



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:30 am GMT

PDB ID : 3E80
Title : Structure of Heparinase II complexed with heparan sulfate degradation disaccharide product
Authors : Shaya, D.; Cygler, M.
Deposited on : 2008-08-19
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

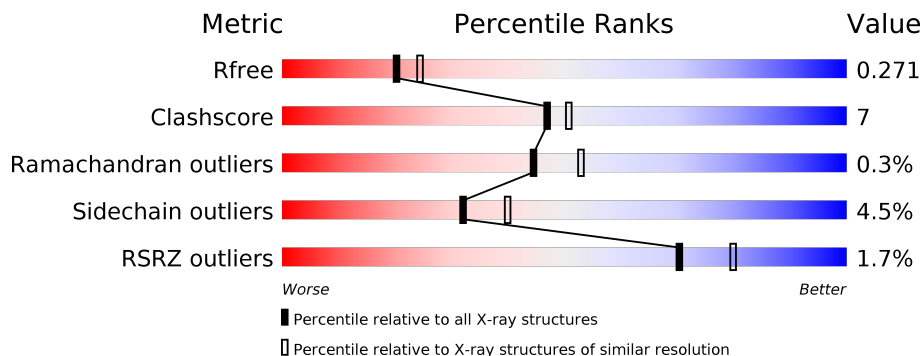
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	749	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 81%; width: 17%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 98%; width: 2%; height: 10px; background-color: orange;"></div> </div> <div>81% 17% .</div> </div>
1	B	749	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 83%; width: 16%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 99%; width: 1%; height: 10px; background-color: orange;"></div> </div> <div>83% 16% .</div> </div>
1	C	749	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 79%; width: 19%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 98%; width: 2%; height: 10px; background-color: orange;"></div> </div> <div>79% 19% .</div> </div>

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
3	XYS	B	776	X	-	-	-
3	GCU	C	775	X	-	-	-
5	PO4	A	3	-	-	-	X
5	PO4	B	7	-	-	-	X
5	PO4	B	8	-	-	-	X
5	PO4	C	6	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 18716 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 Heparinase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5978	3850	1008	1097	23			
1	B	747	Total	C	N	O	S	0	0	0
			5978	3850	1008	1097	23			
1	C	747	Total	C	N	O	S	0	0	0
			5975	3847	1008	1097	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	PCA	GLN	MODIFIED RESIDUE	UNP Q46080
A	758	ALA	PRO	SEE REMARK 999	UNP Q46080
B	26	PCA	GLN	MODIFIED RESIDUE	UNP Q46080
B	758	ALA	PRO	SEE REMARK 999	UNP Q46080
C	26	PCA	GLN	MODIFIED RESIDUE	UNP Q46080
C	758	ALA	PRO	SEE REMARK 999	UNP Q46080

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

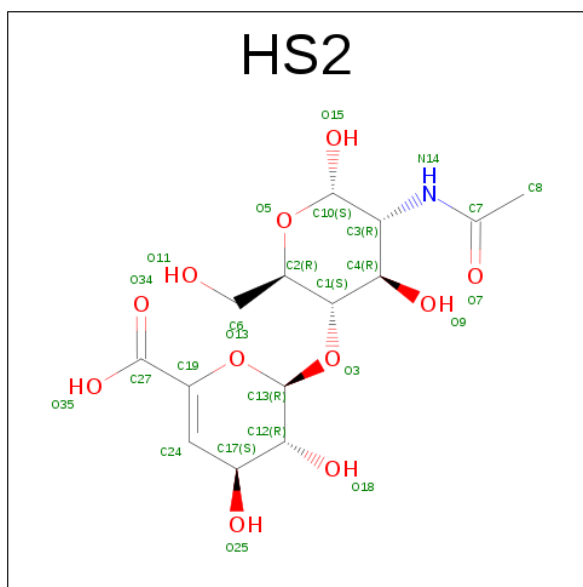
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	4	Total	C	O	0	0
			41	23	18		

