



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:28 AM UTC

PDB ID : 5Z0A / pdb_00005z0a
Title : ST0452(Y97N)-GlcNAc binding form
Authors : Honda, Y.; Nakano, S.; Ito, S.; Dadashipour, M.; Zhang, Z.; Kawarabayasi, Y.
Deposited on : 2017-12-19
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

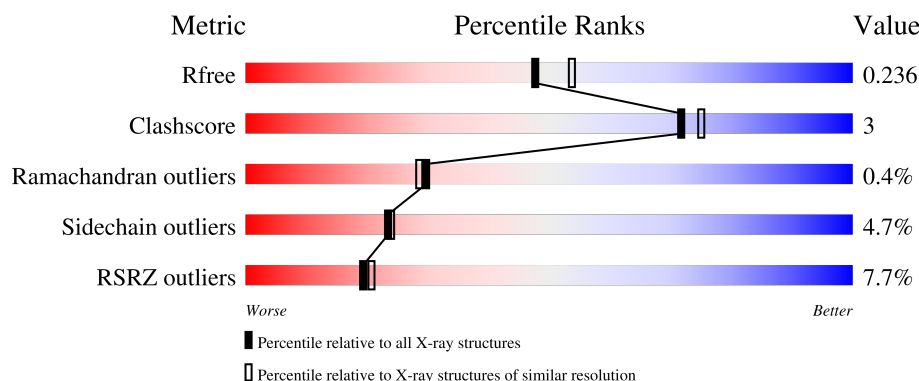
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	409	5% 86% 10% ...
1	B	409	4% 86% 11% ..
1	C	409	6% 87% 9% ..
1	D	409	7% 85% 9% ...
1	E	409	17% 85% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	409	6% 87% 10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19593 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 Dual sugar-1-phosphate nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3129	2011	524	588	6			
1	B	400	Total	C	N	O	S	0	0	0
			3129	2011	524	588	6			
1	C	396	Total	C	N	O	S	0	0	0
			3099	1995	517	581	6			
1	D	400	Total	C	N	O	S	0	0	0
			3129	2011	524	588	6			
1	E	396	Total	C	N	O	S	0	0	0
			3086	1985	515	580	6			
1	F	400	Total	C	N	O	S	0	0	0
			3129	2011	524	588	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ASN	TYR	engineered mutation	UNP Q975F9
A	402	LEU	-	expression tag	UNP Q975F9
A	403	GLU	-	expression tag	UNP Q975F9
A	404	HIS	-	expression tag	UNP Q975F9
A	405	HIS	-	expression tag	UNP Q975F9
A	406	HIS	-	expression tag	UNP Q975F9
A	407	HIS	-	expression tag	UNP Q975F9
A	408	HIS	-	expression tag	UNP Q975F9
A	409	HIS	-	expression tag	UNP Q975F9
B	97	ASN	TYR	engineered mutation	UNP Q975F9
B	402	LEU	-	expression tag	UNP Q975F9
B	403	GLU	-	expression tag	UNP Q975F9
B	404	HIS	-	expression tag	UNP Q975F9
B	405	HIS	-	expression tag	UNP Q975F9
B	406	HIS	-	expression tag	UNP Q975F9
B	407	HIS	-	expression tag	UNP Q975F9
B	408	HIS	-	expression tag	UNP Q975F9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	409	HIS	-	expression tag	UNP Q975F9
C	97	ASN	TYR	engineered mutation	UNP Q975F9
C	402	LEU	-	expression tag	UNP Q975F9
C	403	GLU	-	expression tag	UNP Q975F9
C	404	HIS	-	expression tag	UNP Q975F9
C	405	HIS	-	expression tag	UNP Q975F9
C	406	HIS	-	expression tag	UNP Q975F9
C	407	HIS	-	expression tag	UNP Q975F9
C	408	HIS	-	expression tag	UNP Q975F9
C	409	HIS	-	expression tag	UNP Q975F9
D	97	ASN	TYR	engineered mutation	UNP Q975F9
D	402	LEU	-	expression tag	UNP Q975F9
D	403	GLU	-	expression tag	UNP Q975F9
D	404	HIS	-	expression tag	UNP Q975F9
D	405	HIS	-	expression tag	UNP Q975F9
D	406	HIS	-	expression tag	UNP Q975F9
D	407	HIS	-	expression tag	UNP Q975F9
D	408	HIS	-	expression tag	UNP Q975F9
D	409	HIS	-	expression tag	UNP Q975F9
E	97	ASN	TYR	engineered mutation	UNP Q975F9
E	402	LEU	-	expression tag	UNP Q975F9
E	403	GLU	-	expression tag	UNP Q975F9
E	404	HIS	-	expression tag	UNP Q975F9
E	405	HIS	-	expression tag	UNP Q975F9
E	406	HIS	-	expression tag	UNP Q975F9
E	407	HIS	-	expression tag	UNP Q975F9
E	408	HIS	-	expression tag	UNP Q975F9
E	409	HIS	-	expression tag	UNP Q975F9
F	97	ASN	TYR	engineered mutation	UNP Q975F9
F	402	LEU	-	expression tag	UNP Q975F9
F	403	GLU	-	expression tag	UNP Q975F9
F	404	HIS	-	expression tag	UNP Q975F9
F	405	HIS	-	expression tag	UNP Q975F9
F	406	HIS	-	expression tag	UNP Q975F9
F	407	HIS	-	expression tag	UNP Q975F9
F	408	HIS	-	expression tag	UNP Q975F9
F	409	HIS	-	expression tag	UNP Q975F9

