



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:55 PM UTC

PDB ID : 4YWT / pdb_00004ywt
Title : Crystal structure of full-length glypican-1 core protein after controlled crystal dehydration to 87% relative humidity
Authors : Awad, W.; Mani, K.; Logan, D.T.
Deposited on : 2015-03-21
Resolution : 2.38 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

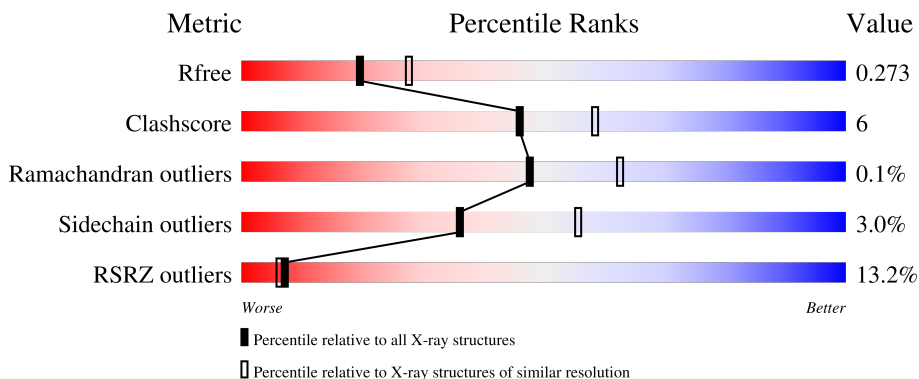
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	526	9% 68% 10% 22%
1	B	526	10% 67% 14% 18%
1	C	526	10% 65% 10% 24%
1	D	526	12% 66% 14% 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13110 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 Glypican-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	4	0
			3166	1981	568	594	23			
1	B	431	Total	C	N	O	S	0	3	0
			3283	2062	581	616	24			
1	C	400	Total	C	N	O	S	0	2	0
			3058	1918	544	575	21			
1	D	429	Total	C	N	O	S	0	4	0
			3254	2043	571	613	27			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP P35052
A	3	PRO	-	expression tag	UNP P35052
A	4	GLN	-	expression tag	UNP P35052
A	5	LEU	-	expression tag	UNP P35052
A	6	HIS	-	expression tag	UNP P35052
A	7	HIS	-	expression tag	UNP P35052
A	8	HIS	-	expression tag	UNP P35052
A	9	HIS	-	expression tag	UNP P35052
A	10	HIS	-	expression tag	UNP P35052
A	11	HIS	-	expression tag	UNP P35052
A	12	ASP	-	expression tag	UNP P35052
A	13	LEU	-	expression tag	UNP P35052
A	14	TYR	-	expression tag	UNP P35052
A	15	GLU	-	expression tag	UNP P35052
A	16	ASN	-	expression tag	UNP P35052
A	17	LEU	-	expression tag	UNP P35052
A	18	TYR	-	expression tag	UNP P35052
A	19	PHE	-	expression tag	UNP P35052
A	20	GLN	-	expression tag	UNP P35052
A	21	GLY	-	expression tag	UNP P35052
A	22	LYS	-	expression tag	UNP P35052

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	-	expression tag	UNP P35052
A	486	ALA	SER	engineered mutation	UNP P35052
A	488	ALA	SER	engineered mutation	UNP P35052
A	490	ALA	SER	engineered mutation	UNP P35052
B	2	ALA	-	expression tag	UNP P35052
B	3	PRO	-	expression tag	UNP P35052
B	4	GLN	-	expression tag	UNP P35052
B	5	LEU	-	expression tag	UNP P35052
B	6	HIS	-	expression tag	UNP P35052
B	7	HIS	-	expression tag	UNP P35052
B	8	HIS	-	expression tag	UNP P35052
B	9	HIS	-	expression tag	UNP P35052
B	10	HIS	-	expression tag	UNP P35052
B	11	HIS	-	expression tag	UNP P35052
B	12	ASP	-	expression tag	UNP P35052
B	13	LEU	-	expression tag	UNP P35052
B	14	TYR	-	expression tag	UNP P35052
B	15	GLU	-	expression tag	UNP P35052
B	16	ASN	-	expression tag	UNP P35052
B	17	LEU	-	expression tag	UNP P35052
B	18	TYR	-	expression tag	UNP P35052
B	19	PHE	-	expression tag	UNP P35052
B	20	GLN	-	expression tag	UNP P35052
B	21	GLY	-	expression tag	UNP P35052
B	22	LYS	-	expression tag	UNP P35052
B	23	LEU	-	expression tag	UNP P35052
B	486	ALA	SER	engineered mutation	UNP P35052
B	488	ALA	SER	engineered mutation	UNP P35052
B	490	ALA	SER	engineered mutation	UNP P35052
C	2	ALA	-	expression tag	UNP P35052
C	3	PRO	-	expression tag	UNP P35052
C	4	GLN	-	expression tag	UNP P35052
C	5	LEU	-	expression tag	UNP P35052
C	6	HIS	-	expression tag	UNP P35052
C	7	HIS	-	expression tag	UNP P35052
C	8	HIS	-	expression tag	UNP P35052
C	9	HIS	-	expression tag	UNP P35052
C	10	HIS	-	expression tag	UNP P35052
C	11	HIS	-	expression tag	UNP P35052
C	12	ASP	-	expression tag	UNP P35052
C	13	LEU	-	expression tag	UNP P35052
C	14	TYR	-	expression tag	UNP P35052

