



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:52 AM UTC

PDB ID : 1N8Z / pdb_00001n8z
Title : Crystal structure of extracellular domain of human HER2 complexed with Herceptin Fab
Authors : Cho, H.-S.; Mason, K.; Ramyar, K.X.; Stanley, A.M.; Gabelli, S.B.; Denney Jr., D.W.; Leahy, D.J.
Deposited on : 2002-11-21
Resolution : 2.52 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

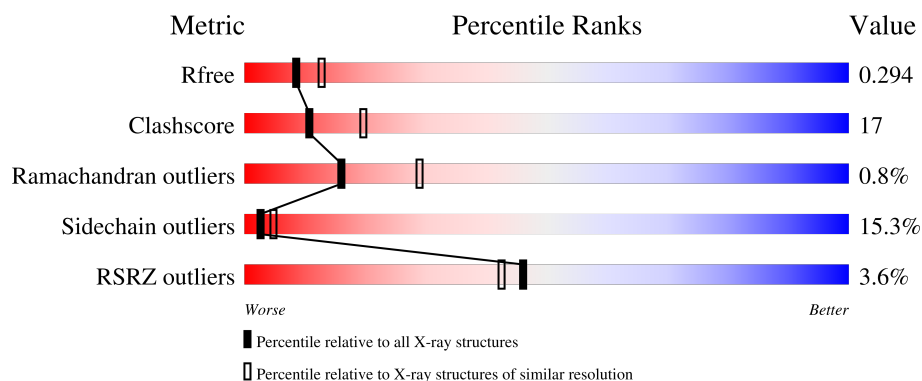
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	214	7% 61% 30% 8%
2	B	220	70% 27%
3	C	607	4% 60% 30% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7890 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 Herceptin Fab (antibody) - light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1645	1029	276	334	6			

- Molecule 2 is a protein called Herceptin Fab (antibody) - heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1642	1036	276	324	6			

- Molecule 3 is a protein called Receptor protein-tyrosine kinase erbB-2.

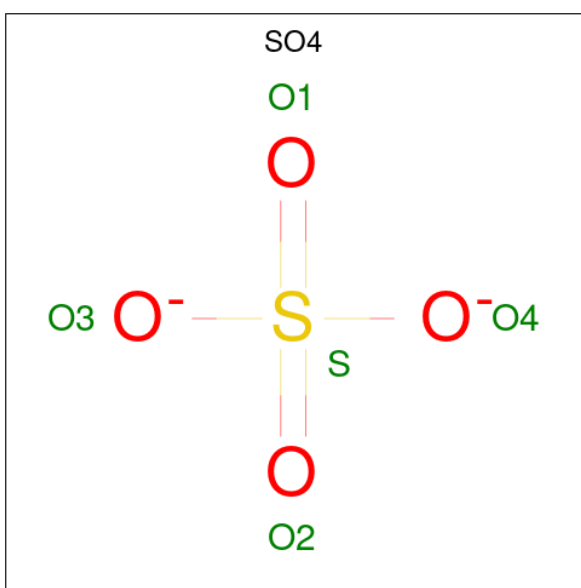
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	581	Total	C	N	O	S	0	0	0
			4491	2796	805	838	52			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		

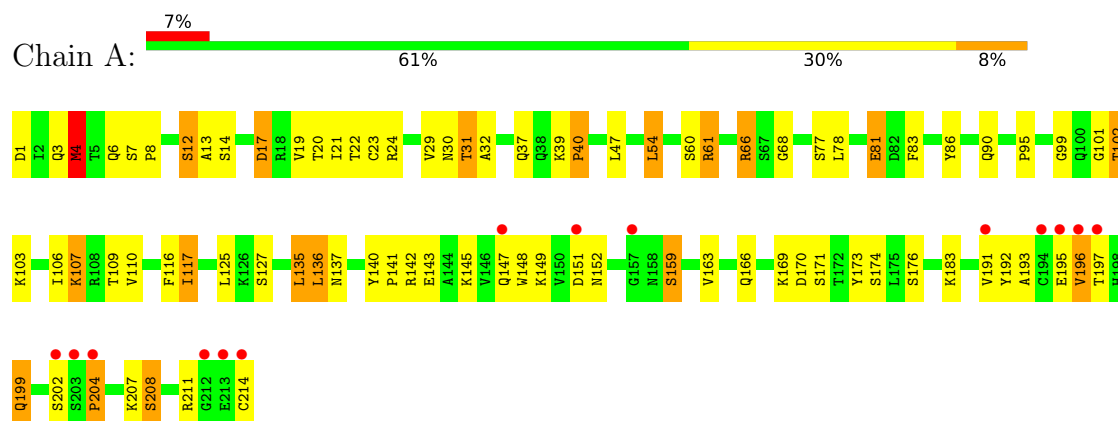
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total 19	O 19	0	0
6	B	13	Total 13	O 13	0	0
6	C	47	Total 47	O 47	0	0

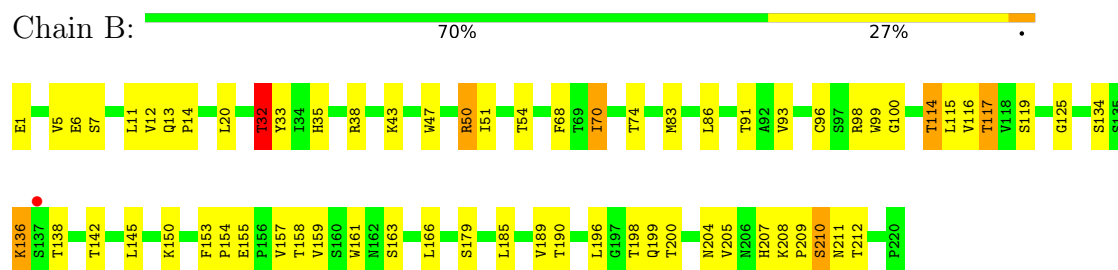
3 Residue-property plots [i](#)

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.