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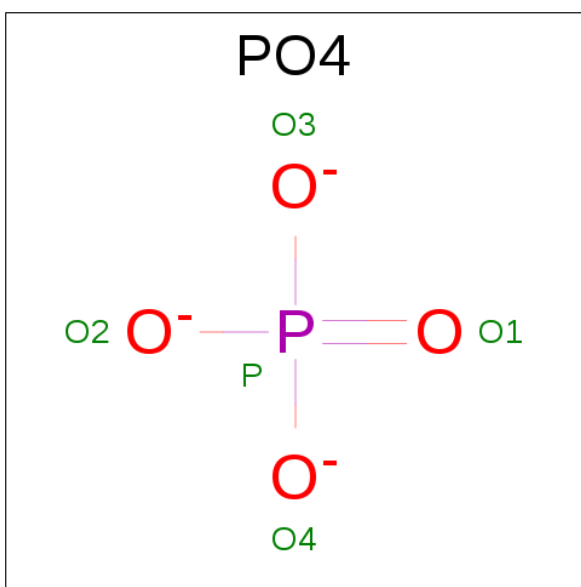
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	4	Total	C	O	0	0
			41	23	18		
3	C	4	Total	C	O	0	0
			41	23	18		

- Molecule 4 is 2-DEOXY-4-O-(4-DEOXY-ALPHA-L-THREO-HEX-4-ENOPYRANURONOSYL)-2-[[[(1R)-1-HYDROXYETHYL]AMINO}-ALPHA-D-GLUCOPYRANOSE (three-letter code: HS2) (formula: C₁₄H₂₁NO₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	14	1	11		
4	B	1	Total	C	N	O	0	0
			26	14	1	11		
4	C	1	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

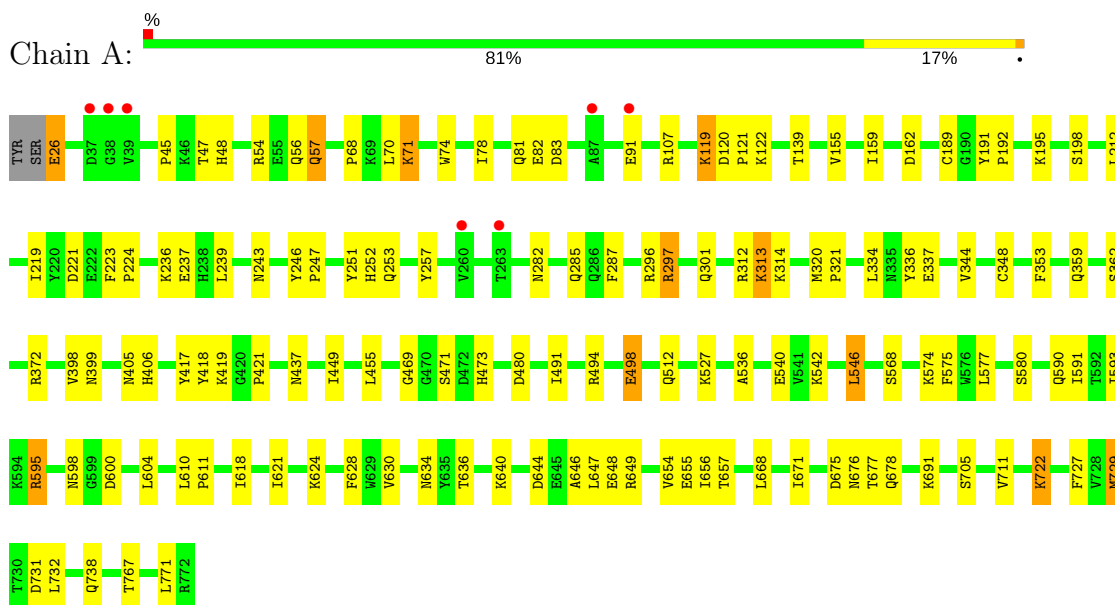
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total	O	0	0
			208	208		
6	B	151	Total	O	0	0
			151	151		
6	C	177	Total	O	0	0
			177	177		