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	GLU	-	expression tag	UNP P35052
C	16	ASN	-	expression tag	UNP P35052
C	17	LEU	-	expression tag	UNP P35052
C	18	TYR	-	expression tag	UNP P35052
C	19	PHE	-	expression tag	UNP P35052
C	20	GLN	-	expression tag	UNP P35052
C	21	GLY	-	expression tag	UNP P35052
C	22	LYS	-	expression tag	UNP P35052
C	23	LEU	-	expression tag	UNP P35052
C	486	ALA	SER	engineered mutation	UNP P35052
C	488	ALA	SER	engineered mutation	UNP P35052
C	490	ALA	SER	engineered mutation	UNP P35052
D	2	ALA	-	expression tag	UNP P35052
D	3	PRO	-	expression tag	UNP P35052
D	4	GLN	-	expression tag	UNP P35052
D	5	LEU	-	expression tag	UNP P35052
D	6	HIS	-	expression tag	UNP P35052
D	7	HIS	-	expression tag	UNP P35052
D	8	HIS	-	expression tag	UNP P35052
D	9	HIS	-	expression tag	UNP P35052
D	10	HIS	-	expression tag	UNP P35052
D	11	HIS	-	expression tag	UNP P35052
D	12	ASP	-	expression tag	UNP P35052
D	13	LEU	-	expression tag	UNP P35052
D	14	TYR	-	expression tag	UNP P35052
D	15	GLU	-	expression tag	UNP P35052
D	16	ASN	-	expression tag	UNP P35052
D	17	LEU	-	expression tag	UNP P35052
D	18	TYR	-	expression tag	UNP P35052
D	19	PHE	-	expression tag	UNP P35052
D	20	GLN	-	expression tag	UNP P35052
D	21	GLY	-	expression tag	UNP P35052
D	22	LYS	-	expression tag	UNP P35052
D	23	LEU	-	expression tag	UNP P35052
D	486	ALA	SER	engineered mutation	UNP P35052
D	488	ALA	SER	engineered mutation	UNP P35052
D	490	ALA	SER	engineered mutation	UNP P35052

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		

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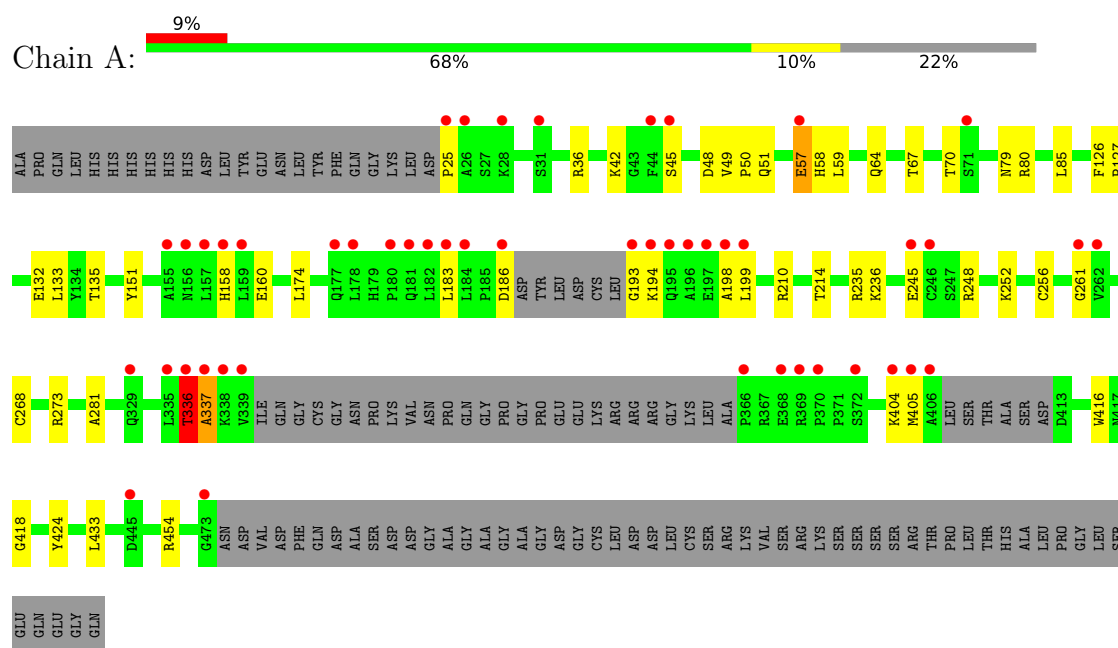
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	86	Total 86	O 86	0	0
4	C	53	Total 53	O 53	0	0
4	D	43	Total 43	O 43	0	0