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			15	8	1	6		

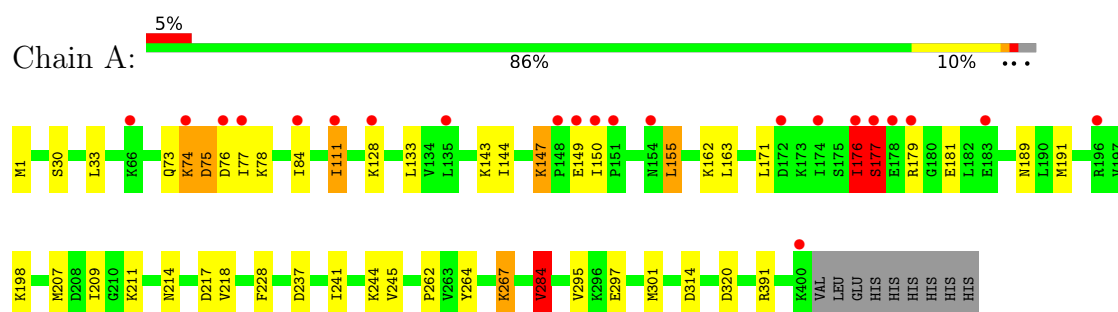
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total	O	0	0
			158	158		
3	B	175	Total	O	0	0
			175	175		
3	C	142	Total	O	0	0
			142	142		
3	D	143	Total	O	0	0
			143	143		
3	E	114	Total	O	0	0
			114	114		
3	F	145	Total	O	0	0
			145	145		

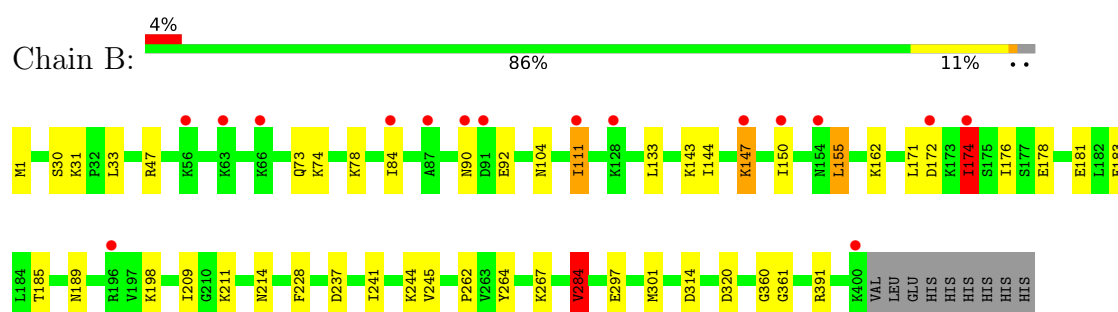
3 Residue-property plots [i](#)

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

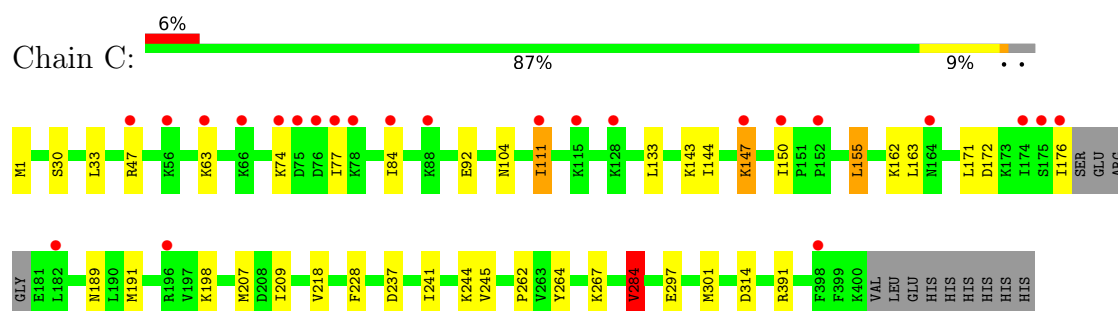
- Molecule 1: Dual sugar-1-phosphate nucleotidyltransferase



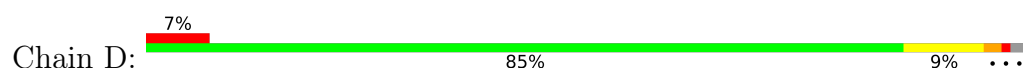
- Molecule 1: Dual sugar-1-phosphate nucleotidyltransferase