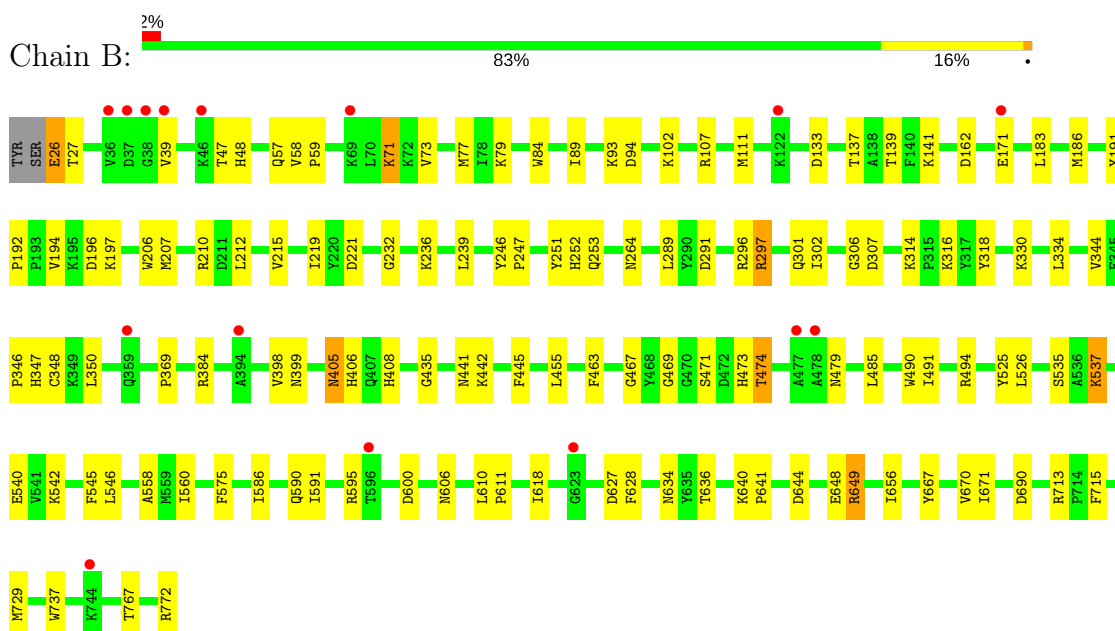
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

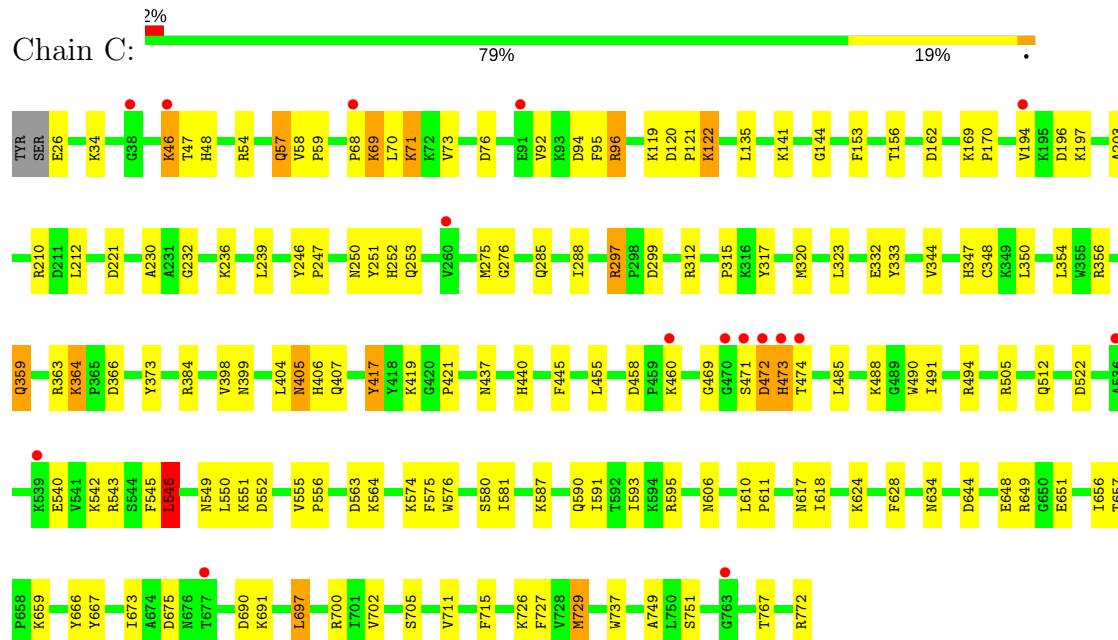
• Molecule 1: Heparinase II protein



• Molecule 1: Heparinase II protein



● Molecule 1: Heparinase II protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	201.28Å 209.36Å 59.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.57 – 2.35 37.57 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.57-2.35) 98.1 (37.57-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.229 , 0.267 0.230 , 0.271	Depositor DCC
R_{free} test set	5152 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18716	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8089e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, XYS, PO4, RAM, HS2, GCU, PCA, MAN