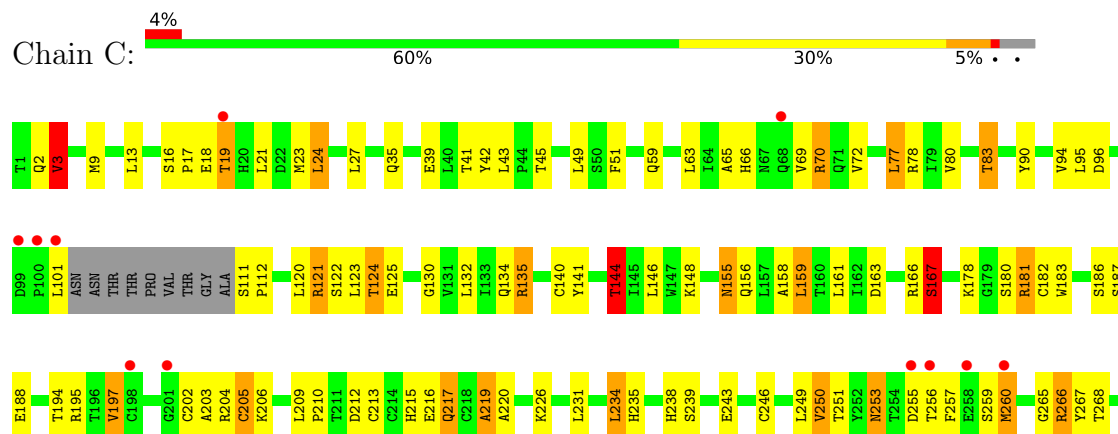
- Molecule 1: Herceptin Fab (antibody) - light chain