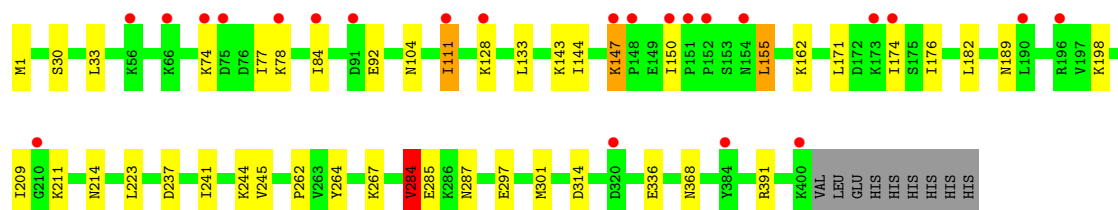


- Molecule 1: Dual sugar-1-phosphate nucleotidyltransferase



- Molecule 1: Dual sugar-1-phosphate nucleotidyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.84Å 94.95Å 101.91Å 110.62° 101.47° 113.03°	Depositor
Resolution (Å)	87.79 – 2.09 87.79 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.5 (87.79-2.09) 96.5 (87.79-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.193 , 0.232 0.199 , 0.236	Depositor DCC
R_{free} test set	7863 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.034 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19593	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	1.14	3/3182 (0.1%)	1.09	8/4294 (0.2%)
1	B	1.13	3/3182 (0.1%)	1.07	7/4294 (0.2%)
1	C	1.07	1/3151 (0.0%)	1.00	3/4252 (0.1%)
1	D	1.12	4/3182 (0.1%)	1.06	11/4294 (0.3%)
1	E	1.16	6/3138 (0.2%)	1.10	14/4236 (0.3%)
1	F	1.09	1/3182 (0.0%)	1.04	8/4294 (0.2%)
All	All	1.12	18/19017 (0.1%)	1.06	51/25664 (0.2%)

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	D	0	1
1	E	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	175	SER	CA-C	12.80	1.58	1.52
1	D	179	ARG	CA-C	7.68	1.62	1.53
1	A	147	LYS	C-O	-7.51	1.20	1.23
1	D	147	LYS	C-O	-7.11	1.20	1.23
1	E	324	GLY	CA-C	6.49	1.57	1.52
1	C	147	LYS	C-O	-6.47	1.20	1.23
1	F	147	LYS	C-O	-6.16	1.20	1.23
1	D	175	SER	N-CA	5.80	1.53	1.46
1	A	295	VAL	C-O	5.69	1.29	1.24
1	E	29	LEU	CA-C	5.46	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	GLY	N-CA	5.34	1.51	1.45
1	B	147	LYS	C-O	-5.20	1.21	1.23
1	A	217	ASP	N-CA	5.16	1.52	1.46
1	D	177	SER	CA-C	5.13	1.63	1.52
1	E	184	LEU	N-CA	5.09	1.52	1.46
1	E	360	GLY	N-CA	5.06	1.52	1.45
1	E	182	LEU	CA-C	5.03	1.59	1.52
1	B	361	GLY	N-CA	-5.02	1.39	1.45

