



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 10:19 PM EDT

PDB ID : 2AJ8
Title : Porcine dipeptidyl peptidase IV (CD26) in complex with 7-Benzyl-1,3-dimethyl-8-piperazin-1-yl-3,7-dihydro-purine-2,6-dione (BDPX)
Authors : Engel, M.; Hoffmann, T.; Manhart, S.; Heiser, U.; Chambre, S.; Huber, R.; Demuth, H.U.; Bode, W.
Deposited on : unknown
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

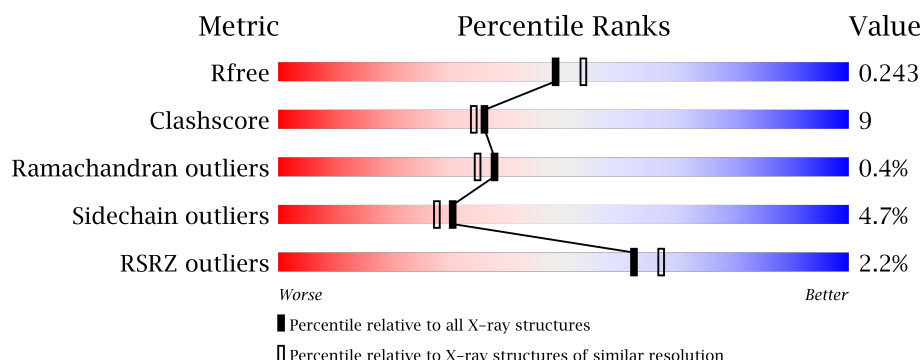
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div></div> </div> <div></div> </div>
1	B	728	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div></div> </div> <div></div> </div>
1	C	728	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div></div> </div> <div></div> </div>
1	D	728	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div></div> </div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	772(A)	-	-	-	X
4	SC3	D	1606	-	-	-	X

2 Entry composition [i](#)

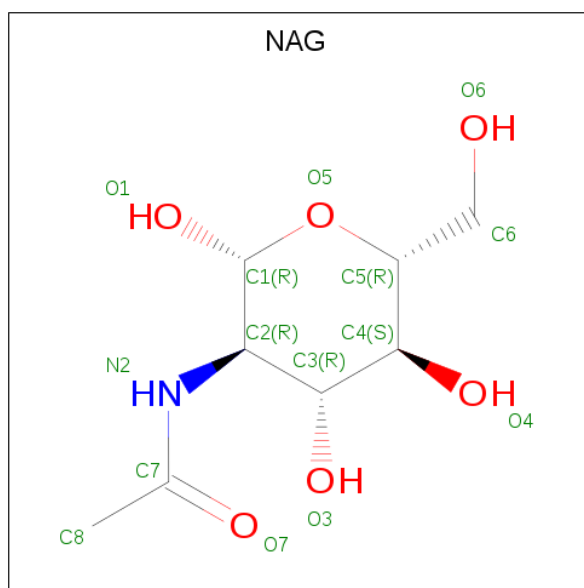
There are 6 unique types of molecules in this entry. The entry contains 26222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	38	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	46	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

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



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

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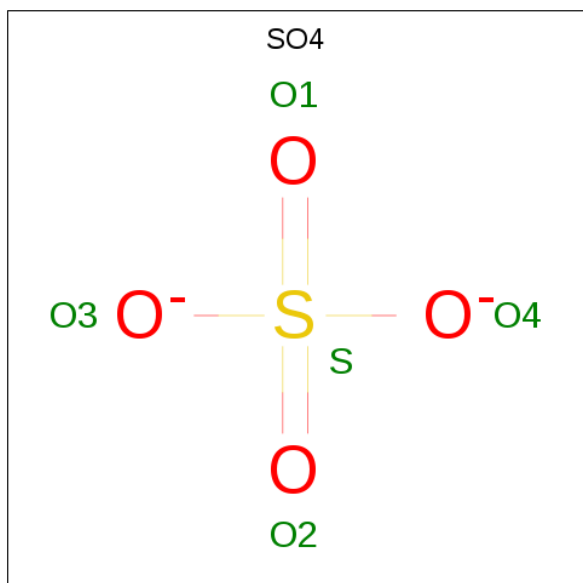
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	3	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



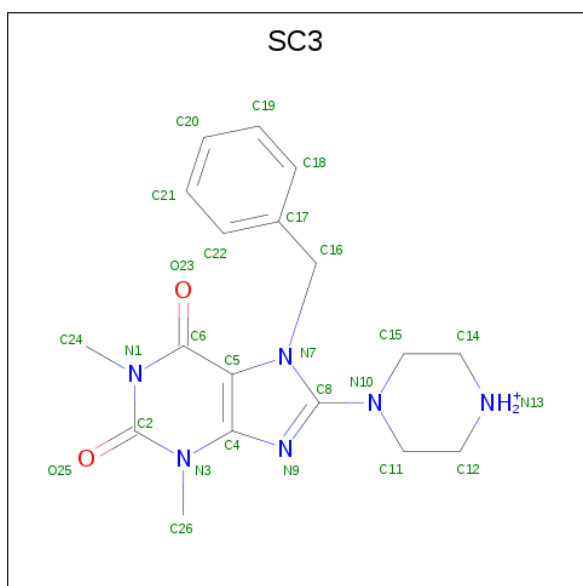
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		

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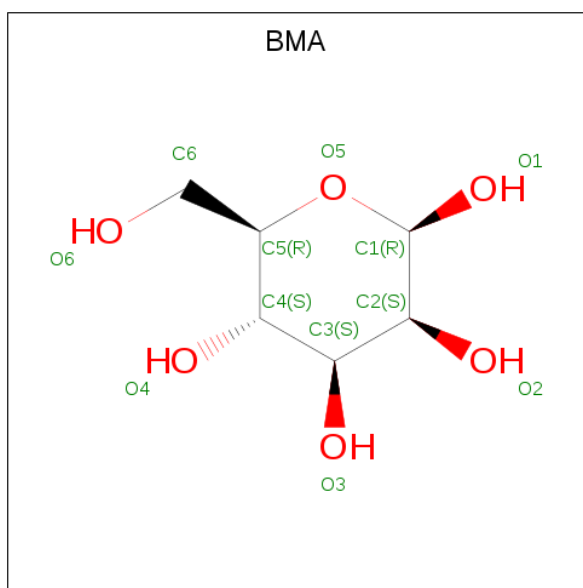
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 7-BENZYL-1,3-DIMETHYL-8-PIPERAZIN-1-YL-3,7-DIHYDRO-PURINE-2,6-DIONE (three-letter code: SC3) (formula: $C_{18}H_{23}N_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	18	6	2		
4	A	1	Total	C	N	O	0	0
			26	18	6	2		
4	B	1	Total	C	N	O	0	0
			26	18	6	2		
4	B	1	Total	C	N	O	0	0
			26	18	6	2		
4	C	1	Total	C	N	O	0	0
			26	18	6	2		
4	C	1	Total	C	N	O	0	0
			26	18	6	2		
4	D	1	Total	C	N	O	0	0
			26	18	6	2		
4	D	1	Total	C	N	O	0	0
			26	18	6	2		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	394	Total	O	0	0
			394	394		
6	B	481	Total	O	0	0
			481	481		
6	C	395	Total	O	0	0
			395	395		
6	D	376	Total	O	0	0
			376	376		

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

Chain A:

2% 77% 21%

S39 T143 E145 P149 M150 N151 T152 Q153 S158 P159 Y160 G161 M168 N169 N170 K175 P178 N179 Q183 T199 E205 E206 W216 N219 A224 F228 P234 E237 L246 Q247 Y248 N119 R125 S131 T134 Y135 N138 K139 R140 L142

Y299 E308 E309 R310 W315 Q320 I327 E332 S333 T334 G335 R336 T346 E347 I348 S349 S370 N377 E378 E379 F387 Q388 T389 D390 K391 S392 N393 T397 T398 K399 E403 E408 L415 K423 R433 L436 N437 D438 Y439 T440 T443 S448

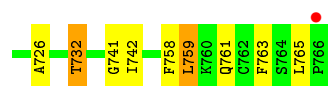
S458 S462 K466 Y467 R471 C472 F473 G474 P475 G476 L477 P478 T481 L482 H483 S486 S487 D488 K489 E490 L491 R492 K502 M503 L504 Q505 D506 V507 Q508 M509 D515 V516 F517 N518 L519 H520 G521 T522 K523 F524 M525 Y526 Q527 P531 D538 Y539 T540 P541 L542 L543

Y547 S552 Q553 K554 V555 L561 Y566 N572 Y585 E608 A654 P655 K658 M659 E660 Y661 V665 R669 E677 D681 R684 E693 K696 L701 H704 V711 S716 M717 Q718 K721 A726 G727 V728 N733 G741 T742