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	0.53	0/6133	0.78	3/8303 (0.0%)
1	B	0.48	0/6133	0.73	3/8303 (0.0%)
1	C	0.51	0/6130	0.74	2/8299 (0.0%)
All	All	0.50	0/18396	0.75	8/24905 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	B	1	0
3	C	1	0
All	All	2	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	PCA	O-C-N	-11.54	104.24	122.70
1	A	26	PCA	O-C-N	-10.11	106.52	122.70
1	A	26	PCA	CA-C-N	10.05	139.31	117.20
1	C	26	PCA	O-C-N	-8.42	109.23	122.70
1	B	26	PCA	C-N-CA	-6.93	104.37	121.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	776	XYS	C1

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Mol	Chain	Res	Type	Atom
3	C	775	GCU	C4

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	PCA	Mainchain

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	5978	0	5889	86	0
1	B	5978	0	5889	72	0
1	C	5975	0	5880	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	41	0	30	0	0
3	B	41	0	30	1	0
3	C	41	0	30	0	0
4	A	26	0	20	0	0
4	B	26	0	20	1	0
4	C	26	0	20	2	0
5	A	20	0	0	0	0
5	B	15	0	0	0	0
5	C	10	0	0	3	0
6	A	208	0	0	9	0
6	B	151	0	0	4	0
6	C	177	0	0	7	0
All	All	18716	0	17808	257	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 7.

The worst 5 of 257 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:GLN:HE22	1:B:405:ASN:HB3	1.26	0.98
1:C:574:LYS:O	1:C:657:THR:HG22	1.74	0.87
1:C:253:GLN:HE22	1:C:405:ASN:HB3	1.46	0.79
1:A:54:ARG:H	1:A:57:GLN:HE21	1.26	0.79
1:B:628:PHE:H	1:B:634:ASN:HD21	1.33	0.74

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	745/749 (100%)	696 (93%)	47 (6%)	2 (0%)	44	53
1	B	745/749 (100%)	695 (93%)	49 (7%)	1 (0%)	55	66
1	C	745/749 (100%)	694 (93%)	48 (6%)	3 (0%)	38	44
All	All	2235/2247 (100%)	2085 (93%)	144 (6%)	6 (0%)	44	53

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	472	ASP
1	A	91	GLU
1	B	399	ASN
1	C	473	HIS
1	A	676	ASN

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	632/634 (100%)	609 (96%)	23 (4%)	40	51
1	B	632/634 (100%)	604 (96%)	28 (4%)	33	41
1	C	631/634 (100%)	597 (95%)	34 (5%)	26	31
All	All	1895/1902 (100%)	1810 (96%)	85 (4%)	32	40

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	314	LYS
1	B	649	ARG
1	C	590	GLN
1	B	346	PRO
1	B	537	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	252	HIS
1	B	473	HIS
1	C	437	ASN
1	B	253	GLN
1	B	347	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	PCA	A	26	1	8,8,9	3.67	2 (25%)	9,10,12	3.34	6 (66%)
1	PCA	B	26	1	8,8,9	2.50	2 (25%)	9,10,12	2.34	5 (55%)
1	PCA	C	26	1	8,8,9	2.90	2 (25%)	9,10,12	2.83	4 (44%)

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	PCA	A	26	1	-	0/0/11/13	0/1/1/1
1	PCA	B	26	1	-	0/0/11/13	0/1/1/1
1	PCA	C	26	1	-	0/0/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	PCA	CA-C	4.61	1.56	1.50
1	B	26	PCA	CD-N	4.89	1.48	1.34
1	C	26	PCA	CD-N	5.01	1.49	1.34
1	A	26	PCA	CD-N	5.14	1.49	1.34
1	C	26	PCA	CA-C	6.00	1.58	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PCA	O-C-CA	-5.38	112.60	125.15
1	A	26	PCA	OE-CD-CG	-5.13	117.42	126.86
1	C	26	PCA	CB-CG-CD	-4.66	96.39	104.30
1	A	26	PCA	CB-CG-CD	-4.43	96.78	104.30
1	B	26	PCA	OE-CD-CG	-4.09	119.34	126.86

