



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 AM GMT

PDB ID : 3FBY
Title : The crystal structure of the signature domain of cartilage oligomeric matrix protein.
Authors : Tan, K.; Lawler, J.
Deposited on : 2008-11-20
Resolution : 3.15 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

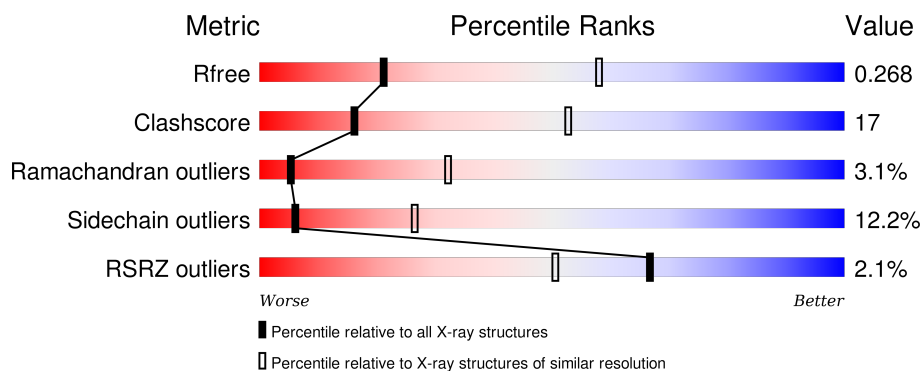
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

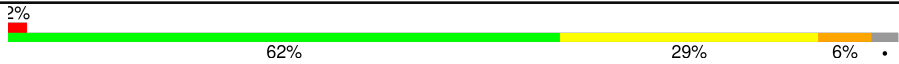


The reported resolution of this entry is 3.15 Å.

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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	551	 2% 62% 29% 6% •
1	B	551	 2% 56% 36% 5% •
1	C	551	 2% 62% 29% 6% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	A	903	X	-	-	-
4	SO4	A	1003	-	-	-	X
4	SO4	C	1003	-	-	-	X
5	NAG	B	901	X	-	-	-
5	MAN	B	903	X	-	-	-
6	MAN	C	903	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12777 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 Cartilage oligomeric matrix protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			
1	B	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			
1	C	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ARG	-	EXPRESSION TAG	UNP P49747
A	210	SER	-	EXPRESSION TAG	UNP P49747
A	211	PRO	-	EXPRESSION TAG	UNP P49747
A	212	TRP	-	EXPRESSION TAG	UNP P49747
A	213	PRO	-	EXPRESSION TAG	UNP P49747
A	214	GLY	-	EXPRESSION TAG	UNP P49747
A	215	VAL	-	EXPRESSION TAG	UNP P49747
A	216	PRO	-	EXPRESSION TAG	UNP P49747
A	217	THR	-	EXPRESSION TAG	UNP P49747
A	218	SER	-	EXPRESSION TAG	UNP P49747
A	219	PRO	-	EXPRESSION TAG	UNP P49747
A	220	VAL	-	EXPRESSION TAG	UNP P49747
A	221	TRP	-	EXPRESSION TAG	UNP P49747
A	222	TRP	-	EXPRESSION TAG	UNP P49747
A	223	ASN	-	EXPRESSION TAG	UNP P49747
A	224	SER	-	EXPRESSION TAG	UNP P49747
A	758	GLY	-	EXPRESSION TAG	UNP P49747
A	759	THR	-	EXPRESSION TAG	UNP P49747
B	209	ARG	-	EXPRESSION TAG	UNP P49747
B	210	SER	-	EXPRESSION TAG	UNP P49747
B	211	PRO	-	EXPRESSION TAG	UNP P49747
B	212	TRP	-	EXPRESSION TAG	UNP P49747
B	213	PRO	-	EXPRESSION TAG	UNP P49747

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Chain	Residue	Modelled	Actual	Comment	Reference
B	214	GLY	-	EXPRESSION TAG	UNP P49747
B	215	VAL	-	EXPRESSION TAG	UNP P49747
B	216	PRO	-	EXPRESSION TAG	UNP P49747
B	217	THR	-	EXPRESSION TAG	UNP P49747
B	218	SER	-	EXPRESSION TAG	UNP P49747
B	219	PRO	-	EXPRESSION TAG	UNP P49747
B	220	VAL	-	EXPRESSION TAG	UNP P49747
B	221	TRP	-	EXPRESSION TAG	UNP P49747
B	222	TRP	-	EXPRESSION TAG	UNP P49747
B	223	ASN	-	EXPRESSION TAG	UNP P49747
B	224	SER	-	EXPRESSION TAG	UNP P49747
B	758	GLY	-	EXPRESSION TAG	UNP P49747
B	759	THR	-	EXPRESSION TAG	UNP P49747
C	209	ARG	-	EXPRESSION TAG	UNP P49747
C	210	SER	-	EXPRESSION TAG	UNP P49747
C	211	PRO	-	EXPRESSION TAG	UNP P49747
C	212	TRP	-	EXPRESSION TAG	UNP P49747
C	213	PRO	-	EXPRESSION TAG	UNP P49747
C	214	GLY	-	EXPRESSION TAG	UNP P49747
C	215	VAL	-	EXPRESSION TAG	UNP P49747
C	216	PRO	-	EXPRESSION TAG	UNP P49747
C	217	THR	-	EXPRESSION TAG	UNP P49747
C	218	SER	-	EXPRESSION TAG	UNP P49747
C	219	PRO	-	EXPRESSION TAG	UNP P49747
C	220	VAL	-	EXPRESSION TAG	UNP P49747
C	221	TRP	-	EXPRESSION TAG	UNP P49747
C	222	TRP	-	EXPRESSION TAG	UNP P49747
C	223	ASN	-	EXPRESSION TAG	UNP P49747
C	224	SER	-	EXPRESSION TAG	UNP P49747
C	758	GLY	-	EXPRESSION TAG	UNP P49747
C	759	THR	-	EXPRESSION TAG	UNP P49747

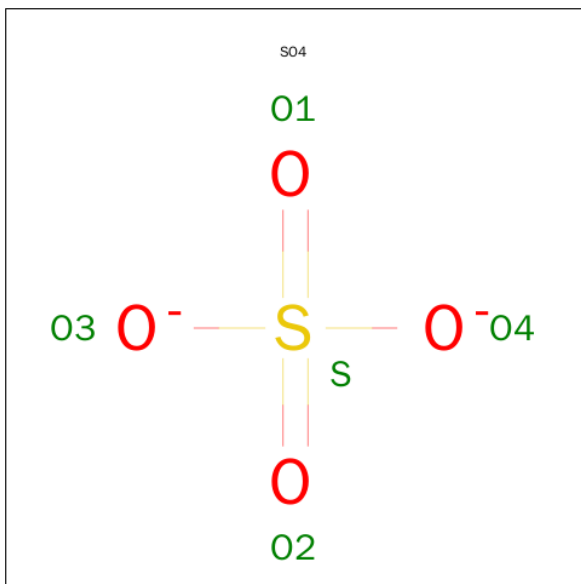
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	29	Total Ca 29 29	0	0
2	A	30	Total Ca 30 30	0	0
2	C	29	Total Ca 29 29	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	5	Total	C	N	O	0	0
			61	34	2	25		

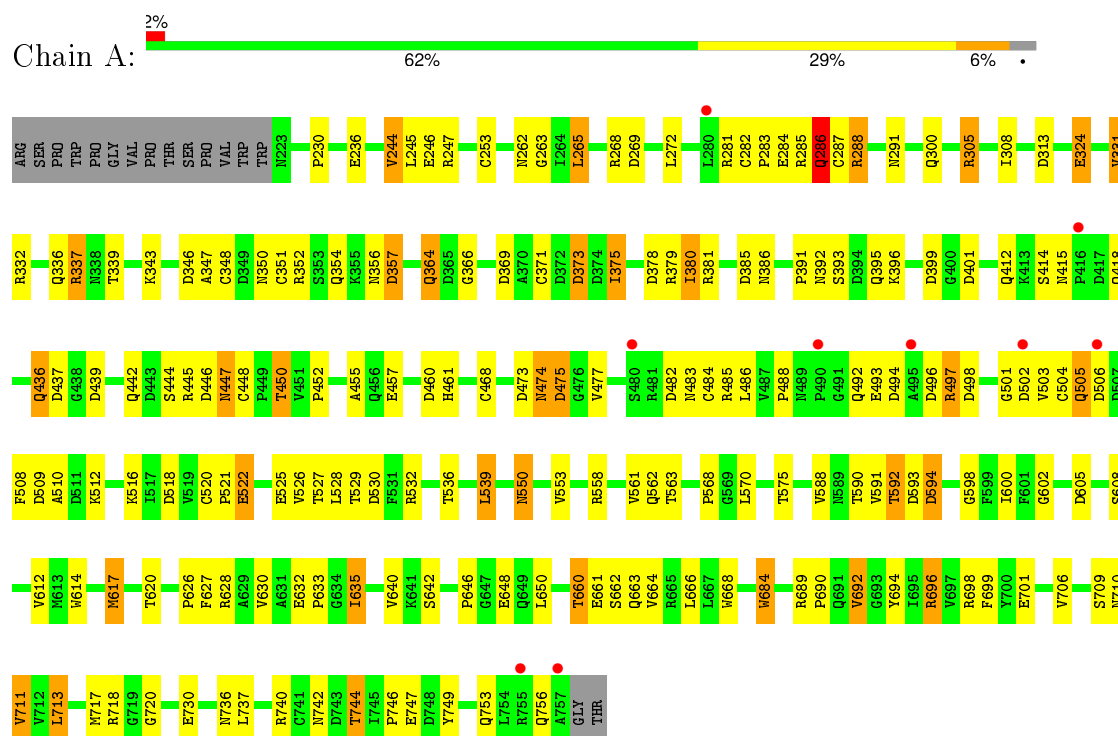
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	3	Total	O	0	0
			3	3		
7	C	2	Total	O	0	0
			2	2		