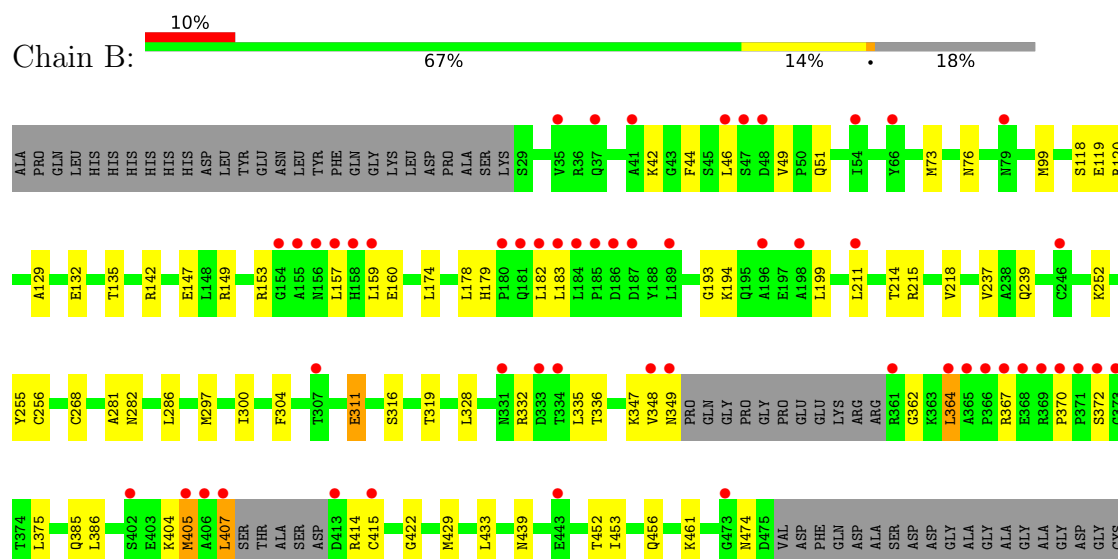
3 Residue-property plots

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

• Molecule 1: Glypican-1



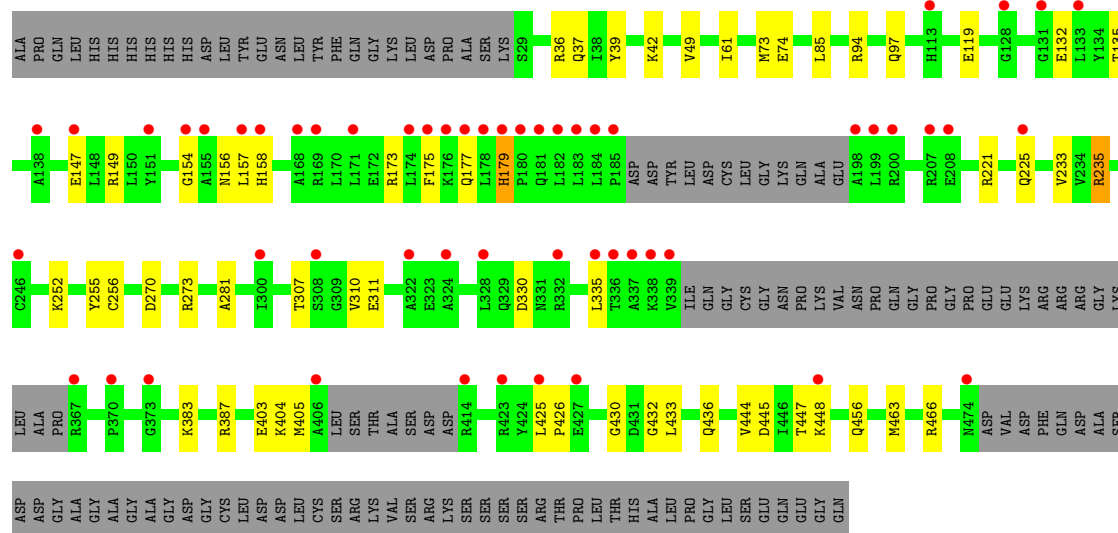
• Molecule 1: Glypican-1



LEU
ASP
GLN
LEU
CYS
SER
ARG
LYS
VAL
SER
ARG
LYS
SER
SER
SER
SER
THR
THR
PRO
LEU
THR
HIS
ALA
LEU
PRO
GLY
LEU
SER
GLN
GLY
GLN