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	LEU	N-CA-CB	9.19	126.02	110.49
1	E	196	ARG	NE-CZ-NH2	8.61	126.95	119.20
1	C	284	VAL	N-CA-C	8.26	119.04	110.62
1	A	284	VAL	N-CA-C	7.80	118.58	110.62
1	E	184	LEU	N-CA-C	-7.33	95.20	110.80
1	E	196	ARG	NE-CZ-NH1	-7.31	114.19	121.50
1	D	176	ILE	CA-C-N	7.22	134.70	121.70
1	D	176	ILE	C-N-CA	7.22	134.70	121.70
1	A	176	ILE	CA-C-N	7.20	134.65	121.70
1	A	176	ILE	C-N-CA	7.20	134.65	121.70
1	E	284	VAL	N-CA-C	6.96	117.72	110.62
1	B	284	VAL	N-CA-C	6.71	117.46	110.62
1	A	77	ILE	N-CA-C	-6.67	98.53	108.46
1	D	284	VAL	N-CA-C	6.60	117.36	110.62
1	E	196	ARG	CB-CA-C	6.50	121.53	110.81
1	F	77	ILE	N-CA-C	-6.33	99.03	108.46
1	D	77	ILE	N-CA-C	-6.30	99.08	108.46
1	B	174	ILE	CB-CA-C	6.29	118.71	110.91
1	F	284	VAL	N-CA-C	6.28	117.03	110.62
1	F	182	LEU	N-CA-C	-6.24	98.37	108.41
1	B	174	ILE	N-CA-CB	6.23	117.51	110.72
1	C	77	ILE	N-CA-C	-5.96	99.58	108.46
1	E	183	GLU	CB-CA-C	5.89	122.15	110.42
1	C	284	VAL	N-CA-CB	5.87	118.52	110.54
1	F	284	VAL	CA-CB-CG2	5.59	119.91	110.40
1	E	176	ILE	CA-C-N	5.58	131.75	121.70
1	E	176	ILE	C-N-CA	5.58	131.75	121.70
1	A	177	SER	N-CA-CB	5.50	119.86	110.50
1	B	284	VAL	CA-CB-CG2	5.50	119.75	110.40
1	D	368	ASN	N-CA-C	5.46	119.23	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	284	VAL	N-CA-CB	5.46	117.96	110.54
1	D	284	VAL	N-CA-CB	5.43	117.93	110.54
1	A	284	VAL	N-CA-CB	5.41	117.90	110.54
1	A	149	GLU	CG-CD-OE1	5.40	130.83	118.40
1	E	384	TYR	CB-CA-C	5.37	117.17	109.11
1	D	284	VAL	CA-CB-CG2	5.35	119.50	110.40
1	F	336	GLU	N-CA-C	5.32	119.07	112.47
1	E	171	LEU	CA-CB-CG	5.31	134.87	116.30
1	E	175	SER	N-CA-C	-5.27	100.08	108.30
1	F	174	ILE	N-CA-C	5.23	117.38	109.12
1	F	368	ASN	N-CA-C	5.21	118.90	112.24
1	D	391	ARG	CG-CD-NE	-5.19	100.58	112.00
1	A	149	GLU	CG-CD-OE2	-5.18	106.48	118.40
1	D	176	ILE	CA-C-O	-5.17	114.32	120.78
1	B	284	VAL	N-CA-CB	5.14	117.53	110.54
1	F	237	ASP	N-CA-CB	5.13	117.70	110.36
1	B	174	ILE	CA-CB-CG2	5.07	119.12	110.50
1	D	175	SER	N-CA-C	5.05	121.56	110.80
1	D	237	ASP	N-CA-CB	5.02	117.53	110.36
1	E	31	LYS	N-CA-C	5.00	117.28	108.82
1	B	31	LYS	N-CA-C	5.00	117.27	108.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	177	SER	Peptide
1	E	176	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3129	0	3232	29	0
1	B	3129	0	3232	21	0
1	C	3099	0	3204	20	0
1	D	3129	0	3232	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3086	0	3177	24	0
1	F	3129	0	3232	14	0
2	F	15	0	15	0	0
3	A	158	0	0	7	0
3	B	175	0	0	3	0
3	C	142	0	0	6	0
3	D	143	0	0	5	0
3	E	114	0	0	0	0
3	F	145	0	0	0	0
All	All	19593	0	19324	127	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 (127) 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:A:320:ASP:HB3	3:A:571:HOH:O	1.37	1.21
1:B:320:ASP:HB3	3:B:514:HOH:O	1.46	1.11
1:D:252:GLU:HG3	3:D:586:HOH:O	1.72	0.88
1:E:176:ILE:HG22	1:E:177:SER:HA	1.55	0.87
1:E:81:GLY:N	1:E:183:GLU:O	2.10	0.85
1:A:176:ILE:HA	1:A:177:SER:HB2	1.58	0.84
1:A:207:MET:HG3	3:A:515:HOH:O	1.84	0.77
1:A:75:ASP:HB3	1:A:76:ASP:HB3	1.66	0.76
1:C:207:MET:HG3	3:C:536:HOH:O	1.89	0.72
1:C:207:MET:CG	3:C:536:HOH:O	2.42	0.68
1:A:207:MET:CG	3:A:515:HOH:O	2.42	0.66
1:E:81:GLY:CA	1:E:183:GLU:O	2.43	0.65
1:B:144:ILE:H	1:B:189:ASN:HD21	1.46	0.63
1:D:382:ARG:HD3	1:D:398:PHE:CE1	2.32	0.63
1:F:144:ILE:H	1:F:189:ASN:HD21	1.47	0.63
1:E:182:LEU:HG	1:E:183:GLU:N	2.14	0.62
1:A:176:ILE:HA	1:A:177:SER:CB	2.30	0.62
1:C:218:VAL:HG11	3:C:536:HOH:O	2.00	0.61
1:A:73:GLN:C	1:A:75:ASP:H	2.09	0.61
1:E:84:ILE:HD11	1:E:171:LEU:HD21	1.82	0.60
1:C:241:ILE:HG23	1:C:245:VAL:HG21	1.82	0.60
1:A:241:ILE:HG23	1:A:245:VAL:HG21	1.83	0.59
1:B:241:ILE:HG23	1:B:245:VAL:HG21	1.84	0.59
1:E:144:ILE:H	1:E:189:ASN:HD21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ILE:HG23	1:E:245:VAL:HG21	1.85	0.59
1:D:241:ILE:HG23	1:D:245:VAL:HG21	1.84	0.58
1:A:74:LYS:O	1:A:75:ASP:O	2.22	0.58
1:D:144:ILE:H	1:D:189:ASN:HD21	1.52	0.58
1:F:241:ILE:HG23	1:F:245:VAL:HG21	1.85	0.58
1:C:144:ILE:H	1:C:189:ASN:HD21	1.50	0.57
1:B:73:GLN:HG2	1:B:74:LYS:N	2.19	0.57
1:E:182:LEU:HG	1:E:183:GLU:H	1.70	0.56
1:A:74:LYS:C	1:A:75:ASP:O	2.48	0.56
1:A:73:GLN:O	1:A:75:ASP:N	2.27	0.56
1:A:144:ILE:H	1:A:189:ASN:HD21	1.52	0.56
1:B:90:ASN:HB3	1:C:63:LYS:HG2	1.88	0.56
1:B:174:ILE:HD11	3:B:543:HOH:O	2.04	0.55
1:E:81:GLY:HA3	1:E:183:GLU:O	2.06	0.55
1:A:30:SER:HB3	1:A:264:TYR:OH	2.07	0.54
1:F:30:SER:HB3	1:F:264:TYR:OH	2.07	0.53
1:C:284:VAL:HG13	1:C:301:MET:HA	1.90	0.53
1:D:218:VAL:HG11	3:D:506:HOH:O	2.08	0.53
1:E:176:ILE:CG2	1:E:177:SER:HA	2.32	0.53
1:A:84:ILE:HD11	1:A:171:LEU:HD11	1.91	0.53