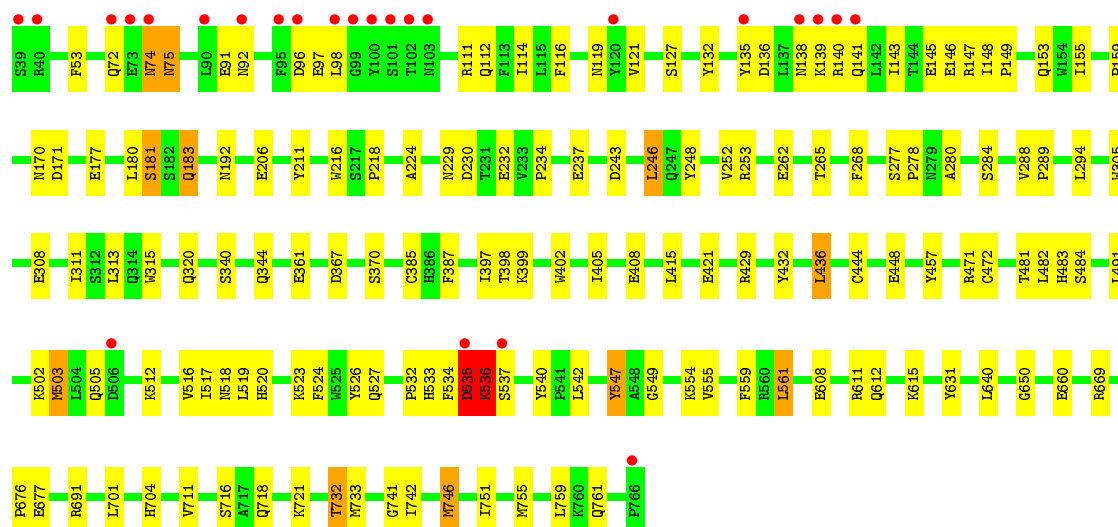
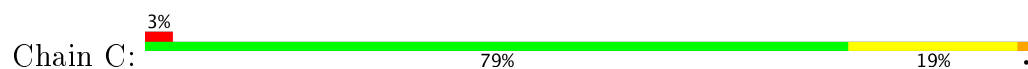
Q761 P766

Chain B:

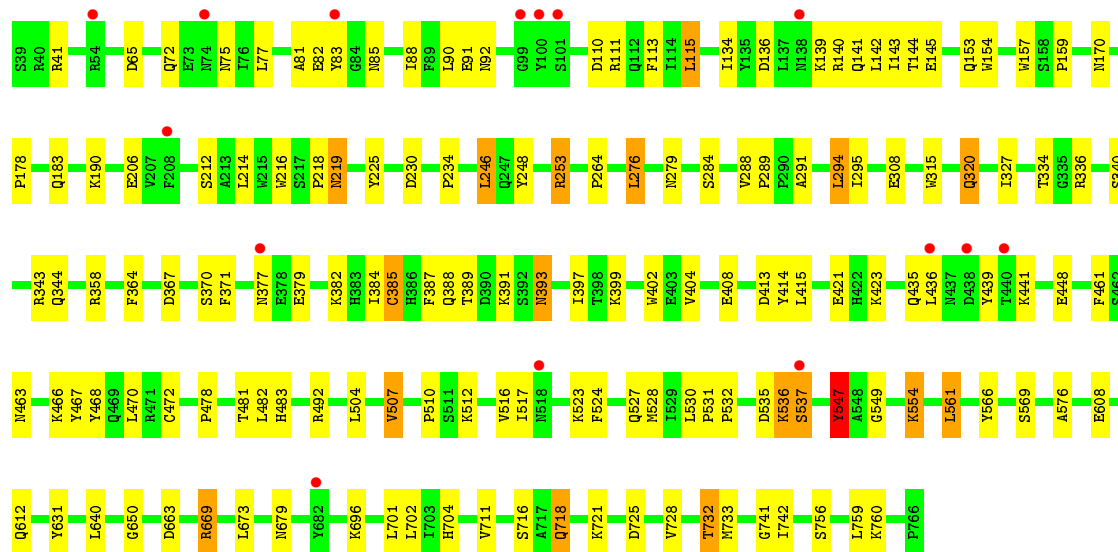
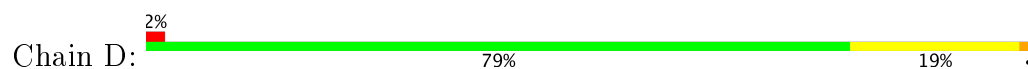
80% 17% 3%



• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.11Å 118.96Å 133.76Å 112.79° 95.74° 90.63°	Depositor
Resolution (Å)	39.45 – 2.11 39.45 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.7 (39.45-2.11) 85.1 (39.45-2.11)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.239 0.203 , 0.243	Depositor DCC
R_{free} test set	9993 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26222	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: BMA, NAG, SC3, SO4

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	0.54	0/6141	0.73	2/8353 (0.0%)
1	B	0.59	0/6141	0.76	4/8353 (0.0%)
1	C	0.56	0/6141	0.74	1/8353 (0.0%)
1	D	0.53	0/6141	0.72	2/8353 (0.0%)
All	All	0.55	0/24564	0.74	9/33412 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	669	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	415	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	669	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	669	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	547	TYR	N-CA-C	-5.20	96.97	111.00
1	D	669	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	542	LEU	CA-CB-CG	5.11	127.04	115.30
1	D	547	TYR	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	700	TYR	Sidechain