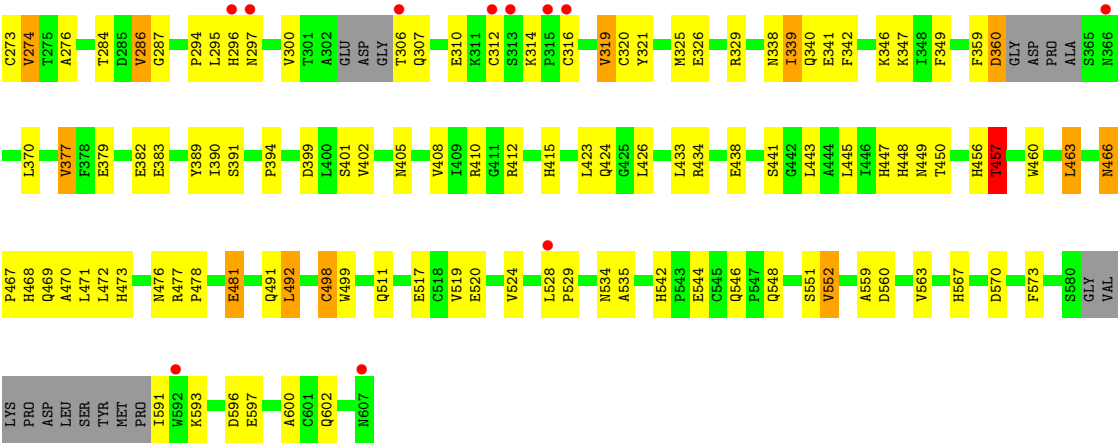


- Molecule 2: Herceptin Fab (antibody) - heavy chain



- Molecule 3: Receptor protein-tyrosine kinase erbB-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.17Å 109.77Å 175.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.52 20.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	92.9 (20.00-2.52) 89.8 (20.00-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.222 , 0.284 (Not available) , 0.294	Depositor DCC
R_{free} test set	1968 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7890	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	2/1682 (0.1%)	1.12	0/2288
2	B	0.90	0/1684	1.09	4/2298 (0.2%)
3	C	0.92	3/4596 (0.1%)	1.19	18/6249 (0.3%)
All	All	0.92	5/7962 (0.1%)	1.16	22/10835 (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
3	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	MET	SD-CE	-7.10	1.61	1.79
3	C	273	CYS	CA-C	-5.66	1.45	1.52
3	C	155	ASN	CA-C	5.56	1.59	1.52
3	C	260	MET	SD-CE	5.41	1.93	1.79
1	A	110	VAL	CA-CB	5.09	1.59	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	VAL	N-CA-C	7.87	119.24	107.75
3	C	457	THR	N-CA-C	-7.67	104.44	113.88
3	C	205	CYS	N-CA-C	7.00	118.40	108.74
2	B	96	CYS	N-CA-C	-6.45	98.47	109.24
3	C	178	LYS	N-CA-C	6.32	118.70	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	457	THR	N-CA-CB	-6.12	102.45	110.59
3	C	219	ALA	CA-C-N	-6.04	112.87	122.29
3	C	219	ALA	C-N-CA	-6.04	112.87	122.29
3	C	144	THR	N-CA-CB	-6.00	102.33	110.67
3	C	181	ARG	N-CA-C	6.00	118.29	108.52
2	B	32	THR	N-CA-C	5.94	116.40	108.38
3	C	412	ARG	N-CA-C	-5.83	106.12	113.18
3	C	573	PHE	N-CA-C	5.72	119.14	109.76
3	C	144	THR	N-CA-C	-5.58	106.83	113.97
2	B	116	VAL	CA-C-N	-5.51	115.02	123.07
2	B	116	VAL	C-N-CA	-5.51	115.02	123.07
3	C	426	LEU	N-CA-C	5.41	120.89	113.97
3	C	377	VAL	CB-CA-C	-5.35	104.24	112.05
3	C	498	CYS	N-CA-C	5.28	116.82	108.96
3	C	319	VAL	N-CA-C	5.13	116.09	108.65
3	C	456	HIS	CA-C-N	5.05	131.04	122.36
3	C	456	HIS	C-N-CA	5.05	131.04	122.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	180	SER	Peptide

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	1645	0	1589	53	0
2	B	1642	0	1584	46	0
3	C	4491	0	4304	160	0
4	C	28	0	26	3	0
5	C	5	0	0	0	0
6	A	19	0	0	1	0
6	B	13	0	0	0	0
6	C	47	0	0	3	0
All	All	7890	0	7503	255	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 17.