1:A:284:VAL:HG13	1:A:301:MET:HA	1.91	0.53
1:E:30:SER:HB3	1:E:264:TYR:OH	2.09	0.52
1:C:84:ILE:HD11	1:C:171:LEU:HD11	1.91	0.52
1:D:30:SER:HB3	1:D:264:TYR:OH	2.10	0.52
1:E:84:ILE:CD1	1:E:171:LEU:HD21	2.38	0.52
1:F:84:ILE:HD11	1:F:171:LEU:HD11	1.92	0.52
1:A:218:VAL:HG11	3:A:515:HOH:O	2.10	0.51
1:B:73:GLN:CG	1:B:74:LYS:N	2.73	0.51
1:C:30:SER:HB3	1:C:264:TYR:OH	2.11	0.51
1:C:207:MET:CB	3:C:536:HOH:O	2.58	0.51
1:B:30:SER:HB3	1:B:264:TYR:OH	2.10	0.51
1:D:84:ILE:HD11	1:D:171:LEU:HD11	1.93	0.50
1:A:267:LYS:HD2	3:A:641:HOH:O	2.12	0.50
1:F:284:VAL:HG13	1:F:301:MET:HA	1.93	0.50
1:B:284:VAL:HG13	1:B:301:MET:HA	1.94	0.50
1:C:207:MET:HB3	3:C:536:HOH:O	2.11	0.50
1:C:244:LYS:O	1:C:262:PRO:HA	2.11	0.50
1:E:182:LEU:O	1:E:183:GLU:HB2	2.12	0.49
1:E:284:VAL:HG13	1:E:301:MET:HA	1.93	0.49
1:D:176:ILE:HG22	1:D:177:SER:HA	1.93	0.49
1:A:133:LEU:HD12	1:A:155:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LYS:O	1:D:75:ASP:C	2.55	0.49
1:F:297:GLU:O	1:F:314:ASP:HA	2.13	0.49
1:B:84:ILE:HD11	1:B:171:LEU:HD11	1.94	0.48
1:C:133:LEU:HD12	1:C:155:LEU:HD13	1.95	0.48
1:D:244:LYS:O	1:D:262:PRO:HA	2.13	0.48
1:E:133:LEU:HD12	1:E:155:LEU:HD13	1.95	0.48
1:C:33:LEU:HD22	1:C:209:ILE:HD12	1.96	0.48
1:D:133:LEU:HD12	1:D:155:LEU:HD13	1.95	0.48
1:A:75:ASP:HB3	1:A:76:ASP:CB	2.39	0.48
1:A:207:MET:CB	3:A:515:HOH:O	2.61	0.48
1:B:244:LYS:O	1:B:262:PRO:HA	2.14	0.48
1:B:133:LEU:HD12	1:B:155:LEU:HD13	1.96	0.47
1:D:284:VAL:HG13	1:D:301:MET:HA	1.96	0.47
1:D:33:LEU:HD22	1:D:209:ILE:HD12	1.95	0.47
1:A:297:GLU:O	1:A:314:ASP:HA	2.14	0.47
1:C:218:VAL:CG1	3:C:536:HOH:O	2.60	0.47
1:A:244:LYS:O	1:A:262:PRO:HA	2.15	0.47
1:F:133:LEU:HD12	1:F:155:LEU:HD13	1.96	0.47
1:C:297:GLU:O	1:C:314:ASP:HA	2.15	0.47
1:B:33:LEU:HD22	1:B:209:ILE:HD12	1.97	0.46
1:E:33:LEU:HD22	1:E:209:ILE:HD12	1.96	0.46
1:C:228:PHE:HB2	1:E:104:ASN:HD21	1.80	0.46
1:E:297:GLU:O	1:E:314:ASP:HA	2.15	0.46
1:F:244:LYS:O	1:F:262:PRO:HA	2.16	0.46
1:F:33:LEU:HD22	1:F:209:ILE:HD12	1.98	0.46
1:D:207:MET:HG3	3:D:506:HOH:O	2.16	0.45
1:F:211:LYS:H	1:F:214:ASN:ND2	2.14	0.45
1:D:364:ARG:HG2	3:D:597:HOH:O	2.16	0.45
1:B:104:ASN:HD21	1:D:228:PHE:HB2	1.82	0.45
1:A:33:LEU:HD22	1:A:209:ILE:HD12	1.98	0.45
1:A:111:ILE:HG23	1:A:162:LYS:HB2	1.99	0.45
1:B:297:GLU:O	1:B:314:ASP:HA	2.17	0.44
1:C:111:ILE:HG23	1:C:162:LYS:HB2	1.99	0.44
1:A:211:LYS:H	1:A:214:ASN:ND2	2.15	0.44
1:E:72:THR:O	1:E:74:LYS:HE2	2.18	0.44
1:B:111:ILE:HG23	1:B:162:LYS:HB2	2.00	0.44
1:D:178:GLU:HA	1:D:180:GLY:O	2.18	0.44
1:E:244:LYS:O	1:E:262:PRO:HA	2.16	0.43
1:A:207:MET:HB3	3:A:515:HOH:O	2.17	0.43
1:B:174:ILE:CD1	3:B:543:HOH:O	2.63	0.43
1:D:178:GLU:OE1	1:D:181:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ASP:HB3	3:D:535:HOH:O	2.18	0.43
1:D:176:ILE:HB	1:D:177:SER:HB3	2.00	0.43
1:A:73:GLN:C	1:A:75:ASP:N	2.71	0.43
1:B:211:LYS:H	1:B:214:ASN:ND2	2.17	0.43
1:D:111:ILE:HG23	1:D:162:LYS:HB2	2.01	0.43
1:D:297:GLU:O	1:D:314:ASP:HA	2.19	0.42
1:C:163:LEU:HD22	1:C:191:MET:HE1	2.02	0.42
1:A:228:PHE:HB2	1:F:104:ASN:HD21	1.85	0.42
1:E:111:ILE:HG23	1:E:162:LYS:HB2	2.02	0.42
1:E:211:LYS:H	1:E:214:ASN:ND2	2.18	0.42
1:B:183:GLU:HG3	1:B:185:THR:OG1	2.20	0.41
1:D:78:LYS:HG3	1:D:181:GLU:HB3	2.01	0.41
1:F:285:GLU:H	1:F:287:ASN:HD21	1.68	0.41
1:A:163:LEU:HD22	1:A:191:MET:HE1	2.02	0.40
1:E:285:GLU:H	1:E:287:ASN:HD21	1.68	0.40
1:F:111:ILE:HG23	1:F:162:LYS:HB2	2.02	0.40
1:F:223:LEU:HG	1:F:262:PRO:HB2	2.02	0.40
1:B:144:ILE:H	1:B:189:ASN:ND2	2.14	0.40
1:D:211:LYS:H	1:D:214:ASN:ND2	2.19	0.40
1:B:228:PHE:HB2	1:D:104:ASN:HD21	1.86	0.40
1:C:104:ASN:HD21	1:E:228:PHE:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/409 (97%)	384 (96%)	11 (3%)	3 (1%)	16	12
1	B	398/409 (97%)	386 (97%)	12 (3%)	0	100	100
1	C	392/409 (96%)	380 (97%)	12 (3%)	0	100	100
1	D	398/409 (97%)	381 (96%)	13 (3%)	4 (1%)	12	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	392/409 (96%)	376 (96%)	13 (3%)	3 (1%)	16	12
1	F	398/409 (97%)	385 (97%)	13 (3%)	0	100	100
All	All	2376/2454 (97%)	2292 (96%)	74 (3%)	10 (0%)	30	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	SER
1	D	74	LYS
1	D	175	SER
1	E	183	GLU
1	A	75	ASP
1	D	75	ASP
1	E	176	ILE
1	E	184	LEU
1	D	176	ILE
1	A	74	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/352 (97%)	327 (95%)	16 (5%)	23	24
1	B	343/352 (97%)	324 (94%)	19 (6%)	19	18
1	C	340/352 (97%)	324 (95%)	16 (5%)	23	24
1	D	343/352 (97%)	327 (95%)	16 (5%)	23	24
1	E	337/352 (96%)	322 (96%)	15 (4%)	24	25
1	F	343/352 (97%)	328 (96%)	15 (4%)	25	26
All	All	2049/2112 (97%)	1952 (95%)	97 (5%)	23	24