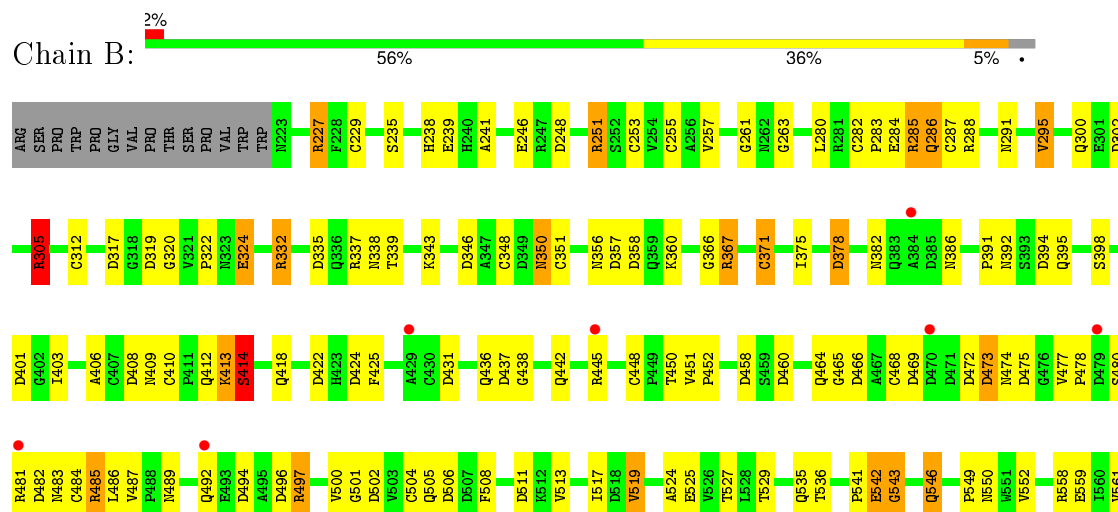
3 Residue-property plots

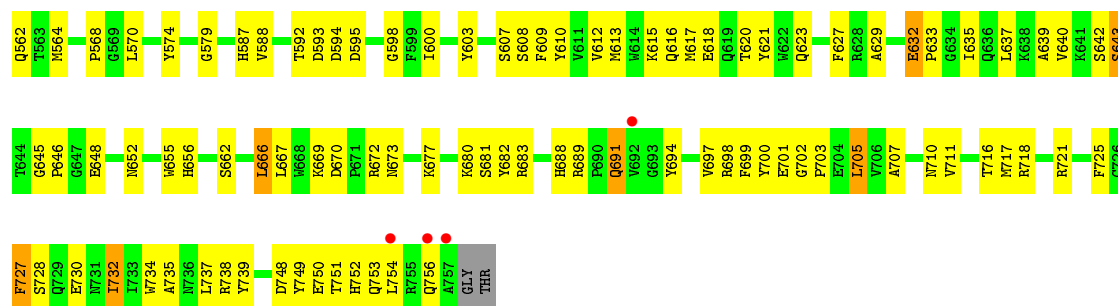
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cartilage oligomeric matrix protein

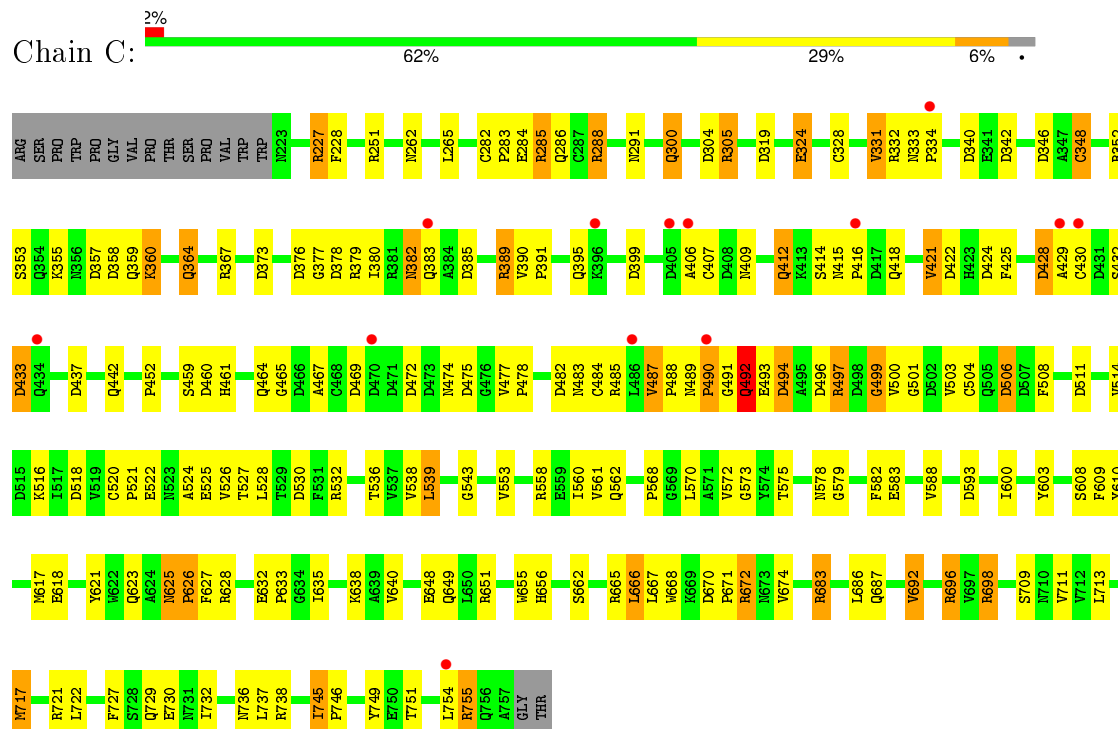


• Molecule 1: Cartilage oligomeric matrix protein





• Molecule 1: Cartilage oligomeric matrix protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.24Å 192.24Å 145.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 3.15 39.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.00-3.15) 99.7 (39.00-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.202 , 0.266 0.204 , 0.268	Depositor DCC
R_{free} test set	2735 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.7	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53803 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	1/4245 (0.0%)	0.82	0/5770
1	B	0.65	3/4245 (0.1%)	0.78	1/5770 (0.0%)
1	C	0.66	0/4245	0.79	1/5770 (0.0%)
All	All	0.68	4/12735 (0.0%)	0.80	2/17310 (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
3	A	1	0
5	B	2	0
6	C	1	0
All	All	4	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	CYS	CB-SG	-7.22	1.70	1.82
1	B	335	ASP	CB-CG	6.03	1.64	1.51
1	A	371	CYS	CB-SG	-5.96	1.72	1.81
1	B	371	CYS	CB-SG	-5.14	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	VAL	CB-CA-C	-5.33	101.27	111.40
1	C	754	LEU	CA-CB-CG	5.05	126.92	115.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	903	MAN	C1
5	B	901	NAG	C1
5	B	903	MAN	C1
6	C	903	MAN	C1

There are no planarity outliers.