All (255) 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)
3:C:457:THR:HG22	3:C:498:CYS:O	1.49	1.10
3:C:266:ARG:HG2	3:C:266:ARG:HH11	1.20	1.03
3:C:124:THR:HG22	3:C:220:ALA:HB1	1.41	1.02
1:A:4:MET:HE2	1:A:23:CYS:SG	2.03	0.99
2:B:207:HIS:CD2	2:B:210:SER:HB2	1.98	0.97
3:C:457:THR:CG2	3:C:498:CYS:O	2.15	0.94
1:A:136:LEU:HD21	1:A:196:VAL:HG11	1.52	0.90
3:C:19:THR:CG2	3:C:472:LEU:HB3	2.03	0.88
3:C:542:HIS:HD2	3:C:544:GLU:H	1.21	0.88
1:A:1:ASP:O	1:A:3:GLN:NE2	2.05	0.88
3:C:284:THR:HG22	3:C:286:VAL:H	1.37	0.87
1:A:8:PRO:O	1:A:102:THR:HB	1.75	0.87
3:C:124:THR:CG2	3:C:220:ALA:O	2.23	0.86
3:C:166:ARG:C	4:C:766:NAG:H83	2.01	0.86
3:C:347:LYS:HE3	3:C:383:GLU:OE1	1.76	0.86
2:B:142:THR:CG2	2:B:190:THR:HG22	2.06	0.85
3:C:144:THR:HG23	3:C:181:ARG:HA	1.58	0.85
3:C:144:THR:CG2	3:C:182:CYS:H	1.90	0.84
3:C:466:ASN:HD22	3:C:468:HIS:H	1.27	0.82
2:B:163:SER:H	2:B:204:ASN:HD21	1.28	0.82
3:C:596:ASP:HB2	3:C:600:ALA:O	1.79	0.82
3:C:96:ASP:OD1	3:C:135:ARG:HD2	1.80	0.81
1:A:12:SER:HB3	1:A:107:LYS:HE3	1.61	0.81
3:C:443:LEU:HD21	3:C:469:GLN:HA	1.64	0.79
3:C:70:ARG:HG3	3:C:70:ARG:HH11	1.47	0.79
3:C:319:VAL:CG1	3:C:320:CYS:N	2.47	0.78
3:C:319:VAL:HG11	3:C:349:PHE:CD1	2.18	0.78
3:C:338:ASN:O	3:C:341:GLU:HB2	1.82	0.78
3:C:19:THR:HG22	3:C:472:LEU:HB3	1.66	0.77
3:C:266:ARG:HH11	3:C:266:ARG:CG	1.97	0.75
3:C:124:THR:HG21	3:C:220:ALA:O	1.85	0.75
3:C:319:VAL:HG12	3:C:320:CYS:N	2.01	0.75
2:B:142:THR:HG23	2:B:190:THR:HG22	1.67	0.75
3:C:141:TYR:O	3:C:144:THR:HB	1.85	0.74
3:C:546:GLN:HE21	3:C:548:GLN:HE22	1.35	0.73
3:C:284:THR:HG22	3:C:286:VAL:N	2.05	0.72
2:B:51:ILE:HB	2:B:70:ILE:CG2	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:447:HIS:HD2	3:C:448:HIS:CD2	2.09	0.71
2:B:207:HIS:HD2	2:B:210:SER:HB2	1.54	0.70
2:B:142:THR:CG2	2:B:190:THR:CG2	2.71	0.69
3:C:294:PRO:O	3:C:297:ASN:HB2	1.93	0.69
3:C:408:VAL:HG12	3:C:438:GLU:HB3	1.75	0.69
3:C:449:ASN:H	3:C:476:ASN:HD22	1.41	0.68
1:A:21:ILE:HG23	1:A:102:THR:HG21	1.75	0.68
2:B:51:ILE:HB	2:B:70:ILE:HG23	1.76	0.67
3:C:443:LEU:HD22	3:C:470:ALA:H	1.58	0.67
3:C:424:GLN:HB3	3:C:447:HIS:CE1	2.30	0.67
3:C:542:HIS:CD2	3:C:544:GLU:H	2.09	0.66
1:A:136:LEU:CD2	1:A:196:VAL:HG11	2.25	0.66
3:C:59:GLN:O	3:C:83:THR:HB	1.96	0.66
3:C:217:GLN:HE22	3:C:235:HIS:HD2	1.44	0.64
1:A:14:SER:O	1:A:17:ASP:HB2	1.98	0.63
3:C:399:ASP:OD2	3:C:401:SER:HB3	1.98	0.63
3:C:443:LEU:CD2	3:C:469:GLN:HA	2.28	0.63
3:C:246:CYS:SG	3:C:268:THR:HG22	2.39	0.62
1:A:6:GLN:OE1	1:A:102:THR:HG22	2.00	0.62
2:B:159:VAL:HG22	2:B:205:VAL:HG22	1.81	0.62
2:B:32:THR:HG22	2:B:33:TYR:H	1.65	0.61
2:B:99:TRP:O	2:B:100:GLY:C	2.42	0.61
3:C:41:THR:HA	3:C:65:ALA:O	2.01	0.61
3:C:319:VAL:CG1	3:C:320:CYS:H	2.14	0.61
3:C:447:HIS:CD2	3:C:448:HIS:HD2	2.20	0.60
1:A:117:ILE:HG22	2:B:136:LYS:HB3	1.83	0.59
2:B:207:HIS:CD2	2:B:210:SER:CB	2.82	0.59
3:C:319:VAL:CG1	3:C:349:PHE:CD1	2.85	0.59
1:A:30:ASN:ND2	1:A:31:THR:HB	2.17	0.59
1:A:166:GLN:HE21	1:A:171:SER:HB3	1.66	0.58
3:C:319:VAL:HG13	3:C:320:CYS:H	1.68	0.58
3:C:542:HIS:CE1	3:C:559:ALA:HB2	2.38	0.58
3:C:389:TYR:CE1	3:C:415:HIS:CE1	2.91	0.58
3:C:443:LEU:CD2	3:C:470:ALA:H	2.16	0.58
3:C:360:ASP:N	3:C:360:ASP:OD1	2.35	0.58
1:A:116:PHE:HD2	1:A:135:LEU:HD23	1.67	0.58
3:C:542:HIS:HD2	3:C:544:GLU:N	1.99	0.58
3:C:447:HIS:CD2	3:C:448:HIS:CD2	2.92	0.58
3:C:326:GLU:O	3:C:329:ARG:HG2	2.04	0.57
3:C:144:THR:HG21	3:C:182:CYS:H	1.68	0.57
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:ASN:ND2	3:C:256:THR:H	2.03	0.57
1:A:21:ILE:CG2	1:A:102:THR:HG21	2.34	0.57
3:C:9:MET:HG2	3:C:39:GLU:OE1	2.05	0.57
2:B:98:ARG:NE	2:B:100:GLY:HA3	2.20	0.56
3:C:544:GLU:OE1	3:C:567:HIS:HD2	1.87	0.56
1:A:197:THR:HG23	1:A:204:PRO:HG3	1.87	0.56
1:A:116:PHE:CD2	1:A:135:LEU:HD23	2.41	0.56
1:A:4:MET:HE3	1:A:4:MET:HA	1.87	0.56
1:A:12:SER:HB3	1:A:107:LYS:CE	2.34	0.56