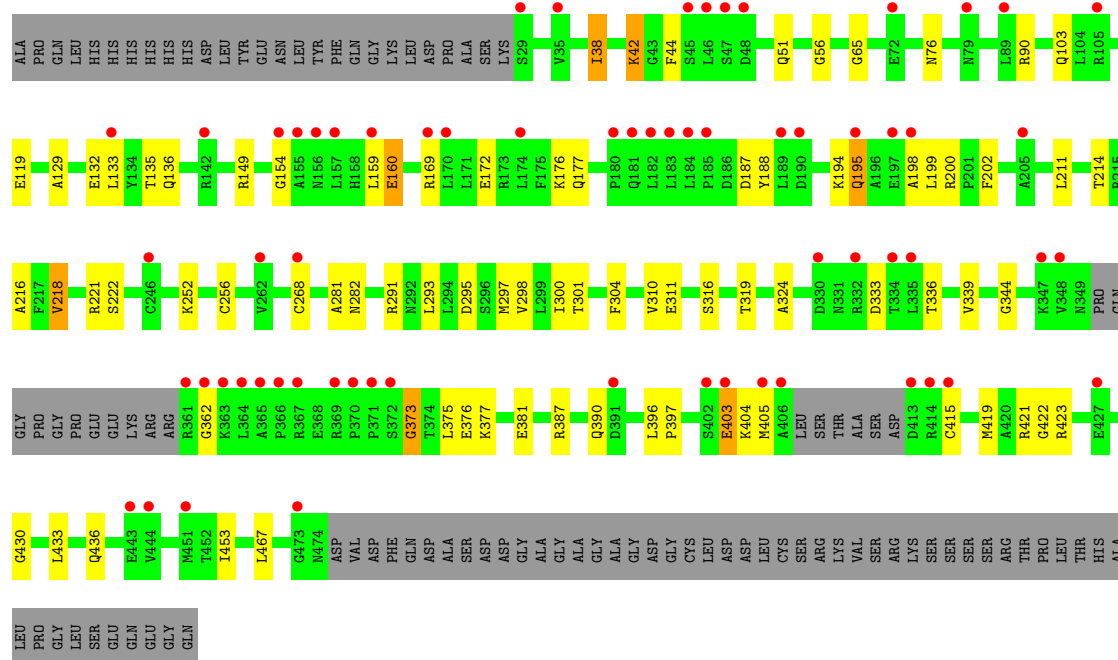
● Molecule 1: Glypican-1

Chain C:  10% 65% 10% 24%



● Molecule 1: Glypican-1

Chain D:  12% 66% 14% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.78Å 166.59Å 137.70Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	43.22 – 2.38 43.22 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.22-2.38) 97.9 (43.22-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.239 , 0.273 0.241 , 0.273	Depositor DCC
R_{free} test set	1985 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13110	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 46.82 % 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 1.0833e-04. 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: NAG, CA

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	0.31	0/3238	0.79	3/4390 (0.1%)
1	B	0.36	0/3352	0.82	4/4550 (0.1%)
1	C	0.34	0/3120	0.78	4/4234 (0.1%)
1	D	0.31	0/3326	0.77	1/4517 (0.0%)
All	All	0.33	0/13036	0.79	12/17691 (0.1%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LEU	N-CA-C	-8.12	102.94	113.17
1	A	336	THR	N-CA-C	7.83	127.49	110.80
1	C	179	HIS	CA-C-N	7.81	127.47	119.19
1	C	179	HIS	C-N-CA	7.81	127.47	119.19
1	B	370	PRO	CA-C-N	6.96	126.44	118.85
1	B	370	PRO	C-N-CA	6.96	126.44	118.85
1	B	193	GLY	N-CA-C	-6.86	105.86	114.16
1	A	337	ALA	N-CA-C	6.39	124.41	110.80
1	C	61	ILE	N-CA-C	5.65	116.30	110.82
1	C	330	ASP	N-CA-C	-5.62	105.15	112.23
1	B	404	LYS	CA-CB-CG	5.32	124.74	114.10
1	D	373	GLY	N-CA-C	-5.14	106.84	115.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	ALA	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	3166	0	3070	30	0
1	B	3283	0	3184	43	0
1	C	3058	0	2949	28	0
1	D	3254	0	3126	45	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	102	0	0	3	0
4	B	86	0	0	4	0
4	C	53	0	0	0	0
4	D	43	0	0	2	0
All	All	13110	0	12381	145	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 6.