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	5966	0	5663	124	0
1	B	5966	0	5663	99	0
1	C	5966	0	5663	110	0
1	D	5966	0	5662	116	0
2	A	112	0	102	2	0
2	B	112	0	101	1	0
2	C	98	0	90	1	0
2	D	140	0	125	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	52	0	46	2	0
4	B	52	0	46	1	0
4	C	52	0	46	1	0
4	D	52	0	46	1	0
5	B	11	0	10	0	0
5	D	11	0	10	0	0
6	A	394	0	0	10	0
6	B	481	0	0	8	0
6	C	395	0	0	9	0
6	D	376	0	0	6	0
All	All	26222	0	23273	433	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 9.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:HG2	1:C:537:SER:H	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:HB2	1:B:466:LYS:HD2	1.45	0.98
1:C:535:ASP:C	1:C:536:LYS:HD3	1.81	0.98
1:B:41:ARG:HD3	1:B:42:THR:O	1.64	0.97
1:C:74:ASN:HB3	1:C:92:ASN:HB2	1.55	0.88
1:C:691:ARG:NE	6:C:1620:HOH:O	2.03	0.88
1:D:536:LYS:O	1:D:537:SER:HB2	1.77	0.82
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.61	0.81
1:B:378:GLU:H	1:B:378:GLU:CD	1.83	0.80
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.80	0.80
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.78	0.80
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.63	0.79
1:B:438:ASP:OD2	1:B:441:LYS:HE3	1.83	0.79
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.65	0.78
1:A:408:GLU:HG2	6:A:1821:HOH:O	1.82	0.77
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.83	0.77
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.49	0.77
1:D:75:ASN:ND2	1:D:92:ASN:H	1.82	0.76
1:D:291:ALA:O	1:D:295:ILE:HG13	1.86	0.76
1:C:253:ARG:HH21	1:D:253:ARG:HH22	1.33	0.76
1:D:704:HIS:HD2	1:D:716:SER:OG	1.69	0.76
1:A:82:GLU:HG2	1:A:467:TYR:OH	1.86	0.75
1:C:704:HIS:HD2	1:C:716:SER:OG	1.70	0.75
1:D:206:GLU:OE1	4:D:1604:SC3:H141	1.85	0.75
1:B:206:GLU:OE1	4:B:1602:SC3:H141	1.87	0.74
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.85	0.74
1:D:75:ASN:HD22	1:D:92:ASN:H	1.36	0.73
1:C:536:LYS:HG2	1:C:537:SER:N	2.02	0.72
1:D:143:ILE:HD13	1:D:178:PRO:HB2	1.74	0.70
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.13	0.69
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.57	0.69
1:D:111:ARG:HD2	6:D:1916:HOH:O	1.91	0.69
1:A:492:ARG:NH2	1:A:492:ARG:HB3	2.08	0.69
1:A:332:GLU:HG3	6:A:1932:HOH:O	1.92	0.68
1:C:111:ARG:HD2	6:C:1809:HOH:O	1.93	0.68
1:C:612:GLN:O	1:C:615:LYS:HG2	1.94	0.68
1:D:81:ALA:O	1:D:82:GLU:HB3	1.95	0.67
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.78	0.66
1:C:253:ARG:NH2	1:D:253:ARG:HH22	1.94	0.66
1:B:334:THR:OG1	1:B:336:ARG:HG2	1.96	0.65
1:B:75:ASN:ND2	1:B:92:ASN:H	1.94	0.64
1:B:393:ASN:H	1:B:393:ASN:HD22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:O	1:B:490:GLU:O	2.14	0.64
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.81	0.64
1:B:393:ASN:ND2	1:B:393:ASN:H	1.96	0.64
1:C:177:GLU:HB2	1:C:180:LEU:HD23	1.80	0.64
1:D:134:ILE:HG21	1:D:178:PRO:HB3	1.79	0.64
1:C:232:GLU:HB3	1:C:262:GLU:HG2	1.79	0.64
1:B:507:VAL:HG13	1:B:509:MET:HG2	1.80	0.63
1:A:71:LYS:HE3	1:A:105:TYR:CE2	2.33	0.63
1:A:206:GLU:OE1	4:A:1601:SC3:H141	1.99	0.62
1:C:746:MET:CE	1:C:746:MET:H	2.12	0.62
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.98	0.62
1:D:516:VAL:HG13	1:D:524:PHE:O	1.99	0.62
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.82	0.62
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.82	0.62
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.20	0.62
1:C:733:MET:HA	1:D:732:THR:CG2	2.30	0.62
1:A:113:PHE:CE1	1:A:178:PRO:HG2	2.35	0.61
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.82	0.61
1:B:232:GLU:HB3	1:B:262:GLU:HG2	1.82	0.61
1:C:74:ASN:HB3	1:C:92:ASN:CB	2.29	0.61
1:D:88:ILE:HG21	1:D:91:GLU:HG3	1.82	0.61
1:B:80:ASN:OD1	1:B:82:GLU:HB2	2.00	0.61
1:C:288:VAL:HG13	1:C:289:PRO:HD2	1.83	0.61
1:B:590:ILE:HD13	6:B:1944:HOH:O	2.01	0.60
1:A:107:VAL:HG22	1:A:114:ILE:HD12	1.83	0.60
1:A:502:LYS:O	1:A:505:GLN:HG2	2.01	0.60
1:A:97:GLU:HB2	6:A:1737:HOH:O	2.00	0.60
1:A:71:LYS:HE3	1:A:105:TYR:HE2	1.66	0.60
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.01	0.60
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.00	0.60
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.84	0.60
1:B:490:GLU:O	1:B:492:ARG:N	2.34	0.60
1:B:370:SER:HB2	1:B:387:PHE:O	2.02	0.59
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.02	0.59
1:C:676:PRO:HG2	1:C:677:GLU:OE2	2.01	0.59
1:C:153:GLN:HE22	1:C:170:ASN:ND2	2.01	0.59
1:B:489:LYS:HG2	1:B:491:LEU:H	1.66	0.59
1:C:72:GLN:O	1:C:74:ASN:N	2.36	0.59
1:C:512:LYS:HD3	6:C:1881:HOH:O	2.02	0.59
1:C:535:ASP:CA	1:C:536:LYS:HD3	2.31	0.59
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:PHE:CE2	1:B:590:ILE:HD12	2.38	0.59
1:B:65:ASP:CB	1:B:466:LYS:HD2	2.27	0.58
1:A:334:THR:OG1	1:A:336:ARG:HG3	2.02	0.58
1:C:535:ASP:O	1:C:536:LYS:HB3	2.04	0.58
1:D:288:VAL:HG13	1:D:289:PRO:HD2	1.85	0.58
1:B:704:HIS:HE1	1:B:711:VAL:O	1.87	0.58
1:B:73:GLU:OE2	1:B:73:GLU:HA	2.04	0.58
2:D:768(A):NAG:H62	2:D:769(B):NAG:HN2	1.67	0.58
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.69	0.57
1:B:704:HIS:HD2	1:B:716:SER:OG	1.86	0.57
1:A:139:LYS:O	1:A:141:GLN:HG3	2.04	0.57
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.34	0.57
1:A:438:ASP:OD1	1:A:440:THR:HB	2.04	0.57
1:C:691:ARG:NH2	6:C:1620:HOH:O	2.36	0.57
1:D:414:TYR:HA	1:D:436:LEU:HD13	1.87	0.57
1:B:111:ARG:HD2	6:B:1884:HOH:O	2.04	0.57
1:C:183:GLN:HE22	1:C:278:PRO:HD3	1.69	0.57
1:D:327:ILE:HD12	1:D:389:THR:HG23	1.87	0.57
1:C:733:MET:HA	1:D:732:THR:HG22	1.86	0.56
1:A:516:VAL:HG11	1:A:523:LYS:HB2	1.87	0.56
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.87	0.56
1:A:502:LYS:HD2	1:A:505:GLN:OE1	2.05	0.56
1:C:691:ARG:CZ	6:C:1620:HOH:O	2.47	0.56
1:D:288:VAL:CG1	1:D:289:PRO:HD2	2.36	0.56
1:D:139:LYS:O	1:D:141:GLN:HG3	2.05	0.55
1:D:230:ASP:OD1	1:D:264:PRO:HB3	2.06	0.55
1:D:153:GLN:HE22	1:D:170:ASN:HD21	1.52	0.55
1:D:718:GLN:HE21	1:D:718:GLN:HA	1.71	0.55
1:D:377:ASN:HB3	1:D:379:GLU:H	1.70	0.55
1:D:72:GLN:HE21	1:D:77:LEU:HD12	1.70	0.55
1:A:143:ILE:HD12	1:A:143:ILE:H	1.71	0.55
1:A:219:ASN:N	1:A:308:GLU:OE2	2.33	0.55
1:B:332:GLU:HG3	6:B:2014:HOH:O	2.07	0.55
1:A:519:LEU:HD22	1:A:608:GLU:OE2	2.07	0.55
1:B:519:LEU:HB3	1:B:520:HIS:CE1	2.40	0.55
1:C:536:LYS:N	1:C:536:LYS:HD3	2.20	0.55
1:B:278:PRO:HG2	2:B:772(A):NAG:H82	1.88	0.55
1:C:516:VAL:HG13	1:C:524:PHE:O	2.08	0.54
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.42	0.54
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.90	0.54
1:C:534:PHE:O	1:C:535:ASP:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:GLN:HE22	1:C:721:LYS:NZ	2.06	0.54
1:B:291:ALA:O	1:B:295:ILE:HG23	2.07	0.54
1:B:422:HIS:CD2	1:B:423:LYS:HD3	2.43	0.54
1:B:516:VAL:HG11	1:B:523:LYS:HD2	1.90	0.54
1:C:114:ILE:CG2	1:C:135:TYR:HB3	2.38	0.54
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.43	0.54
1:C:516:VAL:CG1	1:C:523:LYS:HB2	2.36	0.54
1:A:237:GLU:OE2	1:A:253:ARG:HD3	2.08	0.53
1:D:143:ILE:CD1	1:D:178:PRO:HB2	2.38	0.53
1:D:704:HIS:CD2	1:D:716:SER:OG	2.57	0.53
1:C:112:GLN:HB3	1:C:138:ASN:HD21	1.72	0.53
1:A:143:ILE:HD12	1:A:143:ILE:N	2.23	0.53
1:A:183:GLN:HG2	1:A:276:LEU:HD22	1.91	0.53
1:A:704:HIS:HD2	1:A:716:SER:OG	1.92	0.53
1:A:75:ASN:HB3	1:A:92:ASN:N	2.24	0.53
1:C:206:GLU:OE1	4:C:1603:SC3:H141	2.08	0.53
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.91	0.53
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.29	0.52
1:D:408:GLU:HG2	6:D:1887:HOH:O	2.09	0.52
1:B:308:GLU:HG2	6:B:1862:HOH:O	2.09	0.52
1:C:704:HIS:HE1	1:C:711:VAL:O	1.91	0.52
1:A:109:PRO:HG2	1:A:161:GLY:O	2.10	0.52
1:C:53:PHE:CD1	1:C:503:MET:HG2	2.44	0.52
1:B:522:THR:HG21	1:B:590:ILE:HD11	1.91	0.52
1:C:502:LYS:O	1:C:505:GLN:HG2	2.08	0.52
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.45	0.52
1:D:413:ASP:O	1:D:436:LEU:HD13	2.10	0.52
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.91	0.52
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.92	0.52
1:D:470:LEU:HD12	1:D:483:HIS:CE1	2.45	0.52
1:A:253:ARG:NH2	1:B:253:ARG:HH21	2.08	0.52
1:D:741:GLY:O	1:D:742:ILE:C	2.48	0.52
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.45	0.52
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.92	0.52
1:C:519:LEU:HD22	1:C:608:GLU:OE1	2.11	0.51
1:C:746:MET:HG3	1:D:725:ASP:OD1	2.10	0.51
1:C:140:ARG:NH1	1:C:140:ARG:HG2	2.24	0.51
1:C:305:TRP:CE2	1:C:311:ILE:HD12	2.44	0.51
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.45	0.51
1:B:218:PRO:HD2	1:B:308:GLU:OE2	2.10	0.51
1:B:543:LEU:HG	1:B:759:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASP:HB2	1:C:143:ILE:HD11	1.93	0.51
1:C:148:ILE:HD13	1:C:155:ILE:CD1	2.41	0.51
1:C:518:ASN:O	1:C:519:LEU:HD23	2.11	0.51
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.92	0.51
1:C:253:ARG:NH2	1:D:253:ARG:NH2	2.57	0.51
1:D:718:GLN:HE22	1:D:721:LYS:NZ	2.09	0.51
1:A:677:GLU:N	1:A:677:GLU:OE1	2.37	0.50
1:C:732:THR:HG22	1:D:733:MET:HA	1.93	0.50
1:B:285:TYR:CE1	1:B:336:ARG:HB3	2.46	0.50
1:C:535:ASP:C	1:C:536:LYS:CD	2.69	0.50
1:D:382:LYS:HE2	6:D:1761:HOH:O	2.10	0.50
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.94	0.50
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.57	0.50
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.46	0.50
1:A:490:GLU:HG3	1:A:490:GLU:O	2.11	0.50
1:B:73:GLU:O	1:B:74:ASN:HB2	2.12	0.50
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.76	0.50
1:B:301:CYS:HB2	6:B:2059:HOH:O	2.11	0.50
1:D:219:ASN:HB2	1:D:308:GLU:CD	2.32	0.50
1:C:516:VAL:HG12	1:C:517:ILE:N	2.27	0.50
1:A:370:SER:HB2	1:A:387:PHE:O	2.11	0.49
1:B:524:PHE:HE2	1:B:590:ILE:HD12	1.77	0.49
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.41	0.49
1:A:538:LYS:HD3	1:A:540:TYR:CZ	2.47	0.49
2:A:768(A):NAG:H83	2:A:768(A):NAG:O3	2.11	0.49
1:C:146:GLU:OE1	1:C:181:SER:HA	2.13	0.49
1:A:693:GLU:OE1	1:A:696:LYS:HE2	2.12	0.49
1:A:75:ASN:HD22	1:A:92:ASN:ND2	2.09	0.49
1:D:183:GLN:HG2	1:D:276:LEU:HG	1.94	0.49
1:D:385:CYS:HB3	1:D:387:PHE:CE1	2.46	0.49
1:D:517:ILE:HB	1:D:612:GLN:HE22	1.77	0.49
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.48	0.49
1:A:489:LYS:HG3	1:A:491:LEU:H	1.76	0.49
1:C:415:LEU:HB2	1:C:436:LEU:HD11	1.95	0.49
1:A:507:VAL:HG13	1:A:509:MET:HG2	1.94	0.49
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.47	0.49
1:B:718:GLN:HE22	1:B:721:LYS:HZ1	1.59	0.49
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.94	0.49
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.48	0.49
1:A:150:ASN:O	1:A:151:ASN:HB2	2.13	0.49
1:A:327:ILE:CD1	1:A:389:THR:HG23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LYS:NZ	1:A:726:ALA:O	2.44	0.49
1:C:116:PHE:O	1:C:132:TYR:HA	2.13	0.49
1:B:718:GLN:HE21	1:B:718:GLN:HA	1.78	0.48
1:A:115:LEU:HD23	1:A:134:ILE:HG12	1.95	0.48
1:B:72:GLN:HG2	1:B:73:GLU:HG2	1.96	0.48
1:C:741:GLY:O	1:C:742:ILE:C	2.51	0.48