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	4161	0	3698	124	0
1	B	4161	0	3698	160	0
1	C	4161	0	3698	120	0
2	A	30	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
3	A	50	0	43	3	0
4	A	25	0	0	0	0
4	B	10	0	0	0	0
4	C	15	0	0	1	0
5	B	39	0	34	0	0
6	C	61	0	52	0	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	2	0	0	0	0
All	All	12777	0	11223	403	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 (403) 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:251:ARG:HH11	1:B:251:ARG:HG3	1.04	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:CYS:HB2	1:A:263:GLY:HA3	1.39	1.01
1:B:749:TYR:O	1:B:753:GLN:HG2	1.69	0.93
1:B:570:LEU:HD22	1:B:600:ILE:CD1	1.99	0.92
1:A:337:ARG:HH21	1:A:337:ARG:HG3	1.35	0.89
1:A:520:CYS:HB2	1:A:526:VAL:HG13	1.56	0.88
1:B:246:GLU:HA	1:B:246:GLU:OE1	1.73	0.87
1:C:482:ASP:HA	1:C:492:GLN:OE1	1.75	0.85
1:C:626:PRO:HD3	1:C:648:GLU:HB3	1.61	0.82
1:B:478:PRO:O	1:B:482:ASP:HB2	1.79	0.82
1:A:253:CYS:CB	1:A:263:GLY:HA3	2.10	0.81
1:A:305:ARG:NH1	1:A:305:ARG:HB3	1.94	0.81
1:B:251:ARG:HG3	1:B:251:ARG:NH1	1.80	0.79
1:C:291:ASN:H	1:C:300:GLN:HE22	1.30	0.79
1:A:339:THR:HG23	1:A:346:ASP:OD1	1.84	0.78
1:A:539:LEU:HB2	1:A:568:PRO:HB2	1.67	0.77
1:A:520:CYS:HB2	1:A:526:VAL:CG1	2.13	0.77
1:B:570:LEU:HD22	1:B:600:ILE:HD12	1.67	0.76
1:C:483:ASN:HB2	1:C:499:GLY:O	1.85	0.76
1:C:424:ASP:O	1:C:425:PHE:HB2	1.84	0.76
1:B:635:ILE:H	1:B:635:ILE:HD12	1.50	0.76
1:A:305:ARG:HH11	1:A:305:ARG:HB3	1.51	0.75
1:A:230:PRO:HB2	1:A:245:LEU:HD22	1.69	0.75
1:A:617:MET:CE	1:A:617:MET:HA	2.16	0.75
1:C:672:ARG:HB3	1:C:674:VAL:HG23	1.68	0.75
1:B:367:ARG:NH2	1:B:371:CYS:HB3	2.03	0.73
1:B:689:ARG:HB2	1:B:694:TYR:HB3	1.71	0.72
1:C:437:ASP:HB2	1:C:452:PRO:HG3	1.70	0.72
1:A:337:ARG:HH21	1:A:337:ARG:CG	2.01	0.72
1:A:337:ARG:NH2	1:A:339:THR:HG22	2.04	0.72
1:A:494:ASP:HB3	1:A:496:ASP:O	1.89	0.71
1:B:613:MET:HG2	1:B:725:PHE:CE2	2.26	0.71
1:B:305:ARG:HH11	1:B:305:ARG:HB3	1.56	0.70
1:B:610:TYR:CE1	1:B:717:MET:HB2	2.25	0.70
1:A:284:GLU:O	1:A:285:ARG:C	2.29	0.70
1:C:227:ARG:HH21	1:C:227:ARG:HG2	1.54	0.70
1:C:573:GLY:O	1:C:721:ARG:HD2	1.90	0.70
1:C:227:ARG:HH21	1:C:227:ARG:CG	2.03	0.69
1:C:331:VAL:HG11	1:C:348:CYS:HB3	1.75	0.69
1:A:378:ASP:OD2	1:A:391:PRO:HA	1.93	0.69
1:B:295:VAL:HG21	1:B:312:CYS:HB3	1.75	0.68
1:C:415:ASN:HD22	1:C:418:GLN:HA	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ARG:HB2	1:A:694:TYR:HB3	1.76	0.68
1:B:497:ARG:HA	1:B:497:ARG:HH21	1.59	0.67
1:C:340:ASP:HB3	1:C:353:SER:HA	1.77	0.67
1:C:487:VAL:CG2	1:C:504:CYS:HB3	2.24	0.67
1:B:618:GLU:HG2	1:B:633:PRO:HD3	1.78	0.66
1:A:364:GLN:NE2	1:A:364:GLN:HA	2.11	0.66
1:A:473:ASP:O	1:A:474:ASN:HB2	1.94	0.66
1:B:378:ASP:OD2	1:B:391:PRO:HA	1.96	0.66
1:B:483:ASN:HD21	1:B:492:GLN:HA	1.61	0.65
1:B:629:ALA:HB1	1:B:656:HIS:HB2	1.78	0.65
1:A:497:ARG:C	1:A:497:ARG:HD3	2.18	0.64
1:C:692:VAL:HG21	1:C:749:TYR:CZ	2.32	0.64
1:C:625:ASN:HA	1:C:627:PHE:N	2.12	0.64
1:A:285:ARG:O	1:A:287:CYS:N	2.30	0.64
1:A:291:ASN:H	1:A:300:GLN:HE22	1.45	0.63
1:B:494:ASP:HA	1:B:502:ASP:OD1	1.98	0.63
1:C:399:ASP:HB3	1:C:412:GLN:O	1.98	0.63
1:A:286:GLN:H	1:A:286:GLN:CD	2.02	0.63
1:C:626:PRO:CD	1:C:648:GLU:HB3	2.29	0.63
1:C:409:ASN:OD1	1:C:415:ASN:ND2	2.31	0.63
1:A:364:GLN:NE2	1:A:364:GLN:CA	2.62	0.62
1:C:751:THR:O	1:C:755:ARG:HB2	2.00	0.62
1:A:337:ARG:HH22	1:A:339:THR:HG22	1.62	0.62
1:A:285:ARG:HA	1:A:288:ARG:HD3	1.80	0.62
1:A:262:ASN:HD21	1:A:282:CYS:HB3	1.65	0.62
1:B:617:MET:HE2	1:B:617:MET:HA	1.81	0.62
1:A:642:SER:HB2	1:A:650:LEU:HD13	1.82	0.62
1:A:617:MET:HA	1:A:617:MET:HE3	1.80	0.61
1:C:618:GLU:HB2	1:C:633:PRO:HD3	1.81	0.61
1:A:550:ASN:ND2	1:A:563:THR:OG1	2.30	0.61
1:B:643:SER:HB3	1:B:662:SER:HB3	1.83	0.60
1:C:635:ILE:H	1:C:635:ILE:HD12	1.66	0.60
1:B:392:ASN:ND2	1:B:395:GLN:HA	2.16	0.60
1:B:519:VAL:CG2	1:B:739:TYR:O	2.50	0.60
1:B:253:CYS:CB	1:B:263:GLY:HA3	2.32	0.60
1:C:610:TYR:CE1	1:C:717:MET:HG2	2.38	0.59
1:A:627:PHE:CZ	1:A:660:THR:HG21	2.37	0.59
1:B:677:LYS:HE3	1:B:680:LYS:HD2	1.83	0.59
1:A:530:ASP:OD1	1:A:532:ARG:HG2	2.02	0.59
1:A:262:ASN:HD21	1:A:282:CYS:CB	2.16	0.59
1:A:539:LEU:HD21	1:A:570:LEU:HG	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ASP:HB3	1:B:524:ALA:O	2.03	0.59
1:C:285:ARG:O	1:C:288:ARG:HD3	2.03	0.59
1:A:558:ARG:NH2	1:A:736:ASN:OD1	2.37	0.58
1:B:618:GLU:CG	1:B:633:PRO:HD3	2.33	0.58
1:B:251:ARG:CG	1:B:251:ARG:NH1	2.58	0.58
1:B:570:LEU:CD2	1:B:600:ILE:CD1	2.78	0.58
1:A:594:ASP:HB2	1:A:617:MET:HB2	1.84	0.58
1:B:451:VAL:HG21	1:B:468:CYS:HB3	1.84	0.58
1:B:375:ILE:HG23	1:B:382:ASN:HD21	1.69	0.58
1:A:369:ASP:CG	1:A:375:ILE:HD12	2.24	0.58
1:A:401:ASP:HB3	1:A:414:SER:HA	1.86	0.58
1:B:598:GLY:HA3	1:B:612:VAL:O	2.04	0.58
1:A:350:ASN:HB2	1:A:366:GLY:O	2.04	0.58
1:C:511:ASP:HB3	1:C:524:ALA:HA	1.84	0.57
1:A:380:ILE:HG22	1:A:385:ASP:HB2	1.86	0.57
1:B:610:TYR:HE1	1:B:717:MET:HB2	1.66	0.57
1:A:285:ARG:O	1:A:288:ARG:HG2	2.04	0.57
1:C:608:SER:HA	1:C:640:VAL:O	2.04	0.57
1:A:364:GLN:HE21	1:A:364:GLN:CA	2.17	0.57
1:A:308:ILE:HG22	1:A:313:ASP:HB2	1.87	0.57
1:C:324:GLU:CD	1:C:324:GLU:H	2.07	0.57
1:B:305:ARG:NH1	1:B:305:ARG:HB3	2.19	0.57
1:B:483:ASN:ND2	1:B:492:GLN:HA	2.19	0.57
1:A:455:ALA:HB3	1:A:457:GLU:OE1	2.05	0.56
1:B:489:ASN:O	1:B:492:GLN:NE2	2.38	0.56
1:B:253:CYS:HB3	1:B:263:GLY:HA3	1.88	0.56
1:A:436:GLN:HE22	1:A:450:THR:HG23	1.71	0.56
1:C:465:GLY:O	1:C:469:ASP:HB2	2.06	0.56
1:B:529:THR:HG22	1:B:558:ARG:HG2	1.86	0.56
1:B:694:TYR:CE1	1:B:711:VAL:HG12	2.41	0.56
1:B:477:VAL:HG21	1:B:492:GLN:NE2	2.21	0.56
1:C:621:TYR:HB2	1:C:655:TRP:CD1	2.41	0.56
1:A:475:ASP:OD2	1:A:488:PRO:HA	2.06	0.56
1:B:621:TYR:CE2	1:B:623:GLN:HB2	2.41	0.56
1:B:410:CYS:C	1:B:412:GLN:H	2.08	0.56
1:C:487:VAL:HG21	1:C:504:CYS:HB3	1.88	0.55
1:B:285:ARG:O	1:B:288:ARG:HG2	2.06	0.55
1:C:494:ASP:HB2	1:C:501:GLY:HA2	1.88	0.55
1:A:701:GLU:HG2	1:A:706:VAL:HG11	1.88	0.55
1:B:486:LEU:HD12	1:B:508:PHE:HD2	1.72	0.55
1:B:464:GLN:OE1	1:B:469:ASP:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ILE:HG21	1:A:699:PHE:CE2	2.41	0.55
1:A:509:ASP:HB3	1:A:522:GLU:HA	1.88	0.55
1:B:699:PHE:HB2	1:B:707:ALA:HB3	1.89	0.54