All (145) 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:407:LEU:HD22	1:B:415:CYS:HB3	1.66	0.77
1:A:25:PRO:HD2	1:A:261:GLY:HA2	1.67	0.76
1:B:319:THR:HG21	1:B:367:ARG:HA	1.69	0.74
1:B:268[B]:CYS:SG	4:B:781:HOH:O	2.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:HB2	1:B:364:LEU:HD11	1.70	0.72
1:C:119:GLU:OE1	1:C:149:ARG:NH2	2.23	0.71
1:B:147:GLU:HG3	1:B:157:LEU:HD21	1.75	0.69
1:A:245:GLU:OE1	1:A:248:ARG:NH2	2.25	0.68
1:A:51:GLN:H	1:A:51:GLN:CD	2.02	0.67
1:D:119:GLU:OE1	1:D:149:ARG:NH2	2.28	0.67
1:D:187:ASP:OD1	1:D:188:TYR:N	2.30	0.65
1:A:268[B]:CYS:SG	4:A:790:HOH:O	2.54	0.65
1:D:268[B]:CYS:SG	4:D:741:HOH:O	2.54	0.65
1:B:178:LEU:HD22	1:B:332:ARG:HD3	1.79	0.64
1:A:194:LYS:N	1:A:194:LYS:HD3	2.13	0.64
1:D:160:GLU:N	1:D:160:GLU:OE1	2.28	0.63
1:B:311:GLU:HG3	1:B:375:LEU:HD22	1.81	0.63
1:B:118:SER:OG	4:B:701:HOH:O	2.16	0.62
1:D:195:GLN:O	1:D:199:LEU:HB2	1.98	0.62
1:A:273:ARG:NH2	4:A:702:HOH:O	2.32	0.62
1:D:129:ALA:HA	1:D:362:GLY:HA2	1.82	0.62
1:C:403:GLU:HG3	1:C:404:LYS:HD3	1.85	0.59
1:B:282:ASN:HB3	1:B:453:ILE:HD12	1.84	0.59
1:B:281:ALA:HB1	1:B:433:LEU:HA	1.85	0.59
1:A:193:GLY:C	1:A:194:LYS:HD3	2.28	0.59
1:A:85:LEU:HD13	1:A:405:MET:HE1	1.86	0.58
1:D:333:ASP:HA	1:D:336:THR:HG22	1.84	0.58
1:C:36:ARG:HA	1:C:49:VAL:HG21	1.86	0.58
1:B:348:VAL:HG12	1:B:349:ASN:H	1.69	0.58
1:C:157:LEU:HD12	1:C:158:HIS:H	1.69	0.57
1:D:282:ASN:HB3	1:D:453:ILE:HD12	1.85	0.57
1:D:160:GLU:H	1:D:160:GLU:CD	2.13	0.57
1:D:211:LEU:O	1:D:214:THR:OG1	2.21	0.56
1:B:179:HIS:NE2	1:B:336:THR:OG1	2.39	0.54
1:B:237:VAL:HG21	1:B:286:LEU:HD11	1.90	0.54
1:B:119:GLU:OE1	1:B:149:ARG:NH2	2.33	0.54
1:B:304:PHE:HB3	1:B:375:LEU:HD21	1.90	0.54
1:B:414:ARG:HD2	1:B:422:GLY:HA2	1.89	0.54
1:D:281:ALA:HB1	1:D:433:LEU:HA	1.90	0.53
1:D:316:SER:O	1:D:319:THR:OG1	2.23	0.53
1:C:270:ASP:OD1	1:C:273:ARG:NH2	2.39	0.53
1:B:429:MET:HG3	1:B:439:ASN:HD22	1.74	0.53
1:A:281:ALA:HB1	1:A:433:LEU:HA	1.91	0.52
1:D:421:ARG:NH2	4:D:703:HOH:O	2.42	0.52
1:B:51:GLN:H	1:B:51:GLN:CD	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:GLY:O	1:C:436:GLN:NE2	2.41	0.52
1:A:416:TRP:CE2	1:A:418:GLY:HA2	2.45	0.52
1:C:85:LEU:HD13	1:C:405:MET:HE1	1.91	0.52
1:B:120:ARG:NH1	4:B:709:HOH:O	2.43	0.52
1:D:169:ARG:HD3	1:D:169:ARG:C	2.35	0.52
1:B:132:GLU:HA	1:B:135:THR:OG1	2.10	0.52
1:C:281:ALA:HB1	1:C:433:LEU:HA	1.90	0.52
1:A:57:GLU:HG3	1:A:58:HIS:N	2.24	0.51
1:B:99:MET:HE3	1:B:385:GLN:HB3	1.92	0.51
1:A:59:LEU:HD21	1:A:67:THR:HG21	1.92	0.51
1:C:154:GLY:HA2	1:C:221:ARG:HD2	1.92	0.51
1:C:252:LYS:HA	1:C:256:CYS:SG	2.50	0.51
1:B:211:LEU:O	1:B:214:THR:OG1	2.27	0.51
1:D:297:MET:O	1:D:300:ILE:HG22	2.11	0.50
1:C:36:ARG:HB2	1:C:49:VAL:HG11	1.93	0.50
1:D:415:CYS:O	1:D:422:GLY:N	2.38	0.50
1:C:425:LEU:HG	1:C:426:PRO:HD3	1.94	0.49
1:D:252:LYS:HA	1:D:256:CYS:SG	2.53	0.49
1:B:46:LEU:O	1:B:49:VAL:HG12	2.12	0.49
1:D:430:GLY:O	1:D:436:GLN:NE2	2.45	0.49
1:A:252:LYS:HA	1:A:256:CYS:SG	2.52	0.49
1:C:173:ARG:O	1:C:177:GLN:HG2	2.13	0.49
1:D:298:VAL:O	1:D:301:THR:OG1	2.30	0.49
1:A:158:HIS:HE2	1:A:214:THR:HG23	1.77	0.49
1:C:233:VAL:HG13	1:C:456:GLN:HB3	1.94	0.48
1:D:172:GLU:O	1:D:176:LYS:HG3	2.14	0.48
1:D:291:ARG:HG2	1:D:390:GLN:HG3	1.96	0.48
1:A:210:ARG:NH1	4:A:711:HOH:O	2.40	0.47
1:D:188:TYR:OH	1:D:344:GLY:O	2.30	0.47
1:D:222:SER:HB3	1:D:467:LEU:HD23	1.97	0.47
1:C:132:GLU:HA	1:C:135:THR:HB	1.97	0.47