3:C:19:THR:HG21	3:C:445:LEU:CD1	2.36	0.56
3:C:478:PRO:O	3:C:481:GLU:HB2	2.06	0.56
3:C:447:HIS:HD2	3:C:448:HIS:HD2	1.49	0.55
3:C:528:LEU:HB2	3:C:529:PRO:HD3	1.89	0.55
1:A:95:PRO:HB3	2:B:47:TRP:CZ3	2.42	0.55
1:A:136:LEU:HD12	1:A:136:LEU:N	2.22	0.55
3:C:274:VAL:HG13	3:C:276:ALA:O	2.06	0.55
3:C:210:PRO:O	3:C:213:CYS:HB2	2.07	0.54
2:B:207:HIS:HD2	2:B:210:SER:CB	2.19	0.54
2:B:12:VAL:HG12	2:B:13:GLN:O	2.08	0.54
1:A:148:TRP:CD1	1:A:159:SER:HG	2.26	0.54
1:A:192:TYR:O	1:A:208:SER:HA	2.08	0.54
3:C:391:SER:HB2	6:C:1031:HOH:O	2.07	0.54
2:B:33:TYR:CD2	2:B:50:ARG:HD2	2.43	0.54
3:C:253:ASN:HD22	3:C:255:ASP:H	1.56	0.54
1:A:6:GLN:HE21	1:A:99:GLY:HA3	1.73	0.53
3:C:434:ARG:HA	3:C:499:TRP:CD1	2.43	0.53
3:C:96:ASP:CG	3:C:135:ARG:HD2	2.33	0.53
3:C:408:VAL:HG23	3:C:408:VAL:O	2.09	0.53
2:B:11:LEU:HD11	2:B:153:PHE:HE1	1.75	0.52
3:C:215:HIS:HD2	3:C:217:GLN:H	1.58	0.52
3:C:266:ARG:HG2	3:C:266:ARG:NH1	2.00	0.52
3:C:319:VAL:HG11	3:C:349:PHE:CE1	2.44	0.52
3:C:125:GLU:OE1	3:C:219:ALA:O	2.26	0.52
3:C:466:ASN:ND2	3:C:468:HIS:H	2.03	0.52
1:A:19:VAL:HG21	1:A:78:LEU:HD13	1.92	0.52
1:A:22:THR:HG22	1:A:23:CYS:N	2.24	0.52
3:C:156:GLN:C	3:C:158:ALA:H	2.15	0.52
2:B:142:THR:HG21	2:B:190:THR:CG2	2.40	0.51
2:B:210:SER:HB3	2:B:212:THR:OG1	2.09	0.51
1:A:193:ALA:HA	1:A:208:SER:HB2	1.93	0.51
3:C:135:ARG:HH11	3:C:135:ARG:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:MET:SD	1:A:90:GLN:HB3	2.51	0.51
3:C:19:THR:HG22	3:C:472:LEU:HD13	1.92	0.51
3:C:321:TYR:CE2	3:C:326:GLU:HG3	2.44	0.51
1:A:13:ALA:HB3	1:A:78:LEU:HD22	1.92	0.51
3:C:49:LEU:HD13	3:C:72:VAL:HG12	1.93	0.51
3:C:194:THR:HG23	3:C:205:CYS:O	2.10	0.51
2:B:98:ARG:CZ	2:B:100:GLY:HA3	2.41	0.50
3:C:24:LEU:CD2	3:C:43:LEU:HD21	2.42	0.50
3:C:209:LEU:O	3:C:212:ASP:HB2	2.12	0.50
1:A:86:TYR:O	1:A:101:GLY:HA2	2.12	0.50
3:C:249:LEU:HD11	3:C:267:TYR:CE2	2.46	0.50
1:A:83:PHE:CE1	1:A:166:GLN:HB3	2.46	0.50
1:A:125:LEU:O	1:A:183:LYS:HD2	2.11	0.50
3:C:286:VAL:HG13	3:C:286:VAL:O	2.12	0.50
3:C:466:ASN:HD22	3:C:468:HIS:N	2.05	0.50
3:C:266:ARG:CG	3:C:266:ARG:NH1	2.63	0.49
2:B:33:TYR:HD2	2:B:50:ARG:HD2	1.77	0.49
3:C:253:ASN:ND2	3:C:255:ASP:H	2.11	0.49
1:A:30:ASN:HD21	3:C:602:GLN:HE22	1.60	0.49
3:C:195:ARG:HG3	3:C:203:ALA:O	2.12	0.49
3:C:267:TYR:HA	3:C:287:GLY:O	2.13	0.49
3:C:24:LEU:HD23	3:C:43:LEU:HD21	1.93	0.49
3:C:466:ASN:ND2	3:C:468:HIS:HB2	2.27	0.49
2:B:91:THR:HG23	2:B:117:THR:HA	1.95	0.48
3:C:130:GLY:HA3	3:C:159:LEU:O	2.14	0.48
1:A:39:LYS:NZ	1:A:81:GLU:O	2.35	0.48
2:B:98:ARG:NE	2:B:100:GLY:CA	2.76	0.48
3:C:94:VAL:O	3:C:95:LEU:HD23	2.13	0.48
2:B:134:SER:O	2:B:138:THR:HG23	2.13	0.48
3:C:466:ASN:HD21	3:C:468:HIS:HB2	1.79	0.47
3:C:560:ASP:OD1	3:C:560:ASP:C	2.56	0.47
1:A:30:ASN:HD22	1:A:31:THR:HB	1.79	0.47
1:A:140:TYR:CG	1:A:141:PRO:HA	2.49	0.47
3:C:42:TYR:HA	3:C:66:HIS:O	2.15	0.47
3:C:70:ARG:HG3	3:C:70:ARG:NH1	2.21	0.47
3:C:600:ALA:O	3:C:602:GLN:NE2	2.47	0.47
1:A:61:ARG:HB3	6:A:228:HOH:O	2.15	0.47
2:B:154:PRO:O	2:B:207:HIS:HE1	1.98	0.47
3:C:382:GLU:HA	3:C:405:ASN:O	2.15	0.47
3:C:460:TRP:CE3	3:C:463:LEU:HD23	2.50	0.47
3:C:473:HIS:O	3:C:473:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:HIS:HD2	3:C:243:GLU:OE2	1.98	0.47
1:A:4:MET:CE	1:A:23:CYS:SG	2.92	0.46
3:C:424:GLN:HA	3:C:447:HIS:O	2.15	0.46
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.98	0.46
3:C:253:ASN:HB3	3:C:257:PHE:H	1.80	0.46
3:C:524:VAL:HG13	3:C:552:VAL:HG22	1.96	0.46
3:C:466:ASN:HB2	3:C:467:PRO:HD2	1.96	0.46
1:A:61:ARG:NH2	1:A:81:GLU:OE1	2.49	0.46
3:C:215:HIS:HD2	3:C:217:GLN:HB2	1.81	0.46
1:A:199:GLN:H	1:A:199:GLN:HG2	1.34	0.46
1:A:208:SER:O	2:B:136:LYS:HD2	2.15	0.46
2:B:51:ILE:HB	2:B:70:ILE:HG21	1.97	0.46
3:C:90:TYR:CD2	3:C:132:LEU:HB2	2.51	0.46
3:C:250:VAL:HG21	3:C:259:SER:HB3	1.98	0.46