1:B:607:SER:HB3	1:B:642:SER:HB3	1.90	0.54
1:A:494:ASP:CB	1:A:496:ASP:O	2.55	0.54
1:C:582:PHE:HB3	1:C:686:LEU:HD23	1.88	0.54
1:B:574:TYR:HA	1:B:721:ARG:HH11	1.71	0.54
1:B:543:GLY:O	1:B:546:GLN:NE2	2.40	0.54
1:C:625:ASN:HA	1:C:626:PRO:C	2.28	0.54
1:B:711:VAL:HG21	1:B:752:HIS:CG	2.43	0.54
1:C:415:ASN:ND2	1:C:418:GLN:HA	2.23	0.54
1:B:617:MET:HA	1:B:617:MET:CE	2.37	0.54
1:B:284:GLU:H	1:B:284:GLU:CD	2.11	0.54
1:A:632:GLU:HB3	1:A:633:PRO:HD2	1.90	0.54
1:B:666:LEU:HD11	1:B:669:LYS:HB2	1.91	0.54
1:C:333:ASN:ND2	1:C:333:ASN:O	2.41	0.53
1:C:390:VAL:HB	1:C:407:CYS:HB3	1.90	0.53
1:B:350:ASN:HB2	1:B:366:GLY:O	2.07	0.53
1:B:317:ASP:O	1:B:332:ARG:HD2	2.08	0.53
1:B:431:ASP:HA	1:B:442:GLN:HE22	1.73	0.53
1:A:381:ARG:O	1:A:385:ASP:HB2	2.07	0.53
1:B:324:GLU:CD	1:B:324:GLU:H	2.11	0.53
1:C:409:ASN:H	1:C:418:GLN:HE22	1.57	0.53
1:C:464:GLN:O	1:C:464:GLN:HG3	2.09	0.53
1:B:448:CYS:HB2	1:B:465:GLY:HA3	1.90	0.53
1:C:527:THR:HG23	1:C:528:LEU:HB2	1.91	0.53
1:A:446:ASP:O	1:A:448:CYS:N	2.40	0.52
1:C:283:PRO:HD2	1:C:284:GLU:OE1	2.09	0.52
1:C:648:GLU:HG2	1:C:651:ARG:HH22	1.74	0.52
1:B:409:ASN:HB2	1:B:425:PHE:O	2.10	0.52
1:A:740:ARG:HD2	3:A:901:NAG:H81	1.92	0.52
1:B:227:ARG:O	1:B:235:SER:HB3	2.10	0.52
1:C:485:ARG:HB3	1:C:508:PHE:HZ	1.75	0.52
1:B:466:ASP:HA	1:B:469:ASP:HB3	1.92	0.52
1:B:549:PRO:HA	1:B:562:GLN:HE21	1.75	0.52
1:B:562:GLN:HE22	1:B:564:MET:HB2	1.74	0.52
1:B:473:ASP:OD2	1:B:485:ARG:O	2.27	0.51
1:B:339:THR:HG23	1:B:346:ASP:OD1	2.09	0.51
1:B:408:ASP:HA	1:B:418:GLN:HE22	1.76	0.51
1:A:439:ASP:HB3	1:A:452:PRO:HA	1.93	0.51
1:B:541:PRO:C	1:B:543:GLY:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:TYR:CE2	1:B:705:LEU:HB2	2.46	0.51
1:A:282:CYS:HB2	1:A:284:GLU:OE1	2.11	0.51
1:B:587:HIS:HD2	1:B:681:SER:OG	1.93	0.51
1:A:598:GLY:HA3	1:A:612:VAL:O	2.10	0.50
1:B:367:ARG:HD3	1:B:371:CYS:HB3	1.92	0.50
1:A:460:ASP:O	1:A:461:HIS:HB2	2.10	0.50
1:B:319:ASP:HB3	1:B:332:ARG:HB3	1.92	0.50
1:A:262:ASN:ND2	1:A:282:CYS:CB	2.74	0.50
1:C:603:TYR:HA	1:C:609:PHE:HB3	1.93	0.50
1:C:459:SER:HB2	1:C:472:ASP:O	2.12	0.50
1:A:331:VAL:HG21	1:A:347:ALA:O	2.12	0.50
1:C:478:PRO:O	1:C:482:ASP:HB2	2.11	0.50
1:B:732:ILE:HB	1:B:734:TRP:CZ3	2.47	0.49
1:C:376:ASP:HB3	1:C:389:ARG:O	2.12	0.49
1:A:709:SER:O	1:A:710:ASN:HB2	2.12	0.49
1:A:694:TYR:CE2	1:A:746:PRO:HG2	2.46	0.49
1:B:343:LYS:HG3	1:B:357:ASP:OD1	2.12	0.49
1:C:291:ASN:N	1:C:300:GLN:HE22	2.06	0.49
1:B:613:MET:HG2	1:B:725:PHE:HE2	1.72	0.49
1:C:583:GLU:HG2	1:C:738:ARG:HB2	1.94	0.49
1:A:626:PRO:HD3	1:A:648:GLU:HG2	1.95	0.49
1:A:373:ASP:OD1	1:A:373:ASP:N	2.43	0.49
1:A:529:THR:HG22	1:A:558:ARG:HG2	1.94	0.49
1:B:642:SER:HG	1:B:645:GLY:H	1.59	0.49
1:B:464:GLN:HG2	1:B:469:ASP:HB2	1.95	0.49
1:B:438:GLY:O	1:B:718:ARG:HG3	2.13	0.49
1:C:570:LEU:HD22	1:C:600:ILE:HG13	1.95	0.49
1:C:483:ASN:OD1	1:C:484:CYS:N	2.46	0.48
1:B:748:ASP:HA	1:B:751:THR:OG1	2.12	0.48
1:C:539:LEU:HB2	1:C:568:PRO:HB2	1.94	0.48
1:A:694:TYR:CE1	1:A:711:VAL:HB	2.48	0.48
1:B:561:VAL:HG23	1:B:732:ILE:O	2.14	0.48
1:C:262:ASN:HB3	1:C:284:GLU:HG3	1.95	0.48
1:A:505:GLN:HG3	1:A:506:ASP:OD2	2.14	0.48
1:B:483:ASN:OD1	1:B:501:GLY:HA3	2.13	0.48
1:A:415:ASN:ND2	1:A:418:GLN:OE1	2.47	0.48
1:C:340:ASP:O	1:C:355:LYS:HE3	2.14	0.48
1:B:337:ARG:HG3	1:B:337:ARG:HH21	1.78	0.48
1:B:367:ARG:HH21	1:B:371:CYS:HB3	1.75	0.47
1:A:660:THR:HB	1:A:663:GLN:HB2	1.96	0.47
1:B:466:ASP:O	1:B:469:ASP:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASP:OD2	1:B:360:LYS:HB2	2.14	0.47
1:B:473:ASP:O	1:B:475:ASP:N	2.42	0.47
1:A:494:ASP:OD1	1:A:501:GLY:HA2	2.14	0.47
1:B:487:VAL:HG11	1:B:504:CYS:HB3	1.97	0.47
1:C:583:GLU:CG	1:C:738:ARG:HB2	2.45	0.47
1:B:670:ASP:OD1	1:B:672:ARG:HG3	2.14	0.47
1:A:269:ASP:OD1	1:A:272:LEU:N	2.47	0.47
1:A:527:THR:HG23	1:A:528:LEU:HB2	1.95	0.47
1:B:241:ALA:HA	1:B:255:CYS:HA	1.97	0.47
1:C:746:PRO:HB3	4:C:1003:SO4:O1	2.15	0.47
1:C:626:PRO:HG3	1:C:649:GLN:HA	1.97	0.47
1:C:583:GLU:HG3	1:C:683:ARG:NH2	2.30	0.47
1:A:570:LEU:HD22	1:A:600:ILE:HG13	1.97	0.47
1:C:692:VAL:CG2	1:C:749:TYR:CZ	2.97	0.47
1:A:446:ASP:C	1:A:448:CYS:H	2.18	0.47
1:B:550:ASN:H	1:B:562:GLN:HE21	1.63	0.47
1:A:640:VAL:HG22	1:A:664:VAL:HG22	1.96	0.47
1:C:638:LYS:HG2	1:C:666:LEU:HA	1.97	0.47
1:B:238:HIS:CG	1:B:239:GLU:H	2.33	0.47
1:B:238:HIS:CG	1:B:239:GLU:N	2.83	0.46
1:C:432:SER:O	1:C:433:ASP:C	2.53	0.46
1:B:568:PRO:HG3	1:B:727:PHE:CE2	2.50	0.46
1:B:285:ARG:O	1:B:287:CYS:N	2.49	0.46
1:B:513:VAL:HG21	1:B:527:THR:OG1	2.15	0.46
1:C:304:ASP:C	1:C:305:ARG:HG2	2.34	0.46
1:C:560:ILE:HG22	1:C:561:VAL:N	2.29	0.46
1:B:750:GLU:HA	1:B:753:GLN:HB2	1.97	0.46
1:C:333:ASN:N	1:C:334:PRO:HD3	2.30	0.46
1:B:698:ARG:HB3	1:B:705:LEU:HD11	1.96	0.46
1:C:475:ASP:HB3	1:C:488:PRO:CB	2.46	0.46
1:C:500:VAL:HG23	1:C:504:CYS:SG	2.55	0.46
1:B:403:ILE:HG21	1:B:418:GLN:NE2	2.30	0.46
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.71	0.46
1:C:428:ASP:C	1:C:430:CYS:H	2.19	0.46
1:B:248:ASP:OD1	1:B:248:ASP:N	2.47	0.46
1:B:542:GLU:N	1:B:542:GLU:OE1	2.48	0.46
1:A:337:ARG:NH2	1:A:337:ARG:CG	2.69	0.46
1:A:457:GLU:H	1:A:457:GLU:CD	2.19	0.46
1:B:409:ASN:O	1:B:445:ARG:NH2	2.48	0.46
1:B:291:ASN:H	1:B:300:GLN:HE22	1.63	0.46
1:C:506:ASP:HB3	1:C:514:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:CYS:CB	1:A:526:VAL:CG1	2.90	0.46
1:A:497:ARG:HD3	1:A:498:ASP:N	2.30	0.46
1:C:489:ASN:HD21	1:C:492:GLN:HG2	1.81	0.46
1:B:711:VAL:HG21	1:B:752:HIS:CB	2.46	0.46
1:C:464:GLN:HG3	1:C:469:ASP:OD2	2.14	0.46
1:C:227:ARG:NH2	1:C:227:ARG:CG	2.69	0.45
1:C:692:VAL:HG21	1:C:749:TYR:CE2	2.51	0.45
1:B:550:ASN:O	1:B:562:GLN:HA	2.16	0.45
1:B:320:GLY:O	1:B:322:PRO:HD3	2.17	0.45
1:C:319:ASP:HB3	1:C:332:ARG:HB3	1.97	0.45
1:A:550:ASN:HD21	1:A:563:THR:HG1	1.62	0.45
1:C:686:LEU:HG	1:C:687:GLN:N	2.28	0.45
1:B:239:GLU:HG3	1:C:228:PHE:CE2	2.51	0.45
1:A:482:ASP:OD1	1:A:483:ASN:N	2.49	0.45
1:C:378:ASP:C	1:C:380:ILE:H	2.20	0.45
1:C:331:VAL:CG1	1:C:348:CYS:HB3	2.45	0.45
1:B:337:ARG:HG3	1:B:337:ARG:NH2	2.32	0.45
1:A:692:VAL:HG22	1:A:749:TYR:OH	2.17	0.45
1:B:682:TYR:CE2	1:B:701:GLU:HG3	2.51	0.45
1:A:475:ASP:HB3	1:A:488:PRO:HA	1.98	0.45
1:C:422:ASP:N	1:C:422:ASP:OD2	2.49	0.45