1:D:311:GLU:HB2	1:D:375:LEU:HD22	1.96	0.46
1:D:304:PHE:HB3	1:D:375:LEU:HD21	1.97	0.46
1:A:158:HIS:CE1	1:A:160:GLU:H	2.34	0.46
1:C:383:LYS:HB3	1:C:387:ARG:HH12	1.79	0.46
1:A:42:LYS:O	1:A:80:ARG:NH2	2.38	0.46
1:D:154:GLY:HA2	1:D:221:ARG:HD2	1.98	0.46
1:C:383:LYS:HB3	1:C:387:ARG:NH1	2.30	0.46
1:D:38:ILE:O	1:D:42:LYS:HG3	2.15	0.45
1:B:252:LYS:HA	1:B:256:CYS:SG	2.56	0.45
1:C:463:MET:HE3	1:C:466:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HA	1:A:49:VAL:HG21	1.98	0.45
1:B:199:LEU:HD13	1:B:335:LEU:HD12	1.98	0.45
1:D:132:GLU:HA	1:D:135:THR:OG1	2.17	0.45
1:A:268[B]:CYS:SG	1:A:424:TYR:HB3	2.57	0.44
1:B:174:LEU:HD23	1:B:328:LEU:HD23	1.99	0.44
1:B:347:LYS:HG2	1:B:348:VAL:H	1.81	0.44
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.81	0.44
1:C:387:ARG:NH1	1:D:376:GLU:OE1	2.50	0.44
1:D:295:ASP:OD1	1:D:387:ARG:NH1	2.49	0.44
1:A:45:SER:HB2	1:A:48:ASP:OD2	2.17	0.44
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.76	0.44
1:D:202:PHE:HB3	1:D:324:ALA:HB1	2.00	0.43
1:D:216:ALA:HB1	1:D:310:VAL:HA	1.99	0.43
1:A:133:LEU:HD22	1:A:174:LEU:HD22	1.99	0.43
1:B:179:HIS:CE1	1:B:332:ARG:HH11	2.36	0.43
1:D:132:GLU:HA	1:D:135:THR:HG1	1.83	0.43
1:A:59:LEU:HD12	1:A:64:GLN:HA	2.00	0.43
1:B:297:MET:O	1:B:300:ILE:HG22	2.18	0.43
1:B:42:LYS:HE3	1:B:255:TYR:CE1	2.53	0.43
1:B:405:MET:H	1:B:405:MET:HG3	1.40	0.43
1:D:195:GLN:OE1	1:D:339:VAL:HA	2.18	0.43
1:C:97:GLN:NE2	1:C:235:ARG:HA	2.34	0.43
1:D:198:ALA:HA	1:D:200:ARG:HH11	1.84	0.43
1:A:336:THR:O	1:A:336:THR:CG2	2.67	0.43
1:B:129:ALA:HA	1:B:362:GLY:HA2	2.00	0.43
1:C:310:VAL:HG12	1:C:311:GLU:H	1.84	0.43
1:D:403:GLU:OE1	1:D:404:LYS:HB2	2.19	0.43
1:A:454:ARG:HD3	1:A:454:ARG:HA	1.81	0.42
1:B:452:THR:O	1:B:456:GLN:HG2	2.19	0.42
1:C:448:LYS:HD2	1:C:448:LYS:C	2.44	0.42
1:D:159:LEU:N	1:D:160:GLU:OE1	2.52	0.42
1:C:432:GLY:O	1:C:436:GLN:HG2	2.19	0.42
1:B:316:SER:O	1:B:319:THR:OG1	2.25	0.42
1:D:214:THR:O	1:D:218:VAL:HB	2.20	0.42
1:A:235:ARG:NH2	1:A:236:LYS:HE3	2.35	0.42
1:C:42:LYS:HE2	1:C:255:TYR:OH	2.19	0.42
1:C:175:PHE:O	1:C:179:HIS:CD2	2.73	0.42
1:C:39:TYR:CZ	1:C:73:MET:HG2	2.55	0.42
1:B:183:LEU:HD13	1:B:347:LYS:HD3	2.01	0.41
1:D:44:PHE:CE1	1:D:76:ASN:HB3	2.55	0.41
1:A:126:PHE:N	1:A:127:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HA	1:D:177:GLN:OE1	2.20	0.41
1:B:414:ARG:HD3	1:B:414:ARG:HA	1.69	0.41
1:D:373:GLY:O	1:D:377:LYS:HG2	2.20	0.41
1:D:56:GLY:HA3	1:D:65:GLY:O	2.20	0.41
1:D:293:LEU:HG	1:D:297:MET:HE2	2.02	0.41
1:B:215:ARG:O	1:B:218:VAL:HG12	2.20	0.41
1:D:199:LEU:HD12	1:D:199:LEU:HA	1.85	0.41
1:B:49:VAL:HG23	1:B:73:MET:HE1	2.03	0.41
1:B:44:PHE:CE1	1:B:76:ASN:HB3	2.55	0.41
1:B:159:LEU:HD12	1:B:159:LEU:HA	1.91	0.41
1:B:372:SER:HB3	4:B:705:HOH:O	2.21	0.41
1:C:156:ASN:ND2	1:C:221:ARG:HH12	2.19	0.41
1:A:151:TYR:CE1	1:A:158:HIS:HA	2.57	0.40
1:A:50:PRO:HD3	1:A:70:THR:HG23	2.04	0.40
1:A:132:GLU:HA	1:A:135:THR:OG1	2.21	0.40
1:C:445:ASP:OD2	1:C:447:THR:OG1	2.25	0.40
1:D:396:LEU:HB2	1:D:397:PRO:HD3	2.04	0.40
1:B:99:MET:HE1	1:B:386:LEU:HD23	2.04	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	407/526 (77%)	401 (98%)	4 (1%)	2 (0%)	24	34
1	B	428/526 (81%)	412 (96%)	16 (4%)	0	100	100
1	C	394/526 (75%)	385 (98%)	9 (2%)	0	100	100
1	D	427/526 (81%)	418 (98%)	9 (2%)	0	100	100
All	All	1656/2104 (79%)	1616 (98%)	38 (2%)	2 (0%)	48	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	THR
1	A	337	ALA