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	78	LYS
1	A	111	ILE
1	A	128	LYS
1	A	143	LYS
1	A	147	LYS
1	A	150	ILE
1	A	155	LEU
1	A	176	ILE
1	A	179	ARG
1	A	181	GLU
1	A	198	LYS
1	A	237	ASP
1	A	267	LYS
1	A	284	VAL
1	A	391	ARG
1	B	1	MET
1	B	47	ARG
1	B	78	LYS
1	B	92	GLU
1	B	111	ILE
1	B	143	LYS
1	B	147	LYS
1	B	150	ILE
1	B	155	LEU
1	B	172	ASP
1	B	174	ILE
1	B	176	ILE
1	B	178	GLU
1	B	181	GLU
1	B	198	LYS
1	B	237	ASP
1	B	267	LYS
1	B	284	VAL
1	B	391	ARG
1	C	1	MET
1	C	47	ARG
1	C	74	LYS
1	C	92	GLU
1	C	111	ILE
1	C	143	LYS
1	C	147	LYS
1	C	150	ILE

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Mol	Chain	Res	Type
1	C	155	LEU
1	C	172	ASP
1	C	176	ILE
1	C	198	LYS
1	C	237	ASP
1	C	267	LYS
1	C	284	VAL
1	C	391	ARG
1	D	1	MET
1	D	74	LYS
1	D	76	ASP
1	D	78	LYS
1	D	111	ILE
1	D	143	LYS
1	D	147	LYS
1	D	150	ILE
1	D	155	LEU
1	D	176	ILE
1	D	181	GLU
1	D	198	LYS
1	D	237	ASP
1	D	284	VAL
1	D	385	PRO
1	D	391	ARG
1	E	1	MET
1	E	74	LYS
1	E	92	GLU
1	E	111	ILE
1	E	143	LYS
1	E	147	LYS
1	E	150	ILE
1	E	155	LEU
1	E	171	LEU
1	E	175	SER
1	E	176	ILE
1	E	198	LYS
1	E	267	LYS
1	E	284	VAL
1	E	391	ARG
1	F	1	MET
1	F	74	LYS
1	F	78	LYS