1:A:614:TRP:CD2	1:A:635:ILE:HD13	2.52	0.45
1:C:729:GLN:HB3	1:C:732:ILE:HD11	1.97	0.45
1:A:502:ASP:C	1:A:504:CYS:H	2.19	0.45
1:B:689:ARG:HB3	1:B:691:GLN:HE21	1.82	0.45
1:A:668:TRP:CE2	1:A:709:SER:HA	2.52	0.45
1:C:378:ASP:O	1:C:380:ILE:HG22	2.16	0.45
1:A:337:ARG:NH2	1:A:337:ARG:HG3	2.14	0.45
1:C:638:LYS:NZ	1:C:656:HIS:O	2.50	0.45
1:B:473:ASP:HB3	1:B:486:LEU:O	2.16	0.44
1:A:518:ASP:OD1	1:A:521:PRO:HA	2.16	0.44
1:C:378:ASP:O	1:C:380:ILE:N	2.51	0.44
1:C:380:ILE:HG12	1:C:385:ASP:HB2	1.98	0.44
1:B:392:ASN:O	1:B:392:ASN:CG	2.55	0.44
1:C:621:TYR:CE2	1:C:623:GLN:HB2	2.53	0.44
1:C:475:ASP:HB3	1:C:488:PRO:HA	1.99	0.44
1:B:627:PHE:O	1:B:652:ASN:ND2	2.50	0.44
1:C:520:CYS:C	1:C:522:GLU:H	2.21	0.44
1:B:261:GLY:HA2	1:B:286:GLN:O	2.17	0.44
1:A:590:THR:OG1	1:A:592:THR:HG23	2.18	0.44
1:B:410:CYS:O	1:B:412:GLN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ASP:OD2	1:B:472:ASP:HA	2.18	0.44
1:C:668:TRP:CE2	1:C:709:SER:HA	2.52	0.44
1:B:612:VAL:HG22	1:B:637:LEU:HD23	2.00	0.44
1:B:424:ASP:O	1:B:425:PHE:HB2	2.18	0.44
1:C:648:GLU:HA	1:C:651:ARG:NH2	2.33	0.44
1:B:637:LEU:HD12	1:B:667:LEU:HB2	2.00	0.44
1:B:351:CYS:HB2	1:B:356:ASN:ND2	2.33	0.44
1:C:286:GLN:CD	1:C:286:GLN:H	2.22	0.44
1:C:662:SER:O	1:C:662:SER:OG	2.35	0.44
1:C:373:ASP:HA	1:C:382:ASN:ND2	2.32	0.44
1:A:386:ASN:H	1:A:395:GLN:HE22	1.65	0.43
1:C:582:PHE:CD2	1:C:722:LEU:HD22	2.53	0.43
1:B:552:VAL:HB	1:B:561:VAL:HG13	1.99	0.43
1:C:421:VAL:HG23	1:C:428:ASP:OD2	2.18	0.43
1:C:518:ASP:OD1	1:C:521:PRO:HA	2.18	0.43
1:A:740:ARG:HH11	3:A:901:NAG:C8	2.31	0.43
1:B:608:SER:HA	1:B:640:VAL:O	2.18	0.43
1:C:415:ASN:O	1:C:416:PRO:C	2.57	0.43
1:B:386:ASN:OD1	1:B:392:ASN:ND2	2.48	0.43
1:A:635:ILE:HG12	1:A:635:ILE:H	1.42	0.43
1:B:559:GLU:HG3	1:B:735:ALA:HA	1.99	0.43
1:A:684:TRP:CD1	1:A:684:TRP:C	2.92	0.43
1:A:503:VAL:O	1:A:503:VAL:HG12	2.18	0.43
1:C:625:ASN:N	1:C:625:ASN:OD1	2.51	0.43
1:A:437:ASP:O	1:A:718:ARG:HD2	2.18	0.43
1:B:486:LEU:HD12	1:B:508:PHE:CD2	2.52	0.43
1:A:265:LEU:HA	1:A:265:LEU:HD13	1.84	0.43
1:C:583:GLU:HG3	1:C:683:ARG:HH21	1.82	0.43
1:B:437:ASP:OD2	1:B:452:PRO:HA	2.18	0.43
1:A:620:THR:HG21	1:A:628:ARG:NH1	2.34	0.43
1:C:399:ASP:HB2	1:C:414:SER:OG	2.19	0.43
1:A:532:ARG:H	1:A:532:ARG:HG2	1.55	0.43
1:B:732:ILE:HB	1:B:734:TRP:CH2	2.54	0.43
1:A:696:ARG:HG2	1:A:710:ASN:O	2.18	0.43
1:B:632:GLU:HG2	1:B:673:ASN:OD1	2.18	0.43
1:C:460:ASP:HB2	1:C:474:ASN:ND2	2.33	0.43
1:B:574:TYR:HA	1:B:721:ARG:NH1	2.33	0.43
1:B:603:TYR:HA	1:B:609:PHE:HB3	2.01	0.42
1:A:364:GLN:HE21	1:A:364:GLN:N	2.17	0.42
1:B:394:ASP:O	1:B:395:GLN:HB2	2.18	0.42
1:B:612:VAL:HG11	1:B:699:PHE:HZ	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:CG2	1:A:313:ASP:HB2	2.48	0.42
1:C:578:ASN:HB3	1:C:579:GLY:H	1.67	0.42
1:B:691:GLN:CD	1:B:691:GLN:H	2.23	0.42
1:A:460:ASP:HB2	1:A:474:ASN:ND2	2.34	0.42
1:A:324:GLU:H	1:A:324:GLU:CD	2.22	0.42
1:B:285:ARG:C	1:B:287:CYS:H	2.23	0.42
1:B:549:PRO:HA	1:B:562:GLN:NE2	2.34	0.42
1:C:342:ASP:HB2	1:C:357:ASP:OD2	2.20	0.42
1:C:670:ASP:HA	1:C:671:PRO:HD3	1.95	0.42
1:B:705:LEU:O	1:B:705:LEU:HD23	2.19	0.42
1:A:484:CYS:O	1:A:486:LEU:N	2.52	0.42
1:A:600:ILE:HA	1:A:600:ILE:HD13	1.87	0.42
1:C:520:CYS:HB2	1:C:526:VAL:HG13	2.01	0.42
1:B:401:ASP:HB3	1:B:414:SER:HA	2.01	0.42
1:B:702:GLY:HA3	1:B:703:PRO:HD2	1.88	0.42
1:B:484:CYS:HB2	1:B:489:ASN:OD1	2.20	0.42
1:B:639:ALA:HB2	1:B:667:LEU:HD11	2.02	0.42
1:C:530:ASP:OD2	1:C:532:ARG:HG2	2.20	0.42
1:B:579:GLY:HA2	1:B:688:HIS:O	2.20	0.42
1:B:367:ARG:CZ	1:B:371:CYS:HB3	2.49	0.42
1:C:459:SER:C	1:C:461:HIS:H	2.23	0.42
1:C:380:ILE:HG21	1:C:395:GLN:OE1	2.19	0.42
1:C:617:MET:HE2	1:C:617:MET:HB2	1.95	0.42
1:C:558:ARG:NH2	1:C:736:ASN:OD1	2.52	0.42
1:A:351:CYS:HB3	1:A:354:GLN:HB3	2.01	0.42
1:B:616:GLN:HG2	1:B:617:MET:HG2	2.02	0.41
1:C:618:GLU:OE1	1:C:632:GLU:HG2	2.20	0.41
1:B:410:CYS:C	1:B:412:GLN:N	2.74	0.41
1:A:447:ASN:O	1:A:448:CYS:HB2	2.20	0.41
1:B:337:ARG:HG2	1:B:338:ASN:N	2.35	0.41
1:A:284:GLU:O	1:A:285:ARG:O	2.37	0.41
1:A:690:PRO:HB3	1:A:718:ARG:C	2.41	0.41
1:B:595:ASP:HB2	1:B:728:SER:O	2.20	0.41
1:B:615:LYS:HE2	1:B:655:TRP:CH2	2.55	0.41
1:C:627:PHE:HD2	1:C:628:ARG:O	2.03	0.41
1:A:747:GLU:HG2	3:A:902:NAG:H83	2.02	0.41
1:A:713:LEU:HD12	1:A:713:LEU:HA	1.94	0.41
1:A:594:ASP:N	1:A:594:ASP:OD1	2.53	0.41
1:B:302:ASP:CG	1:B:305:ARG:HA	2.41	0.41
1:B:505:GLN:OE1	1:B:505:GLN:HA	2.20	0.41
1:B:635:ILE:CD1	1:B:635:ILE:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:C	1:A:287:CYS:H	2.23	0.41
1:C:487:VAL:HG22	1:C:504:CYS:HB3	2.02	0.41
1:B:422:ASP:N	1:B:422:ASP:OD2	2.53	0.41
1:B:727:PHE:CD2	1:B:727:PHE:C	2.94	0.41
1:C:378:ASP:OD2	1:C:391:PRO:HA	2.21	0.41
1:A:602:GLY:HA2	1:A:720:GLY:HA3	2.02	0.41
1:A:244:VAL:O	1:A:244:VAL:CG2	2.64	0.41
1:C:265:LEU:HD13	1:C:265:LEU:HA	1.76	0.41
1:A:747:GLU:C	1:A:749:TYR:H	2.23	0.41
1:A:742:ASN:OD1	1:A:744:THR:HG23	2.20	0.41
1:C:358:ASP:OD1	1:C:360:LYS:HB2	2.21	0.41
1:C:745:ILE:H	1:C:745:ILE:HG12	1.56	0.41
1:B:494:ASP:HB2	1:B:501:GLY:HA2	2.03	0.41
1:B:253:CYS:HB2	1:B:263:GLY:HA3	2.02	0.41
1:A:305:ARG:CZ	1:A:305:ARG:HB3	2.48	0.41
1:C:328:CYS:HB2	1:C:333:ASN:OD1	2.21	0.41
1:A:508:PHE:O	1:A:508:PHE:CD2	2.74	0.41
1:C:497:ARG:HA	1:C:497:ARG:HD3	1.50	0.41
1:B:483:ASN:CG	1:B:484:CYS:N	2.75	0.41
1:B:484:CYS:HB2	1:B:489:ASN:ND2	2.36	0.41
1:C:621:TYR:HB2	1:C:655:TRP:NE1	2.35	0.41
1:A:605:ASP:OD1	1:A:608:SER:N	2.53	0.41
1:B:549:PRO:CA	1:B:562:GLN:HE21	2.34	0.40
1:B:615:LYS:HE2	1:B:655:TRP:CZ2	2.56	0.40
1:A:477:VAL:HG21	1:A:492:GLN:NE2	2.36	0.40
1:C:696:ARG:CZ	1:C:698:ARG:NH2	2.84	0.40
1:B:284:GLU:O	1:B:285:ARG:C	2.59	0.40
1:A:284:GLU:HB2	1:A:286:GLN:NE2	2.36	0.40
1:B:485:ARG:NH2	1:B:486:LEU:HD21	2.35	0.40
1:A:343:LYS:HG3	1:A:357:ASP:OD1	2.21	0.40
1:C:291:ASN:H	1:C:300:GLN:NE2	2.10	0.40
1:B:412:GLN:O	1:B:413:LYS:HE3	2.21	0.40
1:C:490:PRO:HB2	1:C:491:GLY:H	1.71	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	533/551 (97%)	443 (83%)	74 (14%)	16 (3%)	5	34
1	B	533/551 (97%)	435 (82%)	82 (15%)	16 (3%)	5	34
1	C	533/551 (97%)	443 (83%)	72 (14%)	18 (3%)	5	29
All	All	1599/1653 (97%)	1321 (83%)	228 (14%)	50 (3%)	5	32