2:B:14:PRO:HD3	2:B:119:SER:C	2.41	0.46
3:C:219:ALA:HB2	3:C:234:LEU:HA	1.97	0.45
3:C:78:ARG:HD3	3:C:231:LEU:HB3	1.98	0.45
3:C:511:GLN:HB2	3:C:519:VAL:O	2.16	0.45
3:C:155:ASN:O	3:C:158:ALA:HB2	2.16	0.45
3:C:265:GLY:O	3:C:266:ARG:HG2	2.16	0.45
1:A:170:ASP:OD1	1:A:170:ASP:C	2.59	0.45
2:B:115:LEU:CD2	2:B:155:GLU:HB3	2.47	0.45
3:C:491:GLN:OE1	3:C:491:GLN:HA	2.17	0.45
3:C:124:THR:CG2	3:C:220:ALA:HB1	2.30	0.45
3:C:197:VAL:HG13	3:C:197:VAL:O	2.17	0.45
2:B:98:ARG:NH2	2:B:100:GLY:HA3	2.32	0.45
3:C:186:SER:C	3:C:188:GLU:N	2.74	0.45
3:C:359:PHE:CZ	3:C:394:PRO:HD3	2.51	0.45
2:B:20:LEU:HG	2:B:83:MET:HE2	1.99	0.44
1:A:54:LEU:HD11	1:A:60:SER:HA	1.99	0.44
3:C:156:GLN:C	3:C:158:ALA:N	2.76	0.44
3:C:424:GLN:CB	3:C:447:HIS:CE1	3.00	0.44
1:A:29:VAL:O	1:A:29:VAL:CG1	2.65	0.44
3:C:167:SER:N	4:C:766:NAG:H83	2.31	0.44
2:B:68:PHE:CD1	2:B:68:PHE:N	2.85	0.44
3:C:249:LEU:HD11	3:C:267:TYR:CZ	2.52	0.44
2:B:6:GLU:HB3	2:B:114:THR:OG1	2.18	0.44
3:C:238:HIS:CD2	3:C:243:GLU:OE2	2.71	0.44
3:C:94:VAL:C	3:C:95:LEU:HD23	2.43	0.44
3:C:3:VAL:HG11	3:C:35:GLN:HE21	1.83	0.43
3:C:70:ARG:HG3	6:C:1019:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:ARG:O	4:C:766:NAG:H83	2.17	0.43
2:B:13:GLN:HG3	2:B:14:PRO:HD2	2.00	0.43
2:B:12:VAL:HG11	2:B:86:LEU:HD12	2.00	0.43
3:C:186:SER:C	3:C:188:GLU:H	2.26	0.43
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.65	0.43
3:C:96:ASP:HA	3:C:135:ARG:O	2.18	0.43
3:C:215:HIS:CD2	3:C:217:GLN:HB2	2.54	0.43
2:B:161:TRP:HB3	2:B:166:LEU:HD23	1.99	0.43
3:C:140:CYS:O	3:C:141:TYR:HB2	2.19	0.43
3:C:274:VAL:CG1	3:C:276:ALA:O	2.66	0.43
3:C:520:GLU:HB3	6:C:1047:HOH:O	2.19	0.43
3:C:256:THR:O	3:C:257:PHE:HB2	2.18	0.43
3:C:339:ILE:HG23	3:C:340:GLN:HG2	2.00	0.42
3:C:534:ASN:O	3:C:535:ALA:C	2.61	0.42
3:C:121:ARG:HA	3:C:183:TRP:CD1	2.53	0.42
3:C:340:GLN:C	3:C:342:PHE:H	2.27	0.42
3:C:390:ILE:HB	3:C:423:LEU:HD23	2.01	0.42
1:A:142:ARG:HB2	1:A:173:TYR:CE2	2.55	0.42
3:C:383:GLU:HG3	3:C:408:VAL:HG23	2.01	0.42
2:B:83:MET:HE3	2:B:83:MET:HB2	1.76	0.42
2:B:145:LEU:HD12	2:B:189:VAL:HG12	2.02	0.42
1:A:66:ARG:HD2	1:A:68:GLY:O	2.20	0.42
2:B:207:HIS:CE1	2:B:209:PRO:HG2	2.54	0.42
3:C:450:THR:O	3:C:477:ARG:HG3	2.20	0.42
3:C:528:LEU:CB	3:C:529:PRO:HD3	2.50	0.42
1:A:81:GLU:H	1:A:81:GLU:HG3	1.58	0.41
1:A:7:SER:HB2	1:A:8:PRO:HA	2.01	0.41
3:C:78:ARG:CZ	3:C:122:SER:HB3	2.50	0.41
3:C:492:LEU:HD11	3:C:520:GLU:OE1	2.21	0.41
1:A:39:LYS:O	1:A:40:PRO:C	2.62	0.41
3:C:16:SER:HA	3:C:17:PRO:HD3	1.73	0.41
2:B:125:GLY:CA	2:B:210:SER:OG	2.68	0.41
3:C:134:GLN:HA	3:C:163:ASP:HB3	2.02	0.41
3:C:77:LEU:HD13	3:C:123:LEU:HD13	2.02	0.41
3:C:135:ARG:CG	3:C:135:ARG:NH1	2.83	0.41
3:C:286:VAL:O	3:C:286:VAL:CG1	2.69	0.41
3:C:524:VAL:CG1	3:C:552:VAL:HG22	2.51	0.41
3:C:16:SER:OG	3:C:19:THR:OG1	2.36	0.41
3:C:155:ASN:O	3:C:158:ALA:CB	2.69	0.41
2:B:33:TYR:HB3	2:B:50:ARG:HD2	2.02	0.41
3:C:120:LEU:HB2	3:C:183:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLN:NE2	1:A:101:GLY:H	2.18	0.41
1:A:107:LYS:HA	1:A:140:TYR:OH	2.20	0.41
3:C:203:ALA:C	3:C:204:ARG:HG2	2.46	0.41
3:C:433:LEU:HB2	3:C:499:TRP:CZ3	2.56	0.41
1:A:29:VAL:O	1:A:29:VAL:HG12	2.19	0.41
2:B:35:HIS:CE1	2:B:50:ARG:HD3	2.55	0.41
2:B:38:ARG:HA	2:B:93:VAL:O	2.21	0.40
3:C:477:ARG:HA	3:C:478:PRO:HD3	1.95	0.40
3:C:570:ASP:OD2	3:C:593:LYS:NZ	2.35	0.40
3:C:111:SER:HA	3:C:112:PRO:HA	1.86	0.40
3:C:410:ARG:NH1	3:C:410:ARG:HG2	2.36	0.40
3:C:23:MET:HG2	3:C:443:LEU:HD12	2.02	0.40
3:C:231:LEU:HD23	3:C:231:LEU:HA	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	190 (90%)	17 (8%)	5 (2%)	4	7
2	B	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
3	C	571/607 (94%)	518 (91%)	50 (9%)	3 (0%)	24	41
All	All	1001/1041 (96%)	918 (92%)	75 (8%)	8 (1%)	16	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASP
3	C	167	SER
1	A	32	ALA
1	A	152	ASN