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	B	26	PCA	1	0

5.5 Carbohydrates ⓘ

12 carbohydrates 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$
3	RAM	A	773	3	11,11,11	0.68	0	15,16,16	1.28	2 (13%)
3	MAN	A	774	1,3	9,9,12	0.70	0	9,11,17	1.41	2 (22%)
3	GCU	A	775	3	9,12,13	0.71	0	12,17,19	1.40	2 (16%)
3	XYS	A	776	3	9,9,10	1.75	2 (22%)	11,12,14	2.08	3 (27%)
3	RAM	B	773	3	11,11,11	0.59	0	15,16,16	0.89	1 (6%)
3	MAN	B	774	1,3	9,9,12	0.75	0	9,11,17	1.44	2 (22%)
3	GCU	B	775	3	9,12,13	0.86	0	12,17,19	1.30	2 (16%)
3	XYS	B	776	3	9,9,10	1.69	1 (11%)	11,12,14	0.85	0
3	RAM	C	773	3	11,11,11	0.64	0	15,16,16	1.03	0
3	MAN	C	774	1,3	9,9,12	0.63	0	9,11,17	1.20	0
3	GCU	C	775	3	9,12,13	0.78	0	12,17,19	1.24	1 (8%)
3	XYS	C	776	3	9,9,10	1.79	2 (22%)	11,12,14	2.38	5 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RAM	A	773	3	-	0/0/20/20	0/1/1/1
3	MAN	A	774	1,3	-	0/2/12/22	0/1/1/1
3	GCU	A	775	3	-	0/0/20/24	0/1/1/1
3	XYS	A	776	3	-	0/0/14/17	0/1/1/1
3	RAM	B	773	3	-	0/0/20/20	0/1/1/1
3	MAN	B	774	1,3	-	0/2/12/22	0/1/1/1
3	GCU	B	775	3	-	0/0/20/24	0/1/1/1
3	XYS	B	776	3	1/1/3/4	0/0/14/17	0/1/1/1
3	RAM	C	773	3	-	0/0/20/20	0/1/1/1
3	MAN	C	774	1,3	-	0/2/12/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GCU	C	775	3	1/1/5/6	0/0/20/24	0/1/1/1
3	XYS	C	776	3	-	0/0/14/17	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	776	XYS	O5-C1	-4.58	1.36	1.43
3	C	776	XYS	O5-C1	-4.14	1.37	1.43
3	A	776	XYS	O5-C1	-3.89	1.37	1.43
3	A	776	XYS	C3-C2	2.75	1.56	1.52
3	C	776	XYS	C3-C2	2.95	1.56	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	774	MAN	C1-C2-C3	-3.05	105.77	110.19
3	C	775	GCU	C3-C4-C5	-2.97	104.17	109.75
3	B	774	MAN	C1-C2-C3	-2.72	106.25	110.19
3	B	774	MAN	O3-C3-C2	-2.39	104.31	110.10
3	C	776	XYS	O3-C3-C4	-2.32	104.30	110.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	775	GCU	C4
3	B	776	XYS	C1

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
3	B	773	RAM	1	0

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	A	2	-	4,4,4	0.70	0	6,6,6	0.93	0
5	PO4	A	3	-	4,4,4	0.84	0	6,6,6	0.81	0
5	PO4	A	5	-	4,4,4	0.59	0	6,6,6	0.76	0
4	HS2	A	777	-	24,27,27	2.23	3 (12%)	31,39,39	2.54	7 (22%)
5	PO4	A	9	-	4,4,4	0.68	0	6,6,6	1.27	1 (16%)
5	PO4	B	1	-	4,4,4	0.88	0	6,6,6	1.41	1 (16%)
5	PO4	B	7	-	4,4,4	0.85	0	6,6,6	0.65	0
4	HS2	B	777	-	24,27,27	2.36	3 (12%)	31,39,39	1.84	6 (19%)
5	PO4	B	8	-	4,4,4	0.59	0	6,6,6	0.82	0
5	PO4	C	4	-	4,4,4	0.78	0	6,6,6	1.13	1 (16%)
5	PO4	C	6	-	4,4,4	0.40	0	6,6,6	1.44	1 (16%)
4	HS2	C	777	-	24,27,27	2.34	3 (12%)	31,39,39	2.27	12 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	A	2	-	-	0/0/0/0	0/0/0/0
5	PO4	A	3	-	-	0/0/0/0	0/0/0/0
5	PO4	A	5	-	-	0/0/0/0	0/0/0/0
4	HS2	A	777	-	-	0/10/50/50	0/2/2/2
5	PO4	A	9	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1	-	-	0/0/0/0	0/0/0/0
5	PO4	B	7	-	-	0/0/0/0	0/0/0/0
4	HS2	B	777	-	-	0/10/50/50	0/2/2/2
5	PO4	B	8	-	-	0/0/0/0	0/0/0/0
5	PO4	C	4	-	-	0/0/0/0	0/0/0/0
5	PO4	C	6	-	-	0/0/0/0	0/0/0/0
4	HS2	C	777	-	-	0/10/50/50	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	777	HS2	C7-N14	2.90	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	777	HS2	C7-N14	3.07	1.45	1.34
4	B	777	HS2	C7-N14	3.49	1.47	1.34
4	A	777	HS2	O13-C19	4.20	1.45	1.37
4	B	777	HS2	O13-C19	4.36	1.45	1.37