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Mol	Chain	Res	Type
1	F	92	GLU
1	F	111	ILE
1	F	128	LYS
1	F	143	LYS
1	F	147	LYS
1	F	150	ILE
1	F	155	LEU
1	F	176	ILE
1	F	198	LYS
1	F	267	LYS
1	F	284	VAL
1	F	391	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	104	ASN
1	A	189	ASN
1	A	195	HIS
1	A	214	ASN
1	A	225	ASN
1	A	230	GLN
1	A	287	ASN
1	B	73	GLN
1	B	104	ASN
1	B	140	ASN
1	B	189	ASN
1	B	195	HIS
1	B	214	ASN
1	B	225	ASN
1	B	230	GLN
1	B	287	ASN
1	C	73	GLN
1	C	104	ASN
1	C	189	ASN
1	C	195	HIS
1	C	214	ASN
1	C	225	ASN
1	C	230	GLN
1	C	287	ASN
1	D	73	GLN

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Mol	Chain	Res	Type
1	D	104	ASN
1	D	189	ASN
1	D	195	HIS
1	D	214	ASN
1	D	225	ASN
1	D	230	GLN
1	D	287	ASN
1	E	73	GLN
1	E	104	ASN
1	E	189	ASN
1	E	195	HIS
1	E	214	ASN
1	E	225	ASN
1	E	230	GLN
1	E	287	ASN
1	F	73	GLN
1	F	104	ASN
1	F	189	ASN
1	F	195	HIS
1	F	214	ASN
1	F	225	ASN
1	F	230	GLN
1	F	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
2	NAG	F	501	-	15,15,15	1.21	0	21,21,21	2.84	4 (19%)

