	0
5	EDO	A	510	4/4	0.99	0.07	-0.10	16,17,20,21	0
3	FUL	B	505	10/11	0.95	0.09	-0.32	25,28,30,31	0
2	NAG	D	505	14/15	0.98	0.06	-1.36	17,22,28,28	0
2	NAG	C	506	14/15	0.98	0.06	-1.39	17,23,26,28	0
5	EDO	C	510	4/4	0.99	0.05	-2.14	16,19,20,20	0
4	ZN	D	507	1/1	0.99	0.04	-2.77	28,28,28,28	0
4	ZN	C	509	1/1	0.99	0.02	-3.42	33,33,33,33	0
4	ZN	B	508	1/1	1.00	0.03	-4.10	22,22,22,22	0
4	ZN	D	508	1/1	0.99	0.02	-4.48	31,31,31,31	0
4	ZN	C	508	1/1	1.00	0.02	-4.80	29,29,29,29	0
4	ZN	A	509	1/1	1.00	0.02	-5.85	32,32,32,32	0
4	ZN	A	508	1/1	1.00	0.02	-7.20	23,23,23,23	0
4	ZN	B	509	1/1	1.00	0.03	-8.69	29,29,29,29	0
2	NAG	B	507	14/15	0.92	0.10	-	26,35,42,43	0
2	NAG	C	504	14/15	0.79	0.27	-	55,63,72,77	0
2	NAG	C	501	14/15	0.78	0.20	-	52,58,65,69	0
2	NAG	A	502	14/15	0.94	0.09	-	24,28,33,38	0
2	NAG	C	502	14/15	0.95	0.07	-	25,30,36,37	0
2	NAG	A	503	14/15	0.88	0.14	-	33,43,51,54	0
5	EDO	A	511	4/4	0.93	0.17	-	26,27,28,34	0
2	NAG	C	507	14/15	0.96	0.08	-	21,27,36,50	0
2	NAG	B	502	14/15	0.94	0.09	-	21,31,38,42	0
2	NAG	D	506	14/15	0.95	0.10	-	24,27,33,41	0
2	NAG	D	501	14/15	0.93	0.09	-	27,31,35,37	0
2	NAG	D	502	14/15	0.90	0.12	-	45,50,57,58	0
2	NAG	B	501	14/15	0.83	0.20	-	43,53,57,58	0
2	NAG	A	504	14/15	0.90	0.17	-	38,50,56,61	0
2	NAG	C	503	14/15	0.89	0.13	-	43,50,57,60	0
2	NAG	D	503	14/15	0.82	0.26	-	56,62,73,75	0
2	NAG	B	503	14/15	0.94	0.11	-	30,40,47,49	0
2	NAG	A	507	14/15	0.92	0.10	-	25,29,41,47	0
2	NAG	B	504	14/15	0.89	0.16	-	38,47,57,63	0
2	NAG	A	501	14/15	0.88	0.21	-	44,52,56,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.