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Mol	Chain	Res	Type
3	C	51	PHE
3	C	187	SER
1	A	40	PRO
1	A	204	PRO

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	188/189 (100%)	149 (79%)	39 (21%)	1	2
2	B	179/181 (99%)	155 (87%)	24 (13%)	4	7
3	C	503/523 (96%)	433 (86%)	70 (14%)	3	6
All	All	870/893 (97%)	737 (85%)	133 (15%)	3	5

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	12	SER
1	A	17	ASP
1	A	20	THR
1	A	24	ARG
1	A	31	THR
1	A	54	LEU
1	A	61	ARG
1	A	66	ARG
1	A	77	SER
1	A	81	GLU
1	A	102	THR
1	A	103	LYS
1	A	106	ILE
1	A	107	LYS
1	A	109	THR
1	A	117	ILE
1	A	127	SER

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Mol	Chain	Res	Type
1	A	135	LEU
1	A	136	LEU
1	A	137	ASN
1	A	143	GLU
1	A	145	LYS
1	A	147	GLN
1	A	149	LYS
1	A	159	SER
1	A	163	VAL
1	A	169	LYS
1	A	174	SER
1	A	176	SER
1	A	191	VAL
1	A	195	GLU
1	A	196	VAL
1	A	199	GLN
1	A	202	SER
1	A	207	LYS
1	A	208	SER
1	A	211	ARG
1	A	214	CYS
2	B	1	GLU
2	B	5	VAL
2	B	7	SER
2	B	32	THR
2	B	43	LYS
2	B	50	ARG
2	B	54	THR
2	B	70	ILE
2	B	74	THR
2	B	114	THR
2	B	117	THR
2	B	136	LYS
2	B	150	LYS
2	B	157	VAL
2	B	158	THR
2	B	179	SER
2	B	185	LEU
2	B	196	LEU
2	B	198	THR
2	B	199	GLN
2	B	200	THR

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Mol	Chain	Res	Type
2	B	208	LYS
2	B	210	SER
2	B	211	ASN
3	C	2	GLN
3	C	3	VAL
3	C	13	LEU
3	C	18	GLU
3	C	19	THR
3	C	21	LEU
3	C	24	LEU
3	C	27	LEU
3	C	45	THR
3	C	63	LEU
3	C	69	VAL
3	C	70	ARG
3	C	77	LEU
3	C	80	VAL
3	C	83	THR
3	C	101	LEU
3	C	121	ARG
3	C	124	THR
3	C	135	ARG
3	C	144	THR
3	C	146	LEU
3	C	148	LYS
3	C	159	LEU
3	C	161	LEU
3	C	167	SER
3	C	197	VAL
3	C	202	CYS
3	C	206	LYS
3	C	216	GLU
3	C	217	GLN
3	C	226	LYS
3	C	234	LEU
3	C	239	SER
3	C	250	VAL
3	C	251	THR
3	C	253	ASN
3	C	260	MET
3	C	266	ARG
3	C	274	VAL