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	332/439 (76%)	328 (99%)	4 (1%)	63	79
1	B	341/439 (78%)	329 (96%)	12 (4%)	32	50
1	C	317/439 (72%)	308 (97%)	9 (3%)	38	58
1	D	336/439 (76%)	320 (95%)	16 (5%)	23	37
All	All	1326/1756 (76%)	1285 (97%)	41 (3%)	36	54

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	79	ASN
1	A	186	ASP
1	A	404	LYS
1	B	142	ARG
1	B	153	ARG
1	B	160	GLU
1	B	182	LEU
1	B	194	LYS
1	B	239	GLN
1	B	311	GLU
1	B	364	LEU
1	B	405	MET
1	B	407	LEU
1	B	461	LYS
1	B	474	ASN
1	C	37	GLN
1	C	74	GLU
1	C	94	ARG
1	C	147	GLU

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Mol	Chain	Res	Type
1	C	225	GLN
1	C	235	ARG
1	C	307	THR
1	C	335	LEU
1	C	444	VAL
1	D	38	ILE
1	D	42	LYS
1	D	51	GLN
1	D	90	ARG
1	D	103	GLN
1	D	136	GLN
1	D	160	GLU
1	D	194	LYS
1	D	195	GLN
1	D	218	VAL
1	D	381[A]	GLU
1	D	381[B]	GLU
1	D	403	GLU
1	D	405	MET
1	D	419	MET
1	D	423	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	225	GLN
1	B	385	GLN
1	B	436	GLN
1	C	82	HIS
1	C	97	GLN
1	C	103	GLN
1	C	225	GLN
1	C	239	GLN
1	C	282	ASN
1	C	474	ASN
1	D	37	GLN
1	D	110	HIS
1	D	326	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 ⓘ

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	B	601	1	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	C	601	1	14,14,15	0.36	0	17,19,21	0.56	0
2	NAG	D	601	1	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	A	601	1	14,14,15	0.43	0	17,19,21	0.51	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	B	601	1	-	4/6/23/26	0/1/1/1
2	NAG	C	601	1	-	4/6/23/26	0/1/1/1
2	NAG	D	601	1	-	3/6/23/26	0/1/1/1
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NAG	O5-C5-C6-O6
2	B	601	NAG	O5-C5-C6-O6
2	B	601	NAG	C4-C5-C6-O6
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	B	601	NAG	C8-C7-N2-C2
2	B	601	NAG	O7-C7-N2-C2
2	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	D	601	NAG	C8-C7-N2-C2
2	D	601	NAG	O7-C7-N2-C2
2	C	601	NAG	C4-C5-C6-O6
2	D	601	NAG	O5-C5-C6-O6