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	B	474	ASN
1	B	543	GLY
1	C	352	ARG
1	C	379	ARG
1	C	490	PRO
1	C	492	GLN
1	A	283	PRO
1	A	286	GLN
1	A	336	GLN
1	A	379	ARG
1	A	485	ARG
1	B	348	CYS
1	B	414	SER
1	B	594	ASP
1	C	406	ALA
1	C	543	GLY
1	A	392	ASN
1	A	399	ASP
1	A	475	ASP
1	A	510	ALA
1	B	305	ARG
1	C	382	ASN
1	C	421	VAL

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Mol	Chain	Res	Type
1	C	429	ALA
1	A	505	GLN
1	B	350	ASN
1	B	458	ASP
1	C	300	GLN
1	C	364	GLN
1	C	428	ASP
1	C	626	PRO
1	A	348	CYS
1	A	474	ASN
1	A	594	ASP
1	A	661	GLU
1	B	286	GLN
1	B	378	ASP
1	B	406	ALA
1	B	648	GLU
1	C	348	CYS
1	C	467	ALA
1	A	356	ASN
1	B	398	SER
1	B	519	VAL
1	C	359	GLN
1	C	499	GLY
1	B	283	PRO
1	B	646	PRO
1	C	377	GLY

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	459/473 (97%)	394 (86%)	65 (14%)	4	19
1	B	459/473 (97%)	410 (89%)	49 (11%)	8	32
1	C	459/473 (97%)	405 (88%)	54 (12%)	6	28
All	All	1377/1419 (97%)	1209 (88%)	168 (12%)	6	26

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	A	244	VAL
1	A	246	GLU
1	A	247	ARG
1	A	265	LEU
1	A	268	ARG
1	A	281	ARG
1	A	286	GLN
1	A	288	ARG
1	A	305	ARG
1	A	324	GLU
1	A	331	VAL
1	A	332	ARG
1	A	337	ARG
1	A	352	ARG
1	A	357	ASP
1	A	364	GLN
1	A	373	ASP
1	A	375	ILE
1	A	380	ILE
1	A	393	SER
1	A	396	LYS
1	A	412	GLN
1	A	436	GLN
1	A	442	GLN
1	A	444	SER
1	A	445	ARG
1	A	450	THR
1	A	468	CYS
1	A	493	GLU
1	A	497	ARG
1	A	512	LYS
1	A	516	LYS
1	A	522	GLU
1	A	525	GLU
1	A	536	THR
1	A	539	LEU
1	A	550	ASN
1	A	553	VAL
1	A	561	VAL
1	A	562	GLN
1	A	575	THR

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Mol	Chain	Res	Type
1	A	588	VAL
1	A	591	VAL
1	A	592	THR
1	A	593	ASP
1	A	617	MET
1	A	630	VAL
1	A	635	ILE
1	A	646	PRO
1	A	660	THR
1	A	662	SER
1	A	666	LEU
1	A	684	TRP
1	A	692	VAL
1	A	696	ARG
1	A	698	ARG
1	A	711	VAL
1	A	713	LEU
1	A	717	MET
1	A	730	GLU
1	A	737	LEU
1	A	744	THR
1	A	753	GLN
1	A	756	GLN
1	B	227	ARG
1	B	251	ARG
1	B	257	VAL
1	B	280	LEU
1	B	282	CYS
1	B	285	ARG
1	B	305	ARG
1	B	324	GLU
1	B	332	ARG
1	B	367	ARG
1	B	413	LYS
1	B	414	SER
1	B	436	GLN
1	B	450	THR
1	B	460	ASP
1	B	473	ASP
1	B	480	SER
1	B	481	ARG
1	B	485	ARG

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Mol	Chain	Res	Type
1	B	496	ASP
1	B	497	ARG
1	B	500	VAL
1	B	506	ASP
1	B	517	ILE
1	B	525	GLU
1	B	535	GLN
1	B	536	THR
1	B	542	GLU
1	B	546	GLN
1	B	588	VAL
1	B	592	THR
1	B	593	ASP
1	B	620	THR
1	B	632	GLU
1	B	643	SER
1	B	666	LEU
1	B	683	ARG
1	B	691	GLN
1	B	697	VAL
1	B	705	LEU
1	B	710	ASN
1	B	716	THR
1	B	727	PHE
1	B	730	GLU
1	B	732	ILE
1	B	737	LEU
1	B	738	ARG
1	B	754	LEU
1	B	756	GLN
1	C	227	ARG
1	C	251	ARG
1	C	282	CYS
1	C	285	ARG
1	C	288	ARG
1	C	305	ARG
1	C	324	GLU
1	C	331	VAL
1	C	346	ASP
1	C	360	LYS
1	C	364	GLN
1	C	367	ARG