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Mol	Chain	Res	Type
3	C	286	VAL
3	C	295	LEU
3	C	296	HIS
3	C	300	VAL
3	C	306	THR
3	C	307	GLN
3	C	310	GLU
3	C	312	CYS
3	C	314	LYS
3	C	316	CYS
3	C	325	MET
3	C	339	ILE
3	C	346	LYS
3	C	360	ASP
3	C	370	LEU
3	C	377	VAL
3	C	379	GLU
3	C	402	VAL
3	C	441	SER
3	C	457	THR
3	C	463	LEU
3	C	466	ASN
3	C	471	LEU
3	C	481	GLU
3	C	492	LEU
3	C	517	GLU
3	C	551	SER
3	C	552	VAL
3	C	563	VAL
3	C	591	ILE
3	C	597	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	30	ASN
1	A	89	GLN
1	A	91	HIS
1	A	137	ASN
1	A	138	ASN
1	A	189	HIS

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Mol	Chain	Res	Type
2	B	204	ASN
2	B	206	ASN
2	B	207	HIS
2	B	211	ASN
3	C	2	GLN
3	C	26	HIS
3	C	35	GLN
3	C	66	HIS
3	C	68	GLN
3	C	119	GLN
3	C	138	GLN
3	C	215	HIS
3	C	217	GLN
3	C	235	HIS
3	C	238	HIS
3	C	245	HIS
3	C	253	ASN
3	C	296	HIS
3	C	297	ASN
3	C	307	GLN
3	C	415	HIS
3	C	424	GLN
3	C	447	HIS
3	C	448	HIS
3	C	456	HIS
3	C	466	ASN
3	C	476	ASN
3	C	526	GLN
3	C	542	HIS
3	C	546	GLN
3	C	567	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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
5	SO4	C	1001	-	4,4,4	0.21	0	6,6,6	0.71	0
4	NAG	C	766	3	14,14,15	0.84	0	17,19,21	1.97	6 (35%)
4	NAG	C	738	3	14,14,15	0.50	0	17,19,21	1.25	2 (11%)

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
4	NAG	C	766	3	-	4/6/23/26	0/1/1/1
4	NAG	C	738	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	766	NAG	O5-C5-C6	3.27	114.03	107.66
4	C	738	NAG	C3-C4-C5	3.09	115.84	110.23
4	C	766	NAG	C2-N2-C7	-3.07	118.78	122.90
4	C	766	NAG	O3-C3-C4	3.06	117.60	110.38
4	C	766	NAG	C1-O5-C5	-2.86	108.35	112.19
4	C	766	NAG	C6-C5-C4	2.72	119.69	113.02
4	C	738	NAG	C4-C3-C2	2.67	114.92	111.02
4	C	766	NAG	C3-C4-C5	-2.17	106.30	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	766	NAG	C8-C7-N2-C2
4	C	766	NAG	O7-C7-N2-C2
4	C	766	NAG	C4-C5-C6-O6
4	C	766	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	766	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	0.40	14 (6%) 25 22	7, 16, 24, 33	0
2	B	220/220 (100%)	0.05	1 (0%) 87 85	8, 16, 24, 35	0
3	C	581/607 (95%)	0.14	22 (3%) 44 40	2, 16, 25, 38	0
All	All	1015/1041 (97%)	0.18	37 (3%) 46 42	2, 16, 24, 38	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	201	GLY	4.1
1	A	151	ASP	4.0
3	C	315	PRO	3.7
3	C	100	PRO	3.6
3	C	19	THR	3.2
3	C	316	CYS	3.1
1	A	204	PRO	3.0
2	B	137	SER	2.9
1	A	212	GLY	2.9
3	C	297	ASN	2.9
3	C	528	LEU	2.9
3	C	592	TRP	2.8
3	C	296	HIS	2.7
1	A	202	SER	2.7
3	C	258	GLU	2.6
3	C	313	SER	2.6
1	A	197	THR	2.6
3	C	101	LEU	2.5
1	A	214	CYS	2.5
1	A	157	GLY	2.5
1	A	203	SER	2.5
3	C	312	CYS	2.3
1	A	194	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	366	ASN	2.3
3	C	306	THR	2.3
1	A	147	GLN	2.3
3	C	68	GLN	2.3
1	A	191	VAL	2.2
3	C	607	ASN	2.2
1	A	195	GLU	2.2
3	C	198	CYS	2.2
1	A	196	VAL	2.1
3	C	260	MET	2.1
3	C	256	THR	2.1
1	A	213	GLU	2.0
3	C	99	ASP	2.0
3	C	255	ASP	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(Å ²)	Q<0.9
4	NAG	C	766	14/15	0.75	0.19	48,55,58,59	0
5	SO4	C	1001	5/5	0.85	0.16	59,60,61,62	0
4	NAG	C	738	14/15	0.91	0.12	33,43,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.