1:D:415:LEU:C	1:D:415:LEU:HD23	2.33	0.48
1:C:370:SER:HB2	1:C:387:PHE:O	2.14	0.48
1:C:139:LYS:HD3	1:C:141:GLN:NE2	2.29	0.48
1:D:393:ASN:H	1:D:393:ASN:HD22	1.60	0.48
1:B:175:LYS:CG	1:B:182:SER:HB3	2.44	0.48
1:A:41:ARG:NH1	6:A:1831:HOH:O	2.45	0.47
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	0.47
1:A:149:PRO:HB2	1:A:168:TRP:CD1	2.49	0.47
1:A:458:SER:OG	1:A:471:ARG:HD3	2.13	0.47
1:A:482:LEU:O	1:A:490:GLU:O	2.32	0.47
1:A:433:ARG:NH1	1:A:443:THR:HG21	2.29	0.47
1:C:704:HIS:CD2	1:C:716:SER:OG	2.59	0.47
1:D:756:SER:O	1:D:760:LYS:HG3	2.15	0.47
1:A:741:GLY:O	1:A:742:ILE:C	2.53	0.47
1:B:358:ARG:HH11	1:B:358:ARG:HG2	1.79	0.47
1:B:547:TYR:HB3	1:B:554:LYS:HG2	1.97	0.47
1:C:53:PHE:CE1	1:C:503:MET:HG2	2.49	0.47
1:A:175:LYS:NZ	1:A:178:PRO:HA	2.30	0.47
1:B:41:ARG:HG2	6:B:1844:HOH:O	2.14	0.47
1:D:388:GLN:HB3	1:D:391:LYS:HB2	1.96	0.47
1:A:527:GLN:HB3	1:A:555:VAL:HG13	1.95	0.47
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.49	0.47
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.50	0.47
1:A:518:ASN:HD21	1:A:521:GLY:H	1.63	0.47
1:A:515:ASP:HB3	1:A:526:TYR:CE2	2.50	0.47
1:B:214:LEU:O	1:B:214:LEU:HD12	2.15	0.47
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.80	0.47
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.97	0.47
1:C:139:LYS:O	1:C:141:GLN:HG3	2.14	0.47
1:A:472:CYS:O	1:A:478:PRO:HA	2.15	0.46
1:B:214:LEU:HD12	1:B:214:LEU:C	2.36	0.46
1:D:466:LYS:HD3	1:D:467:TYR:HE2	1.80	0.46
2:A:774(B):NAG:H4	6:A:1841:HOH:O	2.16	0.46
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.46	0.46
1:C:405:ILE:HG13	1:C:429:ARG:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD23	1:A:143:ILE:O	2.15	0.46
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.98	0.46
1:D:535:ASP:C	1:D:536:LYS:O	2.50	0.46
1:A:336:ARG:HD3	1:C:277:SER:OG	2.15	0.46
1:C:408:GLU:HG2	6:C:1665:HOH:O	2.15	0.46
1:B:378:GLU:N	1:B:378:GLU:CD	2.61	0.46
1:D:528:MET:HG2	1:D:576:ALA:HB2	1.98	0.46
1:B:463:ASN:HD22	1:B:463:ASN:N	2.14	0.46
1:C:243:ASP:HB2	6:C:1982:HOH:O	2.16	0.46
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.98	0.46
1:A:681:ASP:OD1	1:A:684:ARG:NH2	2.48	0.46
1:D:218:PRO:HD2	1:D:308:GLU:OE1	2.16	0.46
1:D:370:SER:HB2	1:D:387:PHE:O	2.17	0.45
1:D:536:LYS:O	1:D:537:SER:CB	2.52	0.45
1:A:95:PHE:HB2	6:A:1728:HOH:O	2.17	0.45
1:D:696:LYS:CG	1:D:728:VAL:HG22	2.46	0.45
1:C:218:PRO:HD2	1:C:308:GLU:OE2	2.16	0.45
1:D:532:PRO:HD3	1:D:569:SER:HA	1.99	0.45
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.98	0.45
1:D:308:GLU:HA	1:D:308:GLU:OE1	2.16	0.45
1:D:704:HIS:HE1	1:D:711:VAL:O	1.99	0.45
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.97	0.45
1:A:660:GLU:HG3	6:A:1628:HOH:O	2.16	0.45
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.99	0.45
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.97	0.45
1:A:285:TYR:HD1	1:C:280:ALA:HB2	1.81	0.45
1:D:472:CYS:O	1:D:478:PRO:HA	2.17	0.45
1:D:504:LEU:HA	1:D:507:VAL:CG1	2.45	0.45
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.52	0.45
1:A:704:HIS:HE1	1:A:711:VAL:O	1.99	0.45
1:B:47:ASP:HA	1:B:52:THR:HG23	1.98	0.45
1:D:90:LEU:HD12	1:D:140:ARG:NH2	2.31	0.45
1:A:327:ILE:HD13	1:A:389:THR:HG23	1.99	0.45
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.16	0.45
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.59	0.44
1:C:127:SER:HB3	1:C:211:TYR:CG	2.52	0.44
1:C:746:MET:H	1:C:746:MET:HE3	1.81	0.44
1:A:143:ILE:H	1:A:143:ILE:CD1	2.31	0.44
1:A:125:ARG:NH2	1:A:205:GLU:OE2	2.43	0.44
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.14	0.44
1:C:535:ASP:O	1:C:536:LYS:CB	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:LEU:O	1:D:144:THR:HG23	2.17	0.44
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.52	0.44
1:D:435:GLN:HE22	1:D:441:LYS:HD2	1.82	0.44
1:D:492:ARG:HD2	6:D:1922:HOH:O	2.17	0.44
1:A:486:SER:OG	1:A:487:SER:N	2.50	0.44
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.47	0.44
1:C:340:SER:O	1:C:344:GLN:HG3	2.17	0.44
1:B:696:LYS:NZ	1:B:726:ALA:O	2.43	0.44
1:D:279:ASN:OD1	2:D:773(A):NAG:N2	2.51	0.44
1:D:288:VAL:CG1	1:D:294:LEU:HG	2.47	0.44
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.65	0.44
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.17	0.44
1:A:95:PHE:CE1	1:A:102:THR:HG21	2.53	0.44
1:B:109:PRO:HG2	1:B:161:GLY:O	2.17	0.44
1:B:246:LEU:HD13	1:B:248:TYR:O	2.18	0.44
1:A:41:ARG:HD2	6:A:1787:HOH:O	2.17	0.44
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.98	0.44
1:D:190:LYS:NZ	6:D:1833:HOH:O	2.51	0.44
1:A:169:ASN:O	1:A:170:ASN:HB2	2.18	0.43
1:B:586:GLN:NE2	6:B:1626:HOH:O	2.48	0.43
1:C:75:ASN:N	1:C:75:ASN:OD1	2.51	0.43
1:D:393:ASN:H	1:D:393:ASN:ND2	2.16	0.43
1:D:397:ILE:HG22	1:D:439:TYR:CE2	2.53	0.43
1:C:503:MET:HE2	1:C:503:MET:HB2	1.87	0.43
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.53	0.43
1:A:113:PHE:CD1	1:A:178:PRO:HG2	2.53	0.43
1:A:397:ILE:HG22	1:A:439:TYR:CZ	2.53	0.43
1:A:40:ARG:HB3	1:A:506:ASP:O	2.19	0.43
1:B:140:ARG:NH1	1:B:140:ARG:HG2	2.33	0.43
1:D:327:ILE:HB	1:D:343:ARG:HG2	1.99	0.43
1:D:435:GLN:NE2	1:D:441:LYS:HD2	2.34	0.43
1:A:733:MET:HA	1:B:732:THR:CG2	2.47	0.43
1:D:288:VAL:HG12	1:D:294:LEU:HG	2.01	0.43
1:A:75:ASN:HB3	1:A:92:ASN:H	1.83	0.43
1:C:718:GLN:HE22	1:C:721:LYS:HZ1	1.65	0.43
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.54	0.43
1:C:535:ASP:N	1:C:540:TYR:OH	2.42	0.43
1:D:718:GLN:HE22	1:D:721:LYS:HZ1	1.65	0.43
1:A:310:ARG:NH1	6:A:1766:HOH:O	2.51	0.43
1:B:183:GLN:OE1	1:B:278:PRO:HA	2.18	0.43
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ALA:HB3	1:A:728:VAL:HG23	1.99	0.43
1:B:415:LEU:HD13	1:B:416:TYR:N	2.34	0.43
1:B:516:VAL:CG1	1:B:517:ILE:N	2.81	0.43
1:C:288:VAL:CG1	1:C:289:PRO:HD2	2.47	0.43
1:A:237:GLU:HA	1:A:252:VAL:O	2.19	0.42
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.89	0.42
1:A:119:ASN:HB2	1:A:131:SER:HB2	2.01	0.42
1:B:490:GLU:CG	1:B:490:GLU:O	2.67	0.42
1:D:276:LEU:HD13	6:D:1669:HOH:O	2.18	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.42
1:B:758:PHE:O	1:B:761:GLN:HG2	2.20	0.42
1:C:559:PHE:CZ	1:C:561:LEU:HD13	2.54	0.42
1:D:718:GLN:HE21	1:D:718:GLN:CA	2.29	0.42
1:C:432:TYR:CE2	1:C:444:CYS:HB2	2.54	0.42
1:D:340:SER:O	1:D:344:GLN:HG3	2.19	0.42
1:A:654:ALA:N	1:A:655:PRO:CD	2.82	0.42
1:B:219:ASN:H	1:B:308:GLU:CD	2.23	0.42
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.54	0.42
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.54	0.42
1:C:96:ASP:C	1:C:98:LEU:H	2.22	0.42
1:B:140:ARG:HG2	1:B:140:ARG:HH11	1.84	0.42
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.55	0.42
1:A:516:VAL:HG13	1:A:524:PHE:O	2.18	0.42
1:A:547:TYR:CD1	1:A:552:SER:HB2	2.54	0.42
1:B:701:LEU:HD13	1:B:703:ILE:HD11	2.01	0.42
1:D:516:VAL:HG12	1:D:517:ILE:N	2.34	0.42
1:A:397:ILE:HG13	1:A:398:THR:HG23	2.01	0.42
1:A:490:GLU:O	1:A:492:ARG:N	2.52	0.42
1:B:487:SER:O	1:B:488:ASP:HB2	2.19	0.42
1:B:425:MET:HA	1:B:426:PRO:HD2	1.89	0.42
1:A:346:ILE:HG22	1:A:347:GLU:N	2.34	0.41
1:A:492:ARG:HH21	1:A:492:ARG:CB	2.25	0.41
1:A:547:TYR:HB3	1:A:554:LYS:HG2	2.01	0.41
1:A:65:ASP:OD2	1:A:466:LYS:HE2	2.19	0.41
1:D:65:ASP:HA	1:D:463:ASN:HB2	2.01	0.41
1:D:718:GLN:NE2	1:D:718:GLN:HA	2.33	0.41
1:A:711:VAL:HG22	4:A:1601:SC3:H20	2.02	0.41
1:C:457:TYR:HA	1:C:471:ARG:O	2.20	0.41
1:D:547:TYR:HB3	1:D:554:LYS:HG2	2.03	0.41
1:D:561:LEU:HA	1:D:561:LEU:HD12	1.90	0.41
1:A:348:ILE:HG13	1:A:349:SER:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:SER:OG	1:D:336:ARG:HD3	2.20	0.41
1:D:113:PHE:CE1	1:D:143:ILE:HD11	2.56	0.41
1:C:732:THR:CG2	1:D:733:MET:HA	2.49	0.41
1:A:199:THR:HA	1:A:228:PHE:CE2	2.56	0.41
1:B:386:HIS:O	1:B:394:CYS:HB2	2.20	0.41
1:C:148:ILE:HA	1:C:149:PRO:HD3	1.82	0.41
1:A:285:TYR:CD1	1:C:280:ALA:HB2	2.55	0.41
1:C:751:ILE:O	1:C:755:MET:HG3	2.20	0.41
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.21	0.41
1:B:516:VAL:HG12	1:B:517:ILE:N	2.35	0.41
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.94	0.41
1:B:763:PHE:HB2	1:B:765:LEU:HG	2.03	0.41
1:A:377:ASN:HB3	1:A:379:GLU:H	1.86	0.41
1:A:733:MET:HA	1:B:732:THR:HG22	2.02	0.41
1:B:75:ASN:HD22	1:B:91:GLU:HA	1.86	0.41
1:D:115:LEU:HD13	1:D:157:TRP:CZ2	2.55	0.41
1:D:206:GLU:OE2	1:D:663:ASP:OD2	2.38	0.41
1:D:481:THR:OG1	1:D:483:HIS:CE1	2.70	0.41
1:A:474:GLY:HA2	1:A:476:GLY:O	2.20	0.41
1:A:504:LEU:O	1:A:507:VAL:HG12	2.20	0.41
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.87	0.41
1:B:429:ARG:NE	6:B:1629:HOH:O	2.20	0.41
1:C:237:GLU:HA	1:C:252:VAL:O	2.20	0.41
1:C:229:ASN:HB3	1:C:265:THR:OG1	2.20	0.41
1:D:90:LEU:HD12	1:D:140:ARG:HH22	1.86	0.41
1:C:517:ILE:HG23	1:C:526:TYR:CE2	2.56	0.41
1:D:113:PHE:HE1	1:D:143:ILE:HD11	1.85	0.41
1:D:358:ARG:HB3	1:D:358:ARG:HE	1.73	0.41
1:A:150:ASN:HD22	1:A:150:ASN:HA	1.66	0.41
1:A:491:LEU:O	1:A:492:ARG:HB3	2.20	0.41
1:A:660:GLU:CG	6:A:1628:HOH:O	2.69	0.41
1:B:704:HIS:CE1	1:B:711:VAL:O	2.71	0.41
1:C:171:ASP:HB2	6:C:1913:HOH:O	2.20	0.41
1:C:246:LEU:HD13	1:C:248:TYR:O	2.21	0.41
1:C:415:LEU:HD23	1:C:415:LEU:C	2.42	0.41
1:C:532:PRO:O	1:C:533:HIS:C	2.57	0.41
1:C:549:GLY:HA2	1:C:631:TYR:CE1	2.55	0.41
1:D:334:THR:OG1	1:D:336:ARG:HG3	2.20	0.41
1:A:134:ILE:HG21	1:A:178:PRO:HB3	2.03	0.41
1:C:74:ASN:ND2	2:C:768(A):NAG:O7	2.54	0.41
1:D:530:LEU:HA	1:D:531:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:ND2	1:A:92:ASN:ND2	2.68	0.41
1:B:47:ASP:HA	1:B:52:THR:CG2	2.51	0.41
1:C:533:HIS:O	1:C:534:PHE:C	2.60	0.41
1:D:110:ASP:C	1:D:110:ASP:OD1	2.58	0.41
1:D:384:ILE:HG13	1:D:404:VAL:HG21	2.02	0.41
1:D:83:TYR:HB3	1:D:85:ASN:OD1	2.21	0.41
1:C:527:GLN:HB3	1:C:555:VAL:HG13	2.03	0.40
1:D:414:TYR:CA	1:D:436:LEU:HD13	2.50	0.40
1:A:109:PRO:HG3	1:A:158:SER:O	2.22	0.40
1:C:718:GLN:HE21	1:C:718:GLN:CA	2.33	0.40
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.36	0.40
1:C:121:VAL:HG23	6:C:1977:HOH:O	2.21	0.40
1:C:536:LYS:CG	1:C:537:SER:H	2.08	0.40
1:A:219:ASN:HB2	1:A:308:GLU:CD	2.42	0.40
1:D:512:LYS:HE3	1:D:527:GLN:CD	2.42	0.40
1:D:536:LYS:HB3	1:D:536:LYS:NZ	2.36	0.40
1:A:110:ASP:O	1:A:111:ARG:HB2	2.22	0.40
1:A:62:TRP:CG	1:A:462:SER:HA	2.57	0.40
1:A:658:LYS:HB3	1:A:661:TYR:CD2	2.56	0.40
1:B:73:GLU:CA	1:B:73:GLU:OE2	2.69	0.40
1:D:246:LEU:HD13	1:D:248:TYR:O	2.21	0.40
1:D:549:GLY:HA2	1:D:631:TYR:CE1	2.57	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	726/728 (100%)	689 (95%)	35 (5%)	2 (0%)	44	43
1	B	726/728 (100%)	695 (96%)	28 (4%)	3 (0%)	38	35
1	C	726/728 (100%)	692 (95%)	30 (4%)	4 (1%)	28	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	726/728 (100%)	696 (96%)	28 (4%)	2 (0%)	44	43
All	All	2904/2912 (100%)	2772 (96%)	121 (4%)	11 (0%)	38	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ARG
1	C	535	ASP
1	B	82	GLU
1	B	491	LEU
1	C	536	LYS
1	A	40	ARG
1	A	491	LEU
1	D	320	GLN
1	D	537	SER
1	C	74	ASN
1	C	97	GLU