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Mol	Chain	Res	Type
1	C	383	GLN
1	C	389	ARG
1	C	412	GLN
1	C	433	ASP
1	C	442	GLN
1	C	477	VAL
1	C	487	VAL
1	C	492	GLN
1	C	493	GLU
1	C	494	ASP
1	C	496	ASP
1	C	497	ARG
1	C	503	VAL
1	C	506	ASP
1	C	516	LYS
1	C	525	GLU
1	C	536	THR
1	C	538	VAL
1	C	539	LEU
1	C	553	VAL
1	C	562	GLN
1	C	572	VAL
1	C	575	THR
1	C	588	VAL
1	C	593	ASP
1	C	625	ASN
1	C	665	ARG
1	C	666	LEU
1	C	667	LEU
1	C	672	ARG
1	C	683	ARG
1	C	692	VAL
1	C	696	ARG
1	C	698	ARG
1	C	711	VAL
1	C	713	LEU
1	C	717	MET
1	C	727	PHE
1	C	730	GLU
1	C	737	LEU
1	C	745	ILE
1	C	755	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	GLN
1	A	364	GLN
1	A	395	GLN
1	A	436	GLN
1	A	492	GLN
1	A	550	ASN
1	A	555	ASN
1	A	663	GLN
1	A	731	ASN
1	B	223	ASN
1	B	300	GLN
1	B	436	GLN
1	B	442	GLN
1	B	535	GLN
1	B	546	GLN
1	B	562	GLN
1	B	587	HIS
1	B	663	GLN
1	B	691	GLN
1	B	731	ASN
1	B	753	GLN
1	B	756	GLN
1	C	300	GLN
1	C	364	GLN
1	C	383	GLN
1	C	412	GLN
1	C	418	GLN
1	C	423	HIS
1	C	550	ASN
1	C	589	ASN
1	C	649	GLN
1	C	663	GLN
1	C	731	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 ⓘ

12 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	901	1,3	14,14,15	0.57	0	15,19,21	2.10	7 (46%)
3	NAG	A	902	3	14,14,15	0.74	0	15,19,21	1.36	2 (13%)
3	MAN	A	903	3	11,11,12	1.00	1 (9%)	14,15,17	1.29	1 (7%)
3	MAN	A	904	3	11,11,12	0.80	0	14,15,17	1.52	1 (7%)
5	NAG	B	901	1,5	14,14,15	0.85	0	15,19,21	1.23	2 (13%)
5	NAG	B	902	5	14,14,15	0.80	1 (7%)	15,19,21	1.83	4 (26%)
5	MAN	B	903	5	11,11,12	0.64	0	14,15,17	1.60	2 (14%)
6	NAG	C	901	1,6	14,14,15	0.60	0	15,19,21	1.07	1 (6%)
6	NAG	C	902	6	14,14,15	0.87	0	15,19,21	2.05	4 (26%)
6	MAN	C	903	6	11,11,12	0.58	0	14,15,17	1.55	3 (21%)
6	MAN	C	904	6	11,11,12	0.51	0	14,15,17	1.53	2 (14%)
6	MAN	C	905	6	11,11,12	0.81	0	14,15,17	1.96	5 (35%)

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	NAG	A	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	902	3	-	0/6/23/26	0/1/1/1
3	MAN	A	903	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	904	3	-	0/2/19/22	0/1/1/1
5	NAG	B	901	1,5	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	902	5	-	0/6/23/26	0/1/1/1
5	MAN	B	903	5	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	C	901	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	902	6	-	0/6/23/26	0/1/1/1
6	MAN	C	903	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	904	6	-	0/2/19/22	0/1/1/1
6	MAN	C	905	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	NAG	O5-C1	-2.16	1.40	1.43
3	A	903	MAN	C2-C3	2.19	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	902	NAG	C2-N2-C7	-5.38	116.13	123.04
5	B	902	NAG	C4-C3-C2	-3.56	105.69	111.23
6	C	902	NAG	C3-C2-N2	-3.52	102.12	110.56
6	C	902	NAG	O4-C4-C3	-2.96	103.67	110.34
3	A	902	NAG	O4-C4-C3	-2.95	103.70	110.34
5	B	902	NAG	C1-O5-C5	-2.52	109.05	112.25
5	B	902	NAG	O7-C7-C8	-2.43	117.60	122.06
6	C	902	NAG	O6-C6-C5	-2.37	103.52	111.33
3	A	901	NAG	C3-C2-N2	-2.31	105.02	110.56
6	C	901	NAG	O3-C3-C4	-2.20	105.38	110.34
5	B	901	NAG	O4-C4-C3	-2.19	105.40	110.34
3	A	901	NAG	O4-C4-C3	-2.16	105.48	110.34
3	A	902	NAG	C3-C2-N2	-2.14	105.42	110.56
6	C	903	MAN	O4-C4-C3	-2.09	105.63	110.34
6	C	904	MAN	C3-C4-C5	-2.06	106.61	110.20
3	A	901	NAG	O7-C7-C8	-2.00	118.39	122.06
6	C	905	MAN	C1-C2-C3	2.05	111.96	109.54
3	A	901	NAG	O3-C3-C2	2.13	113.34	109.11
6	C	905	MAN	O2-C2-C3	2.30	114.75	110.12
6	C	905	MAN	C2-C3-C4	2.42	115.16	111.04
3	A	901	NAG	C2-N2-C7	2.43	126.16	123.04
3	A	901	NAG	C8-C7-N2	3.03	121.90	116.11
6	C	905	MAN	C3-C4-C5	3.32	115.98	110.20
3	A	903	MAN	C2-C3-C4	3.38	116.79	111.04
5	B	902	NAG	C8-C7-N2	3.40	122.61	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	903	MAN	C1-O5-C5	3.41	116.58	112.25
5	B	901	NAG	C4-C3-C2	3.43	116.56	111.23
5	B	903	MAN	C1-O5-C5	3.53	116.73	112.25
6	C	903	MAN	C3-C4-C5	3.74	116.72	110.20
5	B	903	MAN	C3-C4-C5	3.81	116.84	110.20
3	A	904	MAN	C1-C2-C3	4.32	114.65	109.54
6	C	905	MAN	C1-O5-C5	4.44	117.89	112.25
6	C	904	MAN	C1-O5-C5	4.46	117.91	112.25
3	A	901	NAG	C1-O5-C5	4.69	118.20	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	903	MAN	C1
6	C	903	MAN	C1
3	A	903	MAN	C1
5	B	901	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	NAG	2	0
3	A	902	NAG	1	0

5.6 Ligand geometry

Of 98 ligands modelled in this entry, 88 are monoatomic - leaving 10 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	$\# Z > 2$
4	SO4	A	1001	-	4,4,4	0.21	0	6,6,6	0.37	0
4	SO4	A	1002	-	4,4,4	0.23	0	6,6,6	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1003	-	4,4,4	0.23	0	6,6,6	0.12	0
4	SO4	A	1004	-	4,4,4	0.07	0	6,6,6	0.18	0
4	SO4	A	1005	-	4,4,4	0.18	0	6,6,6	0.10	0
4	SO4	B	1001	-	4,4,4	0.16	0	6,6,6	0.31	0
4	SO4	B	1002	-	4,4,4	0.26	0	6,6,6	0.43	0
4	SO4	C	1001	-	4,4,4	0.27	0	6,6,6	0.21	0
4	SO4	C	1002	-	4,4,4	0.17	0	6,6,6	0.16	0
4	SO4	C	1003	-	4,4,4	0.27	0	6,6,6	0.22	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
4	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1003	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1003	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	535/551 (97%)	-0.09	9 (1%) 73 59	33, 49, 76, 91	0
1	B	535/551 (97%)	0.03	11 (2%) 67 50	24, 54, 70, 82	0
1	C	535/551 (97%)	0.01	13 (2%) 62 45	38, 54, 77, 85	0
All	All	1605/1653 (97%)	-0.02	33 (2%) 67 50	24, 52, 75, 91	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	754	LEU	4.9
1	C	429	ALA	4.0
1	B	757	ALA	3.5
1	A	495	ALA	3.1
1	C	406	ALA	3.1
1	A	490	PRO	3.1
1	A	506	ASP	2.9
1	C	754	LEU	2.9
1	C	490	PRO	2.8
1	A	757	ALA	2.7
1	C	416	PRO	2.5
1	B	756	GLN	2.4
1	A	280	LEU	2.3
1	C	486	LEU	2.3
1	A	755	ARG	2.3
1	A	416	PRO	2.3
1	B	481	ARG	2.3
1	A	480	SER	2.2
1	C	434	GLN	2.2
1	C	470	ASP	2.2
1	B	429	ALA	2.2
1	B	492	GLN	2.2
1	B	692	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	479	ASP	2.2
1	C	430	CYS	2.1
1	C	396	LYS	2.1
1	C	383	GLN	2.1
1	B	445	ARG	2.1
1	B	470	ASP	2.1
1	C	405	ASP	2.1
1	C	334	PRO	2.1
1	A	502	ASP	2.1
1	B	384	ALA	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	B	901	14/15	0.94	0.15	-1.27	78,84,86,87	0
3	NAG	A	901	14/15	0.95	0.14	-1.41	61,67,71,74	0
6	NAG	C	901	14/15	0.96	0.17	-1.87	64,69,72,77	0
6	MAN	C	904	11/12	0.73	0.27	-	84,88,90,90	11
6	MAN	C	905	11/12	0.72	0.40	-	87,91,93,95	11
5	NAG	B	902	14/15	0.91	0.21	-	84,86,90,93	14
5	MAN	B	903	11/12	0.80	0.23	-	85,89,90,90	11
6	MAN	C	903	11/12	0.87	0.19	-	91,93,95,95	11
3	MAN	A	903	11/12	0.89	0.23	-	96,98,101,101	11
6	NAG	C	902	14/15	0.91	0.18	-	79,82,85,90	0
3	NAG	A	902	14/15	0.91	0.19	-	70,81,90,91	0
3	MAN	A	904	11/12	0.86	0.24	-	97,99,100,100	11