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	F	501	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	NAG	O5-C1-C2	10.34	119.91	109.52
2	F	501	NAG	O1-C1-C2	4.13	117.80	109.22
2	F	501	NAG	O1-C1-O5	3.21	119.96	110.41
2	F	501	NAG	O3-C3-C2	-2.75	104.12	109.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	400/409 (97%)	0.20	22 (5%)	30	32	15, 29, 66, 91	0
1	B	400/409 (97%)	0.07	16 (4%)	42	44	16, 28, 56, 80	0
1	C	396/409 (96%)	0.24	24 (6%)	27	29	17, 31, 70, 93	0
1	D	400/409 (97%)	0.27	29 (7%)	21	22	16, 30, 76, 111	0
1	E	396/409 (96%)	0.62	71 (17%)	3	4	15, 31, 81, 134	0
1	F	400/409 (97%)	0.23	23 (5%)	29	30	16, 30, 61, 96	0
All	All	2392/2454 (97%)	0.27	185 (7%)	19	21	15, 30, 70, 134	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	176	ILE	8.6
1	E	150	ILE	7.2
1	E	174	ILE	6.7
1	C	176	ILE	5.9
1	E	184	LEU	5.5
1	F	150	ILE	5.4
1	E	175	SER	5.1
1	E	190	LEU	5.0
1	E	182	LEU	5.0
1	A	176	ILE	4.6
1	F	174	ILE	4.5
1	E	171	LEU	4.5
1	E	185	THR	4.5
1	E	74	LYS	4.3
1	E	192	ALA	4.3
1	F	128	LYS	4.2
1	A	150	ILE	4.2
1	B	174	ILE	4.1
1	E	186	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	80	THR	4.1
1	C	150	ILE	4.1
1	E	147	LYS	4.0
1	B	150	ILE	4.0
1	E	145	ILE	3.9
1	F	384	TYR	3.8
1	D	150	ILE	3.8
1	E	151	PRO	3.7
1	D	77	ILE	3.7
1	E	79	GLY	3.6
1	C	77	ILE	3.6
1	E	81	GLY	3.6
1	D	84	ILE	3.6
1	E	82	ALA	3.6
1	E	128	LYS	3.5
1	D	175	SER	3.5
1	D	180	GLY	3.5
1	C	111	ILE	3.4
1	E	87	ALA	3.4
1	A	77	ILE	3.4
1	E	97	ASN	3.3
1	D	173	LYS	3.3
1	A	178	GLU	3.3
1	F	196	ARG	3.3
1	D	111	ILE	3.2
1	C	128	LYS	3.2
1	E	66	LYS	3.2
1	D	177	SER	3.2
1	E	152	PRO	3.2
1	E	83	ALA	3.2
1	A	177	SER	3.2
1	E	183	GLU	3.1
1	E	154	ASN	3.1
1	B	84	ILE	3.1
1	D	176	ILE	3.1
1	C	66	LYS	3.1
1	D	174	ILE	3.1
1	E	177	SER	3.1
1	A	111	ILE	3.1
1	C	175	SER	3.1
1	C	398	PHE	3.0
1	E	178	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	182	LEU	3.0
1	D	196	ARG	3.0
1	A	151	PRO	3.0
1	F	151	PRO	3.0
1	E	86	SER	3.0
1	D	179	ARG	3.0
1	C	74	LYS	3.0
1	E	84	ILE	3.0
1	D	74	LYS	3.0
1	E	173	LYS	3.0
1	B	196	ARG	2.9
1	E	196	ARG	2.9
1	F	74	LYS	2.9
1	A	172	ASP	2.9
1	F	148	PRO	2.9
1	E	189	ASN	2.9
1	E	96	ILE	2.9
1	A	66	LYS	2.8
1	F	78	LYS	2.8
1	E	168	PHE	2.8
1	E	91	ASP	2.8
1	A	74	LYS	2.8
1	E	85	LEU	2.8
1	A	128	LYS	2.8
1	C	84	ILE	2.8
1	E	111	ILE	2.8
1	F	75	ASP	2.7
1	A	400	LYS	2.7
1	E	144	ILE	2.7
1	F	147	LYS	2.7
1	A	174	ILE	2.7
1	B	111	ILE	2.7
1	C	75	ASP	2.7
1	D	75	ASP	2.7
1	E	187	ALA	2.7
1	C	182	LEU	2.7
1	F	400	LYS	2.7
1	A	196	ARG	2.7
1	E	165	SER	2.6
1	E	88	LYS	2.6
1	A	84	ILE	2.6
1	F	154	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	148	PRO	2.6
1	D	128	LYS	2.6
1	E	134	VAL	2.5
1	D	66	LYS	2.5
1	F	91	ASP	2.5
1	E	135	LEU	2.5
1	E	137	ASN	2.5
1	D	147	LYS	2.5
1	D	164	ASN	2.5
1	D	91	ASP	2.4
1	E	172	ASP	2.4
1	E	170	TYR	2.4
1	C	88	LYS	2.4
1	D	78	LYS	2.4
1	F	173	LYS	2.4
1	A	154	ASN	2.4
1	E	90	ASN	2.4
1	E	164	ASN	2.4
1	F	320	ASP	2.4
1	D	151	PRO	2.4
1	C	115	LYS	2.4
1	F	56	LYS	2.4
1	C	164	ASN	2.4
1	B	66	LYS	2.4
1	C	196	ARG	2.4
1	B	87	ALA	2.4
1	F	84	ILE	2.4
1	B	400	LYS	2.4
1	F	152	PRO	2.4
1	E	131	GLY	2.3
1	E	320	ASP	2.3
1	B	128	LYS	2.3
1	E	188	ILE	2.3
1	A	148	PRO	2.3
1	E	127	PRO	2.3
1	E	89	PHE	2.3
1	E	169	THR	2.3
1	A	135	LEU	2.3
1	D	400	LYS	2.3
1	E	72	THR	2.3
1	B	56	LYS	2.3
1	B	91	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	76	ASP	2.3
1	A	183	GLU	2.2
1	F	111	ILE	2.2
1	E	132	VAL	2.2
1	C	56	LYS	2.2
1	E	193	LYS	2.2
1	E	166	ASP	2.2
1	E	146	GLU	2.2
1	B	154	ASN	2.2
1	C	152	PRO	2.2
1	D	143	LYS	2.2
1	E	143	LYS	2.2
1	C	63	LYS	2.2
1	F	66	LYS	2.2
1	A	149	GLU	2.2
1	D	178	GLU	2.2
1	F	210	GLY	2.2
1	B	90	ASN	2.2
1	D	181	GLU	2.1
1	B	147	LYS	2.1
1	B	63	LYS	2.1
1	D	135	LEU	2.1
1	C	47	ARG	2.1
1	E	167	ILE	2.1
1	E	180	GLY	2.1
1	E	364	ARG	2.1
1	C	78	LYS	2.1
1	F	190	LEU	2.1
1	A	76	ASP	2.1
1	B	172	ASP	2.1
1	E	129	ASP	2.1
1	A	179	ARG	2.1
1	D	68	ILE	2.1
1	D	191	MET	2.0
1	C	147	LYS	2.0
1	E	56	LYS	2.0
1	C	174	ILE	2.0
1	E	149	GLU	2.0
1	E	138	GLN	2.0
1	E	179	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	501	15/15	0.86	0.12	32,47,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.