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	652/652 (100%)	627 (96%)	25 (4%)	38	37
1	B	652/652 (100%)	623 (96%)	29 (4%)	33	31
1	C	652/652 (100%)	614 (94%)	38 (6%)	23	20
1	D	652/652 (100%)	622 (95%)	30 (5%)	31	29
All	All	2608/2608 (100%)	2486 (95%)	122 (5%)	30	28

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	74	ASN
1	A	90	LEU

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Mol	Chain	Res	Type
1	A	145	GLU
1	A	150	ASN
1	A	219	ASN
1	A	246	LEU
1	A	294	LEU
1	A	399	LYS
1	A	415	LEU
1	A	423	LYS
1	A	436	LEU
1	A	448	GLU
1	A	471	ARG
1	A	472	CYS
1	A	492	ARG
1	A	520	HIS
1	A	542	LEU
1	A	543	LEU
1	A	547	TYR
1	A	561	LEU
1	A	566	TYR
1	A	701	LEU
1	A	718	GLN
1	A	761	GLN
1	B	41	ARG
1	B	183	GLN
1	B	246	LEU
1	B	294	LEU
1	B	340	SER
1	B	367	ASP
1	B	378	GLU
1	B	379	GLU
1	B	385	CYS
1	B	393	ASN
1	B	415	LEU
1	B	436	LEU
1	B	450	ASN
1	B	492	ARG
1	B	506	ASP
1	B	520	HIS
1	B	535	ASP
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU