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 [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	411/526 (78%)	0.79	48 (11%) 9 8	19, 48, 96, 119	4 (0%)
1	B	431/526 (81%)	0.91	53 (12%) 8 7	21, 53, 98, 134	3 (0%)
1	C	400/526 (76%)	1.10	54 (13%) 7 6	35, 58, 107, 139	2 (0%)
1	D	429/526 (81%)	1.10	65 (15%) 5 5	31, 60, 104, 135	4 (0%)
All	All	1671/2104 (79%)	0.98	220 (13%) 7 6	19, 56, 102, 139	13 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	VAL	6.1
1	B	407	LEU	5.9
1	B	155	ALA	5.5
1	A	25	PRO	5.4
1	C	185	PRO	5.3
1	A	337	ALA	5.2
1	D	155	ALA	4.8
1	B	366	PRO	4.7
1	C	155	ALA	4.7
1	C	183	LEU	4.5
1	A	156	ASN	4.5
1	A	158	HIS	4.5
1	C	198	ALA	4.5
1	D	361	ARG	4.4
1	A	196	ALA	4.4
1	D	406	ALA	4.4
1	C	180	PRO	4.4
1	D	370	PRO	4.4
1	D	366	PRO	4.3
1	C	158	HIS	4.3
1	A	193	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	4.2
1	C	336	THR	4.2
1	B	156	ASN	4.2
1	A	198	ALA	4.2
1	B	361	ARG	4.2
1	C	157	LEU	4.0
1	A	26	ALA	3.9
1	D	348	VAL	3.8
1	B	184	LEU	3.8
1	A	366	PRO	3.7
1	A	199	LEU	3.6
1	B	364	LEU	3.6
1	C	200	ARG	3.6
1	C	177	GLN	3.6
1	D	154	GLY	3.6
1	B	181	GLN	3.6
1	A	473	GLY	3.6
1	D	157	LEU	3.6
1	A	338	LYS	3.6
1	A	186	ASP	3.5
1	C	367	ARG	3.5
1	A	159	LEU	3.5
1	B	186	ASP	3.4
1	A	372	SER	3.4
1	B	211	LEU	3.4
1	C	178	LEU	3.4
1	C	184	LEU	3.4
1	D	405	MET	3.4
1	B	473	GLY	3.4
1	B	183	LEU	3.4
1	D	183	LEU	3.4
1	C	175	PHE	3.4
1	B	369	ARG	3.4
1	B	371	PRO	3.3
1	B	333	ASP	3.3
1	A	339	VAL	3.3
1	B	331	ASN	3.3
1	C	113	HIS	3.3
1	D	198	ALA	3.3
1	B	373	GLY	3.3
1	C	207[A]	ARG	3.3
1	D	262	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	156	ASN	3.2
1	C	179	HIS	3.2
1	A	181	GLN	3.2
1	C	181	GLN	3.2
1	D	181	GLN	3.2
1	C	199	LEU	3.2
1	D	45	SER	3.2
1	B	415	CYS	3.2
1	B	185	PRO	3.2
1	C	182	LEU	3.2
1	D	48	ASP	3.1
1	B	159	LEU	3.1
1	B	349	ASN	3.1
1	D	46	LEU	3.1
1	D	184	LEU	3.1
1	D	335	LEU	3.1
1	A	194	LYS	3.1
1	C	154	GLY	3.1
1	D	365	ALA	3.1
1	A	262	VAL	3.1
1	D	414	ARG	3.1
1	D	363	LYS	3.0
1	A	157	LEU	3.0
1	C	337	ALA	3.0
1	D	427	GLU	3.0
1	D	47	SER	3.0
1	B	413	ASP	3.0
1	A	177	GLN	3.0
1	C	373	GLY	3.0
1	D	413	ASP	3.0
1	D	332	ARG	2.9
1	D	29	SER	2.9
1	B	187	ASP	2.9
1	B	368	GLU	2.9
1	C	128	GLY	2.9
1	A	368	GLU	2.9
1	C	208	GLU	2.9
1	D	372	SER	2.9
1	C	338	LYS	2.9
1	A	155	ALA	2.9
1	B	46	LEU	2.9
1	D	133	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	48	ASP	2.9
1	D	402	SER	2.8
1	A	178	LEU	2.8
1	D	182	LEU	2.8
1	A	336	THR	2.8
1	B	154	GLY	2.8
1	C	427	GLU	2.8
1	D	195	GLN	2.7
1	B	182	LEU	2.7
1	B	370	PRO	2.7
1	C	246	CYS	2.7
1	D	89	LEU	2.7
1	A	71	SER	2.7
1	C	406	ALA	2.6
1	D	347	LYS	2.6
1	C	131	GLY	2.6
1	B	372	SER	2.6
1	C	474	ASN	2.6
1	D	185	PRO	2.6
1	C	448	LYS	2.6
1	B	406	ALA	2.6
1	A	369	ARG	2.6
1	B	348	VAL	2.6
1	D	180	PRO	2.6
1	B	402	SER	2.6
1	A	335	LEU	2.6
1	C	147	GLU	2.5
1	C	335	LEU	2.5
1	D	371	PRO	2.5
1	D	403	GLU	2.5
1	C	174	LEU	2.5
1	C	328	LEU	2.5
1	D	35	VAL	2.5
1	B	66	TYR	2.5
1	C	425	LEU	2.5
1	B	198	ALA	2.5
1	A	197	GLU	2.5
1	A	370	PRO	2.4
1	B	180	PRO	2.4
1	D	246	CYS	2.4
1	A	182	LEU	2.4
1	B	37	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	334	THR	2.4
1	B	246	CYS	2.4
1	D	415	CYS	2.4
1	D	451	MET	2.4
1	C	171	LEU	2.4
1	D	142	ARG	2.4
1	B	365	ALA	2.4
1	B	158	HIS	2.4
1	D	330	ASP	2.3
1	D	391	ASP	2.3
1	D	473	GLY	2.3
1	A	406	ALA	2.3
1	B	405	MET	2.3
1	C	308	SER	2.3
1	A	28	LYS	2.3
1	B	47	SER	2.3
1	D	369	ARG	2.3
1	C	225	GLN	2.3
1	B	41	ALA	2.3
1	A	45	SER	2.3
1	D	443	GLU	2.3
1	D	174	LEU	2.2
1	A	261	GLY	2.2
1	D	72	GLU	2.2
1	D	205	ALA	2.2
1	A	184	LEU	2.2
1	C	332	ARG	2.2
1	D	79	ASN	2.2
1	A	405	MET	2.2
1	A	57	GLU	2.2
1	A	404	LYS	2.2
1	C	324	ALA	2.2
1	C	151	TYR	2.2
1	B	157	LEU	2.2
1	D	169	ARG	2.2
1	C	176	LYS	2.2
1	D	362	GLY	2.2
1	C	138	ALA	2.2
1	C	169	ARG	2.1
1	D	190	ASP	2.1
1	A	44	PHE	2.1
1	A	180	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	443	GLU	2.1
1	C	133	LEU	2.1
1	A	245	GLU	2.1
1	B	79	ASN	2.1
1	D	197	GLU	2.1
1	A	195	GLN	2.1
1	C	370	PRO	2.1
1	D	268[A]	CYS	2.1
1	B	189	LEU	2.1
1	D	170	LEU	2.1
1	A	445	ASP	2.1
1	B	35	VAL	2.1
1	D	444	VAL	2.1
1	C	423	ARG	2.1
1	C	322	ALA	2.1
1	D	159	LEU	2.1
1	D	364	LEU	2.1
1	B	54	ILE	2.1
1	C	300	ILE	2.1
1	C	414	ARG	2.1
1	D	367	ARG	2.1
1	A	31	SER	2.0
1	B	307	THR	2.0
1	A	329	GLN	2.0
1	D	189	LEU	2.0
1	B	367	ARG	2.0
1	D	105	ARG	2.0
1	D	334	THR	2.0
1	B	196	ALA	2.0
1	C	168	ALA	2.0
1	A	246	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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(Å ²)	Q<0.9
3	CA	C	603	1/1	0.61	0.15	99,99,99,99	0
2	NAG	D	601	14/15	0.75	0.12	80,89,95,96	0
2	NAG	B	601	14/15	0.81	0.13	65,72,80,84	0
3	CA	D	602	1/1	0.81	0.12	93,93,93,93	0
3	CA	A	603	1/1	0.82	0.11	90,90,90,90	0
3	CA	A	602	1/1	0.84	0.08	47,47,47,47	0
3	CA	C	604	1/1	0.84	0.10	60,60,60,60	0
2	NAG	C	601	14/15	0.84	0.14	79,84,89,90	0
3	CA	B	603	1/1	0.85	0.09	43,43,43,43	1
2	NAG	A	601	14/15	0.85	0.12	56,68,78,81	0
3	CA	C	602	1/1	0.88	0.09	71,71,71,71	0
3	CA	D	603	1/1	0.90	0.09	82,82,82,82	0
3	CA	B	602	1/1	0.96	0.08	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.