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	777	HS2	O7-C7-C8	-9.62	104.56	122.06
4	B	777	HS2	O7-C7-C8	-6.52	110.20	122.06
4	C	777	HS2	O7-C7-C8	-5.49	112.07	122.06
4	A	777	HS2	C8-C7-N14	-5.33	106.48	116.11
4	C	777	HS2	C8-C7-N14	-4.67	107.68	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	777	HS2	1	0
5	C	6	PO4	3	0
4	C	777	HS2	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 [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, 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	746/749 (99%)	0.03	7 (0%) 84 91	19, 24, 27, 31	0
1	B	746/749 (99%)	0.20	15 (2%) 65 75	19, 24, 27, 31	0
1	C	746/749 (99%)	0.20	16 (2%) 64 74	19, 24, 28, 34	0
All	All	2238/2247 (99%)	0.14	38 (1%) 70 80	19, 24, 28, 34	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	472	ASP	5.6
1	B	38	GLY	5.4
1	C	470	GLY	5.2
1	C	473	HIS	4.7
1	C	471	SER	4.6

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, 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
1	PCA	B	26	8/9	0.82	0.16	-	30,31,32,33	0
1	PCA	A	26	8/9	0.80	0.23	-	28,29,29,31	0
1	PCA	C	26	8/9	0.85	0.17	-	29,29,30,30	0

6.3 Carbohydrates [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
3	RAM	C	773	11/11	0.97	0.17	1.50	25,26,28,28	0
3	RAM	B	773	11/11	0.94	0.16	0.57	28,29,30,30	0
3	RAM	A	773	11/11	0.95	0.14	-0.02	23,27,29,30	0
3	XYS	A	776	9/10	0.72	0.33	-	42,47,47,47	0
3	MAN	B	774	9/12	0.95	0.12	-	26,27,29,29	0
3	XYS	C	776	9/10	0.72	0.32	-	44,49,50,50	0
3	GCU	A	775	12/13	0.93	0.14	-	33,35,35,36	0
3	MAN	C	774	9/12	0.94	0.13	-	23,27,28,29	0
3	GCU	B	775	12/13	0.90	0.16	-	36,40,41,42	0
3	GCU	C	775	12/13	0.91	0.14	-	32,35,36,37	0
3	XYS	B	776	9/10	0.79	0.31	-	45,48,49,49	0
3	MAN	A	774	9/12	0.94	0.13	-	24,26,28,31	0

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
5	PO4	B	8	5/5	0.94	0.28	5.64	48,49,49,50	0
5	PO4	A	3	5/5	0.95	0.22	5.39	41,41,42,43	0
5	PO4	B	7	5/5	0.92	0.21	2.22	52,52,53,54	0
5	PO4	A	5	5/5	0.87	0.26	1.68	52,53,54,54	0
5	PO4	C	4	5/5	0.97	0.19	1.61	31,31,31,31	0
5	PO4	A	2	5/5	0.93	0.20	1.57	44,45,45,45	0
4	HS2	A	777	26/26	0.91	0.17	0.50	24,30,31,33	0
4	HS2	C	777	26/26	0.84	0.23	0.44	32,36,37,38	0
4	HS2	B	777	26/26	0.93	0.13	-0.25	21,26,28,28	0
5	PO4	B	1	5/5	0.98	0.10	-1.32	27,27,28,29	0
5	PO4	A	9	5/5	0.98	0.09	-1.62	26,26,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	C	3	1/1	1.00	0.02	-4.59	25,25,25,25	0
2	ZN	A	1	1/1	0.99	0.04	-4.61	27,27,27,27	0
2	ZN	B	2	1/1	1.00	0.04	-4.86	26,26,26,26	0
5	PO4	C	6	5/5	0.81	0.33	-	57,57,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.