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Mol	Chain	Res	Type
1	B	547	TYR
1	B	561	LEU
1	B	566	TYR
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	718	GLN
1	B	732	THR
1	B	759	LEU
1	C	75	ASN
1	C	91	GLU
1	C	119	ASN
1	C	145	GLU
1	C	147	ARG
1	C	181	SER
1	C	183	GLN
1	C	192	ASN
1	C	230	ASP
1	C	246	LEU
1	C	284	SER
1	C	294	LEU
1	C	313	LEU
1	C	361	GLU
1	C	367	ASP
1	C	385	CYS
1	C	399	LYS
1	C	436	LEU
1	C	448	GLU
1	C	472	CYS
1	C	482	LEU
1	C	484	SER
1	C	491	LEU
1	C	503	MET
1	C	520	HIS
1	C	535	ASP
1	C	536	LYS
1	C	542	LEU
1	C	547	TYR
1	C	554	LYS
1	C	561	LEU
1	C	611	ARG
1	C	660	GLU

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Mol	Chain	Res	Type
1	C	701	LEU
1	C	732	THR
1	C	746	MET
1	C	759	LEU
1	C	761	GLN
1	D	41	ARG
1	D	115	LEU
1	D	145	GLU
1	D	219	ASN
1	D	246	LEU
1	D	253	ARG
1	D	276	LEU
1	D	284	SER
1	D	294	LEU
1	D	367	ASP
1	D	385	CYS
1	D	393	ASN
1	D	399	LYS
1	D	423	LYS
1	D	448	GLU
1	D	482	LEU
1	D	507	VAL
1	D	536	LYS
1	D	547	TYR
1	D	554	LYS
1	D	561	LEU
1	D	566	TYR
1	D	608	GLU
1	D	673	LEU
1	D	679	ASN
1	D	701	LEU
1	D	702	LEU
1	D	718	GLN
1	D	732	THR
1	D	759	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	74	ASN
1	A	75	ASN

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Mol	Chain	Res	Type
1	A	103	ASN
1	A	123	GLN
1	A	141	GLN
1	A	150	ASN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	192	ASN
1	A	247	GLN
1	A	345	HIS
1	A	369	ASN
1	A	435	GLN
1	A	463	ASN
1	A	483	HIS
1	A	572	ASN
1	A	586	GLN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	A	761	GLN
1	B	75	ASN
1	B	169	ASN
1	B	170	ASN
1	B	176	ASN
1	B	192	ASN
1	B	227	GLN
1	B	247	GLN
1	B	345	HIS
1	B	393	ASN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	586	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN

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Mol	Chain	Res	Type
1	B	761	GLN
1	C	72	GLN
1	C	74	ASN
1	C	123	GLN
1	C	138	ASN
1	C	141	GLN
1	C	169	ASN
1	C	170	ASN
1	C	176	ASN
1	C	183	GLN
1	C	192	ASN
1	C	227	GLN
1	C	247	GLN
1	C	393	ASN
1	C	435	GLN
1	C	463	ASN
1	C	483	HIS
1	C	505	GLN
1	C	586	GLN
1	C	606	GLN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	745	ASN
1	C	761	GLN
1	D	61	GLN
1	D	72	GLN
1	D	75	ASN
1	D	103	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	227	GLN
1	D	247	GLN
1	D	393	ASN
1	D	435	GLN
1	D	483	HIS

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Mol	Chain	Res	Type
1	D	505	GLN
1	D	572	ASN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	731	GLN
1	D	745	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