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	SO4	A	1003	5/5	0.75	0.39	4.89	106,107,107,107	5
4	SO4	C	1003	5/5	0.80	0.37	3.03	97,97,98,98	5
4	SO4	A	1002	5/5	0.87	0.27	1.56	94,94,97,97	5
2	CA	B	828	1/1	0.92	0.20	0.81	69,69,69,69	0
2	CA	C	828	1/1	0.97	0.20	0.78	58,58,58,58	0
2	CA	C	810	1/1	0.85	0.27	0.38	174,174,174,174	0
2	CA	C	801	1/1	0.97	0.20	0.01	52,52,52,52	0
2	CA	A	802	1/1	1.00	0.16	-0.03	58,58,58,58	0
2	CA	B	829	1/1	0.83	0.17	-0.14	89,89,89,89	0
2	CA	B	804	1/1	0.94	0.16	-0.17	83,83,83,83	0
2	CA	A	826	1/1	0.99	0.15	-0.41	86,86,86,86	0
2	CA	C	802	1/1	0.99	0.17	-0.52	50,50,50,50	0
2	CA	B	825	1/1	0.98	0.15	-0.55	111,111,111,111	0
2	CA	A	807	1/1	0.96	0.15	-0.57	61,61,61,61	0
2	CA	B	801	1/1	0.96	0.18	-0.61	70,70,70,70	0
2	CA	A	801	1/1	0.99	0.15	-0.65	56,56,56,56	0
2	CA	B	826	1/1	0.96	0.14	-0.68	86,86,86,86	0
2	CA	B	827	1/1	0.99	0.14	-0.78	62,62,62,62	0
2	CA	B	807	1/1	0.98	0.15	-0.81	56,56,56,56	0
2	CA	C	817	1/1	0.97	0.14	-0.81	105,105,105,105	0
2	CA	C	807	1/1	0.96	0.13	-0.83	65,65,65,65	0
2	CA	A	821	1/1	0.81	0.16	-0.83	104,104,104,104	0
2	CA	B	820	1/1	0.96	0.14	-0.86	118,118,118,118	0
2	CA	B	803	1/1	0.97	0.14	-0.88	65,65,65,65	0
2	CA	A	817	1/1	0.99	0.14	-0.96	81,81,81,81	0
2	CA	A	803	1/1	0.96	0.13	-0.96	76,76,76,76	0
2	CA	B	805	1/1	0.99	0.14	-1.04	55,55,55,55	0
2	CA	A	828	1/1	0.96	0.14	-1.04	54,54,54,54	0
2	CA	B	818	1/1	0.98	0.13	-1.08	106,106,106,106	0
2	CA	B	806	1/1	0.99	0.12	-1.12	54,54,54,54	0
2	CA	C	827	1/1	0.98	0.13	-1.12	47,47,47,47	0
2	CA	A	812	1/1	0.97	0.09	-1.17	70,70,70,70	0
2	CA	B	810	1/1	0.92	0.07	-1.23	109,109,109,109	0
2	CA	C	805	1/1	0.97	0.13	-1.28	75,75,75,75	0
2	CA	A	811	1/1	0.94	0.11	-1.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	827	1/1	0.98	0.14	-1.30	64,64,64,64	0
2	CA	A	800	1/1	0.86	0.16	-1.31	65,65,65,65	0
2	CA	A	805	1/1	0.94	0.12	-1.34	60,60,60,60	0
2	CA	C	806	1/1	0.98	0.09	-1.40	72,72,72,72	0
2	CA	B	817	1/1	0.98	0.09	-1.40	127,127,127,127	0
2	CA	A	806	1/1	0.99	0.10	-1.41	54,54,54,54	0
2	CA	C	809	1/1	0.84	0.09	-1.44	108,108,108,108	0
2	CA	C	821	1/1	0.65	0.12	-1.51	95,95,95,95	0
2	CA	B	815	1/1	0.98	0.07	-1.54	103,103,103,103	0
2	CA	A	818	1/1	0.98	0.09	-1.59	85,85,85,85	0
2	CA	B	821	1/1	0.91	0.10	-1.59	125,125,125,125	0
2	CA	A	823	1/1	0.94	0.07	-1.60	103,103,103,103	0
2	CA	A	825	1/1	0.95	0.11	-1.61	93,93,93,93	0
2	CA	C	820	1/1	0.91	0.06	-1.62	125,125,125,125	0
2	CA	C	812	1/1	0.91	0.11	-1.62	117,117,117,117	0
2	CA	C	811	1/1	0.96	0.10	-1.65	117,117,117,117	0
2	CA	B	808	1/1	0.99	0.11	-1.65	56,56,56,56	0
2	CA	A	822	1/1	0.91	0.09	-1.66	107,107,107,107	0
2	CA	B	823	1/1	0.85	0.09	-1.67	131,131,131,131	0
2	CA	B	811	1/1	0.86	0.07	-1.70	123,123,123,123	0
2	CA	C	825	1/1	0.92	0.08	-1.70	85,85,85,85	0
2	CA	A	820	1/1	0.95	0.06	-1.73	119,119,119,119	0
2	CA	A	808	1/1	0.99	0.09	-1.76	56,56,56,56	0
2	CA	B	819	1/1	0.96	0.08	-1.80	114,114,114,114	0
2	CA	C	803	1/1	0.98	0.10	-1.80	71,71,71,71	0
2	CA	A	819	1/1	0.97	0.07	-1.80	119,119,119,119	0
2	CA	C	808	1/1	0.97	0.09	-1.83	64,64,64,64	0
2	CA	A	810	1/1	0.97	0.07	-1.84	104,104,104,104	0
2	CA	B	809	1/1	0.93	0.07	-1.85	85,85,85,85	0
2	CA	C	818	1/1	0.97	0.12	-1.86	94,94,94,94	0
2	CA	C	826	1/1	0.96	0.10	-1.87	85,85,85,85	0
2	CA	B	812	1/1	0.97	0.04	-1.87	87,87,87,87	0
2	CA	A	824	1/1	0.66	0.08	-1.90	160,160,160,160	0
2	CA	A	804	1/1	0.96	0.07	-1.92	78,78,78,78	0
2	CA	A	809	1/1	0.96	0.08	-1.93	65,65,65,65	0
2	CA	B	824	1/1	0.90	0.06	-2.03	140,140,140,140	0
2	CA	B	822	1/1	0.94	0.09	-2.06	114,114,114,114	0
2	CA	C	823	1/1	0.98	0.04	-2.07	111,111,111,111	0
2	CA	A	813	1/1	0.98	0.06	-2.13	81,81,81,81	0
2	CA	C	819	1/1	0.86	0.04	-2.15	118,118,118,118	0
2	CA	B	802	1/1	0.99	0.14	-2.16	53,53,53,53	0
2	CA	A	829	1/1	0.96	0.12	-2.22	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	813	1/1	0.95	0.08	-2.29	111,111,111,111	0
2	CA	C	814	1/1	0.85	0.05	-2.29	119,119,119,119	0
2	CA	C	822	1/1	0.98	0.05	-2.30	118,118,118,118	0
2	CA	A	815	1/1	0.95	0.05	-2.41	115,115,115,115	0
2	CA	C	813	1/1	0.96	0.05	-2.50	119,119,119,119	0
2	CA	A	814	1/1	0.99	0.04	-2.54	101,101,101,101	0
2	CA	C	824	1/1	0.96	0.04	-2.65	115,115,115,115	0
2	CA	B	814	1/1	0.92	0.05	-2.78	121,121,121,121	0
2	CA	C	829	1/1	0.95	0.09	-2.91	109,109,109,109	0
2	CA	C	815	1/1	0.72	0.07	-2.96	125,125,125,125	0
2	CA	C	804	1/1	0.93	0.06	-4.00	74,74,74,74	0
4	SO4	C	1002	5/5	0.82	0.79	-	96,96,97,97	5
4	SO4	B	1001	5/5	0.95	0.18	-	82,82,85,85	0
2	CA	B	816	1/1	0.88	0.15	-	111,111,111,111	0
4	SO4	C	1001	5/5	0.91	0.30	-	88,89,89,89	5
2	CA	C	816	1/1	0.95	0.12	-	123,123,123,123	0
4	SO4	A	1001	5/5	0.93	0.38	-	104,105,106,106	5
4	SO4	B	1002	5/5	0.88	0.66	-	94,94,95,97	5
4	SO4	A	1005	5/5	0.72	0.54	-	108,108,108,108	5
2	CA	A	816	1/1	0.90	0.18	-	114,114,114,114	0
4	SO4	A	1004	5/5	0.76	0.32	-	105,106,106,106	5

6.5 Other polymers

There are no such residues in this entry.