47 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	$\# Z > 2$
3	SO4	A	1500	-	4,4,4	0.53	0	6,6,6	0.62	0
4	SC3	A	1601	-	21,29,29	3.21	6 (28%)	25,42,42	2.09	5 (20%)
4	SC3	A	1608	-	21,29,29	2.84	9 (42%)	25,42,42	2.12	6 (24%)
2	NAG	A	767(A)	1	14,14,15	0.66	0	15,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	768(A)	1	14,14,15	0.58	0	15,19,21	0.76	0
2	NAG	A	769(A)	1,2	14,14,15	0.60	0	15,19,21	0.77	0
2	NAG	A	770(B)	2	14,14,15	0.48	0	15,19,21	0.85	1 (6%)
2	NAG	A	771(A)	1	14,14,15	0.47	0	15,19,21	0.89	1 (6%)
2	NAG	A	772(A)	1	14,14,15	0.48	0	15,19,21	1.20	2 (13%)
2	NAG	A	773(A)	1,2	14,14,15	0.60	0	15,19,21	0.73	0
2	NAG	A	774(B)	2	14,14,15	0.65	0	15,19,21	0.81	0
3	SO4	B	1501	-	4,4,4	0.51	0	6,6,6	0.64	0
4	SC3	B	1602	-	21,29,29	3.36	9 (42%)	25,42,42	2.09	5 (20%)
4	SC3	B	1605	-	21,29,29	3.29	9 (42%)	25,42,42	2.15	6 (24%)
2	NAG	B	767(A)	1	14,14,15	0.62	0	15,19,21	0.67	0
2	NAG	B	768(A)	1,2	14,14,15	0.61	0	15,19,21	0.99	1 (6%)
2	NAG	B	769(B)	2,5	14,14,15	0.66	0	15,19,21	0.76	0
5	BMA	B	770(C)	2	11,11,12	0.62	0	13,15,17	1.40	3 (23%)
2	NAG	B	771(A)	1	14,14,15	0.46	0	15,19,21	0.78	0
2	NAG	B	772(A)	1	14,14,15	0.64	0	15,19,21	0.66	0
2	NAG	B	773(A)	1	14,14,15	0.60	0	15,19,21	0.92	1 (6%)
2	NAG	B	774(A)	1,2	14,14,15	0.62	0	15,19,21	0.94	1 (6%)
2	NAG	B	775(B)	2	14,14,15	0.70	0	15,19,21	0.86	1 (6%)
3	SO4	C	1502	-	4,4,4	0.49	0	6,6,6	0.59	0
4	SC3	C	1603	-	21,29,29	3.23	7 (33%)	25,42,42	2.42	5 (20%)
4	SC3	C	1607	-	21,29,29	3.23	8 (38%)	25,42,42	2.03	5 (20%)
2	NAG	C	767(A)	1	14,14,15	0.48	0	15,19,21	0.78	0
2	NAG	C	768(A)	1	14,14,15	0.50	0	15,19,21	0.86	0
2	NAG	C	769(A)	1	14,14,15	0.51	0	15,19,21	0.78	0
2	NAG	C	770(A)	1	14,14,15	0.63	0	15,19,21	0.69	0
2	NAG	C	771(A)	1	14,14,15	0.53	0	15,19,21	0.86	0
2	NAG	C	772(A)	1,2	14,14,15	0.59	0	15,19,21	0.80	0
2	NAG	C	773(B)	2	14,14,15	0.58	0	15,19,21	0.96	0
3	SO4	D	1503	-	4,4,4	0.40	0	6,6,6	0.65	0
4	SC3	D	1604	-	21,29,29	3.35	6 (28%)	25,42,42	2.07	5 (20%)
4	SC3	D	1606	-	21,29,29	3.30	10 (47%)	25,42,42	2.11	5 (20%)
2	NAG	D	767(A)	1	14,14,15	0.84	1 (7%)	15,19,21	0.76	0
2	NAG	D	768(A)	1,2	14,14,15	0.57	0	15,19,21	0.73	0
2	NAG	D	769(B)	2,5	14,14,15	0.56	0	15,19,21	0.78	0
5	BMA	D	770(C)	2	11,11,12	0.63	0	13,15,17	0.68	0
2	NAG	D	771(A)	1,2	14,14,15	0.56	0	15,19,21	0.63	0
2	NAG	D	772(B)	2	14,14,15	0.49	0	15,19,21	0.72	0
2	NAG	D	773(A)	1	14,14,15	0.70	0	15,19,21	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	774(A)	1,2	14,14,15	0.56	0	15,19,21	1.02	2 (13%)
2	NAG	D	775(B)	2	14,14,15	0.67	0	15,19,21	0.81	0
2	NAG	D	776(A)	1,2	14,14,15	0.72	0	15,19,21	0.71	0
2	NAG	D	777(B)	2	14,14,15	0.59	0	15,19,21	1.41	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1500	-	-	0/0/0/0	0/0/0/0
4	SC3	A	1601	-	-	0/4/16/16	0/4/4/4
4	SC3	A	1608	-	-	0/4/16/16	1/4/4/4
2	NAG	A	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	768(A)	1	-	1/6/23/26	0/1/1/1
2	NAG	A	769(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	770(B)	2	-	0/6/23/26	0/1/1/1
2	NAG	A	771(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	772(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	A	773(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	774(B)	2	-	0/6/23/26	0/1/1/1
3	SO4	B	1501	-	-	0/0/0/0	0/0/0/0
4	SC3	B	1602	-	-	0/4/16/16	0/4/4/4
4	SC3	B	1605	-	-	0/4/16/16	0/4/4/4
2	NAG	B	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	768(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	769(B)	2,5	-	0/6/23/26	0/1/1/1
5	BMA	B	770(C)	2	-	0/2/19/22	0/1/1/1
2	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	772(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	773(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	B	774(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	775(B)	2	-	0/6/23/26	0/1/1/1
3	SO4	C	1502	-	-	0/0/0/0	0/0/0/0
4	SC3	C	1603	-	-	0/4/16/16	0/4/4/4
4	SC3	C	1607	-	-	0/4/16/16	1/4/4/4
2	NAG	C	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	768(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	770(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	C	771(A)	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	772(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	773(B)	2	-	0/6/23/26	0/1/1/1
3	SO4	D	1503	-	-	0/0/0/0	0/0/0/0
4	SC3	D	1604	-	-	0/4/16/16	0/4/4/4
4	SC3	D	1606	-	-	0/4/16/16	1/4/4/4
2	NAG	D	767(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	D	768(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	769(B)	2,5	-	0/6/23/26	0/1/1/1
5	BMA	D	770(C)	2	-	0/2/19/22	0/1/1/1
2	NAG	D	771(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	772(B)	2	-	0/6/23/26	0/1/1/1
2	NAG	D	773(A)	1	-	0/6/23/26	0/1/1/1
2	NAG	D	774(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	775(B)	2	-	0/6/23/26	0/1/1/1
2	NAG	D	776(A)	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	777(B)	2	-	0/6/23/26	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1606	SC3	C8-N9	-5.46	1.26	1.34
4	C	1607	SC3	C8-N9	-4.76	1.27	1.34
4	B	1605	SC3	C8-N9	-4.56	1.27	1.34
4	D	1604	SC3	C8-N9	-4.08	1.28	1.34
4	A	1608	SC3	C8-N9	-4.05	1.28	1.34
4	C	1603	SC3	C8-N9	-3.69	1.28	1.34
4	A	1601	SC3	C8-N9	-3.37	1.29	1.34
4	B	1602	SC3	C8-N9	-3.30	1.29	1.34
4	D	1606	SC3	C15-N10	2.00	1.49	1.46
4	D	1604	SC3	C20-C19	2.01	1.42	1.38
4	C	1607	SC3	C20-C19	2.04	1.43	1.38
4	C	1603	SC3	C20-C19	2.04	1.43	1.38
4	D	1606	SC3	C21-C20	2.05	1.43	1.38
4	C	1603	SC3	C18-C17	2.06	1.43	1.38
4	A	1608	SC3	C20-C19	2.06	1.43	1.38
4	C	1607	SC3	C11-N10	2.08	1.49	1.46
4	A	1608	SC3	C22-C17	2.10	1.43	1.38
4	C	1607	SC3	C21-C20	2.10	1.43	1.38
4	B	1605	SC3	C22-C17	2.10	1.43	1.38
4	B	1605	SC3	C20-C19	2.11	1.43	1.38
4	D	1606	SC3	C18-C17	2.12	1.43	1.38
4	B	1602	SC3	C21-C22	2.14	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1605	SC3	C11-N10	2.18	1.50	1.46
4	A	1608	SC3	C21-C22	2.18	1.43	1.38
4	D	1606	SC3	C20-C19	2.19	1.43	1.38
4	C	1607	SC3	C22-C17	2.26	1.43	1.38
4	B	1602	SC3	C18-C17	2.29	1.43	1.38
2	D	767(A)	NAG	C1-C2	2.32	1.55	1.52
4	C	1603	SC3	C11-N10	2.41	1.50	1.46
4	A	1608	SC3	C15-N10	2.42	1.50	1.46
4	A	1601	SC3	C22-C17	2.48	1.44	1.38
4	C	1607	SC3	C19-C18	2.48	1.43	1.38
4	B	1602	SC3	C11-N10	2.50	1.50	1.46
4	B	1605	SC3	C21-C22	2.50	1.43	1.38
4	D	1606	SC3	C19-C18	2.53	1.43	1.38
4	A	1601	SC3	C11-N10	2.67	1.50	1.46
4	A	1608	SC3	C19-C18	2.67	1.44	1.38
4	B	1605	SC3	C19-C18	2.69	1.44	1.38
4	D	1606	SC3	C11-N10	2.71	1.50	1.46
4	B	1602	SC3	C22-C17	2.71	1.44	1.38
4	B	1605	SC3	C15-N10	2.78	1.51	1.46
4	D	1604	SC3	C11-N10	2.91	1.51	1.46
4	B	1602	SC3	C20-C19	2.92	1.45	1.38
4	A	1608	SC3	C11-N10	2.94	1.51	1.46
4	D	1606	SC3	C22-C17	3.13	1.45	1.38
4	A	1601	SC3	C6-C5	3.55	1.47	1.41
4	A	1601	SC3	C15-N10	3.93	1.52	1.46
4	C	1603	SC3	C15-N10	4.07	1.52	1.46
4	C	1607	SC3	C6-C5	4.12	1.48	1.41
4	B	1602	SC3	C15-N10	4.26	1.53	1.46
4	C	1603	SC3	C6-C5	4.30	1.48	1.41
4	D	1604	SC3	C15-N10	4.51	1.53	1.46
4	B	1605	SC3	C6-C5	4.58	1.49	1.41
4	B	1602	SC3	C6-C5	4.87	1.49	1.41
4	D	1606	SC3	C6-C5	5.05	1.50	1.41
4	A	1608	SC3	C6-C5	5.05	1.50	1.41
4	D	1604	SC3	C6-C5	5.29	1.50	1.41
4	A	1608	SC3	C4-N9	8.65	1.41	1.33
4	D	1606	SC3	C4-N9	10.93	1.43	1.33
4	B	1605	SC3	C4-N9	11.31	1.43	1.33
4	C	1607	SC3	C4-N9	11.58	1.44	1.33
4	D	1604	SC3	C4-N9	11.77	1.44	1.33
4	C	1603	SC3	C4-N9	11.89	1.44	1.33
4	B	1602	SC3	C4-N9	11.90	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1601	SC3	C4-N9	12.15	1.44	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1603	SC3	C15-N10-C8	-6.44	107.72	122.07
4	A	1601	SC3	C15-N10-C8	-5.69	109.39	122.07
4	B	1602	SC3	C15-N10-C8	-5.65	109.48	122.07
4	A	1608	SC3	C6-C5-C4	-5.48	116.14	119.92
4	D	1604	SC3	C15-N10-C8	-5.31	110.24	122.07
4	B	1605	SC3	C15-N10-C8	-5.12	110.65	122.07
4	D	1606	SC3	C15-N10-C8	-5.09	110.73	122.07
4	D	1606	SC3	C6-C5-C4	-4.95	116.50	119.92
4	C	1607	SC3	C15-N10-C8	-4.84	111.28	122.07
4	A	1601	SC3	C6-C5-C4	-4.83	116.59	119.92
4	B	1602	SC3	C6-C5-C4	-4.83	116.59	119.92
4	A	1608	SC3	C15-N10-C8	-4.73	111.52	122.07
4	D	1606	SC3	C11-N10-C8	-4.73	111.54	122.07
4	C	1603	SC3	C6-C5-C4	-4.57	116.77	119.92
4	C	1607	SC3	C6-C5-C4	-4.52	116.81	119.92
4	D	1604	SC3	C6-C5-C4	-4.49	116.83	119.92
4	A	1608	SC3	C11-N10-C8	-4.43	112.20	122.07
4	B	1605	SC3	C6-C5-C4	-4.25	116.99	119.92
4	C	1603	SC3	C11-N10-C8	-4.14	112.85	122.07
4	A	1601	SC3	C11-N10-C8	-3.95	113.26	122.07
4	C	1607	SC3	C11-N10-C8	-3.84	113.52	122.07
4	B	1605	SC3	C11-N10-C8	-3.71	113.80	122.07
4	C	1603	SC3	C5-C4-N9	-3.68	103.43	110.68
4	A	1601	SC3	C5-C4-N9	-3.66	103.46	110.68
4	C	1607	SC3	C5-C4-N9	-3.62	103.53	110.68
4	A	1608	SC3	C5-C4-N9	-3.55	103.67	110.68
4	D	1606	SC3	C5-C4-N9	-3.52	103.74	110.68
4	D	1604	SC3	C5-C4-N9	-3.50	103.77	110.68
4	D	1604	SC3	C11-N10-C8	-3.48	114.32	122.07
4	B	1605	SC3	C5-C4-N9	-3.48	103.82	110.68
4	B	1602	SC3	C11-N10-C8	-3.48	114.33	122.07
4	B	1602	SC3	C5-C4-N9	-3.46	103.85	110.68
5	B	770(C)	BMA	C6-C5-C4	-2.99	106.02	113.00
2	D	777(B)	NAG	O5-C1-C2	-2.91	107.42	111.47
2	B	774(A)	NAG	C2-N2-C7	-2.44	119.38	122.94
2	A	772(A)	NAG	C4-C3-C2	-2.44	107.44	111.02
4	B	1605	SC3	C5-C6-N1	-2.38	115.55	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	773(A)	NAG	C2-N2-C7	-2.38	119.47	122.94
2	D	773(A)	NAG	C2-N2-C7	-2.29	119.59	122.94
2	A	770(B)	NAG	C2-N2-C7	-2.24	119.67	122.94
2	D	777(B)	NAG	C6-C5-C4	-2.16	107.94	113.00
2	A	771(A)	NAG	C2-N2-C7	-2.11	119.86	122.94
2	D	774(A)	NAG	C2-N2-C7	-2.11	119.87	122.94
2	D	774(A)	NAG	C3-C4-C5	-2.10	106.51	110.22
2	B	775(B)	NAG	C2-N2-C7	-2.08	119.91	122.94
4	A	1608	SC3	C5-C6-N1	-2.04	115.95	118.28
2	A	772(A)	NAG	C2-N2-C7	-2.03	119.97	122.94
2	D	777(B)	NAG	C1-C2-N2	2.08	114.04	110.49
2	B	768(A)	NAG	C1-O5-C5	2.15	115.13	112.17
2	D	777(B)	NAG	C3-C4-C5	2.37	114.39	110.22
5	B	770(C)	BMA	C3-C4-C5	2.46	114.55	110.22
5	B	770(C)	BMA	C1-O5-C5	2.52	115.64	112.17
4	A	1601	SC3	C17-C16-N7	2.75	116.99	112.62
4	B	1602	SC3	C17-C16-N7	3.31	117.88	112.62
4	A	1608	SC3	C17-C16-N7	3.95	118.89	112.62
4	D	1606	SC3	C17-C16-N7	3.99	118.97	112.62
4	D	1604	SC3	C17-C16-N7	4.01	118.99	112.62
4	C	1607	SC3	C17-C16-N7	4.44	119.67	112.62
4	B	1605	SC3	C17-C16-N7	5.76	121.78	112.62
4	C	1603	SC3	C17-C16-N7	6.18	122.44	112.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	768(A)	NAG	O7-C7-N2-C2

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1607	SC3	C11-C12-C14-C15-N10-N13
4	D	1606	SC3	C11-C12-C14-C15-N10-N13
4	A	1608	SC3	C11-C12-C14-C15-N10-N13

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1601	SC3	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	768(A)	NAG	1	0
2	A	774(B)	NAG	1	0
4	B	1602	SC3	1	0
2	B	772(A)	NAG	1	0
4	C	1603	SC3	1	0
2	C	768(A)	NAG	1	0
4	D	1604	SC3	1	0
2	D	768(A)	NAG	1	0
2	D	769(B)	NAG	1	0
2	D	773(A)	NAG	1	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	728/728 (100%)	0.03	16 (2%) 62 67	15, 30, 59, 87	11 (1%)
1	B	728/728 (100%)	-0.21	7 (0%) 82 85	13, 26, 49, 72	12 (1%)
1	C	728/728 (100%)	-0.07	25 (3%) 46 52	15, 29, 60, 99	12 (1%)
1	D	728/728 (100%)	-0.02	15 (2%) 64 68	16, 31, 57, 75	10 (1%)
All	All	2912/2912 (100%)	-0.07	63 (2%) 62 67	13, 29, 56, 99	45 (1%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	TYR	7.9
1	C	39	SER	6.3
1	A	83	TYR	5.8
1	C	95	PHE	5.8
1	C	101	SER	5.4
1	D	83	TYR	5.2
1	B	39	SER	4.6
1	B	83	TYR	4.5
1	C	99	GLY	4.3
1	C	98	LEU	4.1
1	C	40	ARG	3.9
1	C	96	ASP	3.8
1	A	138	ASN	3.8
1	C	139	LYS	3.7
1	A	100	TYR	3.6
1	A	99	GLY	3.6
1	C	102	THR	3.5
1	A	72	GLN	3.4
1	B	54	ARG	3.4
1	D	99	GLY	3.4
1	C	535	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	99	GLY	3.1
1	A	98	LEU	3.1
1	A	85	ASN	3.0
1	C	138	ASN	3.0
1	C	141	GLN	3.0
1	D	436	LEU	2.9
1	C	74	ASN	2.9
1	C	73	GLU	2.8
1	B	138	ASN	2.8
1	A	388	GLN	2.8
1	B	101	SER	2.8
1	D	537	SER	2.8
1	C	506	ASP	2.7
1	A	393	ASN	2.6
1	C	92	ASN	2.5
1	C	103	ASN	2.5
1	D	138	ASN	2.4
1	D	518	ASN	2.4
1	A	101	SER	2.4
1	A	39	SER	2.4
1	D	208	PHE	2.4
1	B	766	PRO	2.3
1	A	150	ASN	2.3
1	C	140	ARG	2.3
1	C	537	SER	2.3
1	A	505	GLN	2.3
1	C	120	TYR	2.3
1	C	72	GLN	2.2
1	C	766	PRO	2.2
1	D	377	ASN	2.2
1	D	54	ARG	2.2
1	C	90	LEU	2.2
1	A	54	ARG	2.2
1	D	101	SER	2.2
1	D	682	TYR	2.2
1	D	100	TYR	2.1
1	A	179	ASN	2.1
1	D	74	ASN	2.1
1	D	440	THR	2.1
1	C	135	TYR	2.1
1	A	90	LEU	2.0
1	D	438	ASP	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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SC3	D	1606	26/26	0.94	0.12	4.01	26,30,42,43	0
2	NAG	C	772(A)	14/15	0.95	0.13	2.38	31,35,40,40	0
4	SC3	A	1601	26/26	0.94	0.19	1.38	22,28,31,33	0
2	NAG	D	774(A)	14/15	0.84	0.18	1.36	55,61,65,66	0
4	SC3	C	1603	26/26	0.94	0.17	1.13	24,30,35,36	0
4	SC3	D	1604	26/26	0.94	0.17	1.12	24,31,33,34	0
2	NAG	B	773(A)	14/15	0.91	0.11	0.87	36,40,45,45	0
2	NAG	B	767(A)	14/15	0.72	0.24	0.81	71,73,74,74	0
2	NAG	A	767(A)	14/15	0.72	0.29	0.77	80,81,83,83	0
2	NAG	C	771(A)	14/15	0.88	0.14	0.67	42,48,50,52	0
4	SC3	B	1602	26/26	0.94	0.15	0.62	21,26,30,32	0
2	NAG	B	771(A)	14/15	0.90	0.12	0.57	29,33,40,40	0
4	SC3	B	1605	26/26	0.95	0.11	0.40	26,28,39,40	0
2	NAG	C	767(A)	14/15	0.87	0.14	0.31	54,57,60,60	0
2	NAG	B	772(A)	14/15	0.88	0.11	0.23	39,41,44,47	0
2	NAG	D	771(A)	14/15	0.92	0.11	0.12	32,37,46,50	0
2	NAG	A	769(A)	14/15	0.93	0.10	0.11	37,42,46,51	0
2	NAG	A	773(A)	14/15	0.93	0.11	0.09	29,37,44,46	0
4	SC3	A	1608	26/26	0.95	0.11	0.04	26,35,42,45	0
2	NAG	C	769(A)	14/15	0.94	0.10	-0.04	32,36,39,40	0
2	NAG	D	776(A)	14/15	0.93	0.10	-0.21	28,35,43,44	0
2	NAG	A	772(A)	14/15	0.91	0.12	-0.41	44,48,50,52	0
3	SO4	D	1503	5/5	0.98	0.09	-0.62	38,40,42,43	0
2	NAG	D	768(A)	14/15	0.83	0.15	-0.70	71,73,74,76	0
2	NAG	B	768(A)	14/15	0.91	0.12	-0.72	42,47,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	C	1502	5/5	0.99	0.09	-0.81	28,28,31,31	0
2	NAG	A	768(A)	14/15	0.75	0.15	-0.91	73,74,74,75	0
4	SC3	C	1607	26/26	0.97	0.09	-0.97	30,34,39,40	0
2	NAG	B	774(A)	14/15	0.96	0.07	-1.03	26,34,41,42	0
3	SO4	A	1500	5/5	0.98	0.10	-1.31	33,33,34,34	0
3	SO4	B	1501	5/5	1.00	0.07	-2.34	26,26,27,27	0
2	NAG	B	775(B)	14/15	0.89	0.20	-	37,45,50,56	0
2	NAG	D	773(A)	14/15	0.68	0.23	-	60,64,67,68	0
5	BMA	D	770(C)	11/12	0.72	0.30	-	76,77,77,77	0
2	NAG	C	770(A)	14/15	0.80	0.14	-	40,41,45,45	0
2	NAG	C	768(A)	14/15	0.59	0.24	-	85,88,89,89	0
5	BMA	B	770(C)	11/12	0.80	0.15	-	50,52,54,54	0
2	NAG	A	771(A)	14/15	0.84	0.12	-	51,53,55,58	3
2	NAG	A	774(B)	14/15	0.90	0.22	-	44,49,53,57	0
2	NAG	A	770(B)	14/15	0.83	0.26	-	58,63,65,65	0
2	NAG	B	769(B)	14/15	0.92	0.11	-	45,46,48,48	0
2	NAG	D	772(B)	14/15	0.77	0.27	-	58,62,66,66	0
2	NAG	D	777(B)	14/15	0.88	0.16	-	47,52,55,56	0
2	NAG	D	775(B)	14/15	0.77	0.31	-	66,68,69,69	0
2	NAG	C	773(B)	14/15	0.89	0.19	-	45,48,51,51	0
2	NAG	D	769(B)	14/15	0.79	0.29	-	76,77,81,82	0
2	NAG	D	767(A)	14/15	0.32	0.45	-	79,81,84,85	0

6.5 Other polymers

There are no such residues in this entry.