



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:49 AM UTC

PDB ID : 3EE6 / pdb_00003ee6
Title : Crystal Structure Analysis of Tripeptidyl peptidase -I
Authors : Pal, A.; Kraetzner, R.; Grapp, M.; Gruene, T.; Schreiber, K.; Granborg, M.;
Urlaub, H.; Asif, A.R.; Becker, S.; Gartner, J.; Sheldrick, G.M.; Steinfeld, R.
Deposited on : 2008-09-04
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

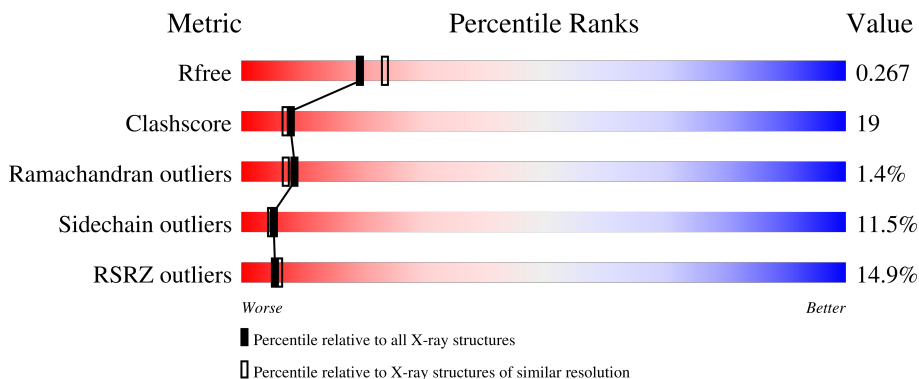
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	571	15% 63% 24% 6% 7%
1	B	571	13% 61% 24% 7% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8361 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.

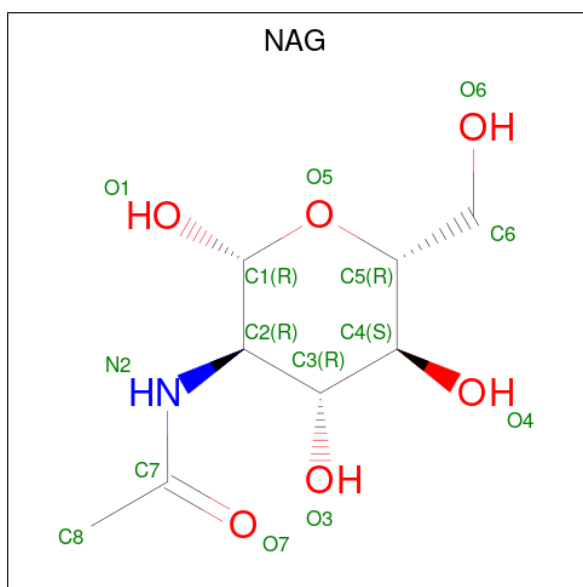
- Molecule 1 is a protein called Tripeptidyl-peptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4082	2588	714	769	11			
1	B	529	Total	C	N	O	S	0	0	0
			4080	2587	714	768	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	ARG	-	expression tag	UNP O14773
A	565	SER	-	expression tag	UNP O14773
A	566	HIS	-	expression tag	UNP O14773
A	567	HIS	-	expression tag	UNP O14773
A	568	HIS	-	expression tag	UNP O14773
A	569	HIS	-	expression tag	UNP O14773
A	570	HIS	-	expression tag	UNP O14773
A	571	HIS	-	expression tag	UNP O14773
B	564	ARG	-	expression tag	UNP O14773
B	565	SER	-	expression tag	UNP O14773
B	566	HIS	-	expression tag	UNP O14773
B	567	HIS	-	expression tag	UNP O14773
B	568	HIS	-	expression tag	UNP O14773
B	569	HIS	-	expression tag	UNP O14773
B	570	HIS	-	expression tag	UNP O14773
B	571	HIS	-	expression tag	UNP O14773

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Zn	0	0
			4	4		
3	B	4	Total	Zn	0	0
			4	4		

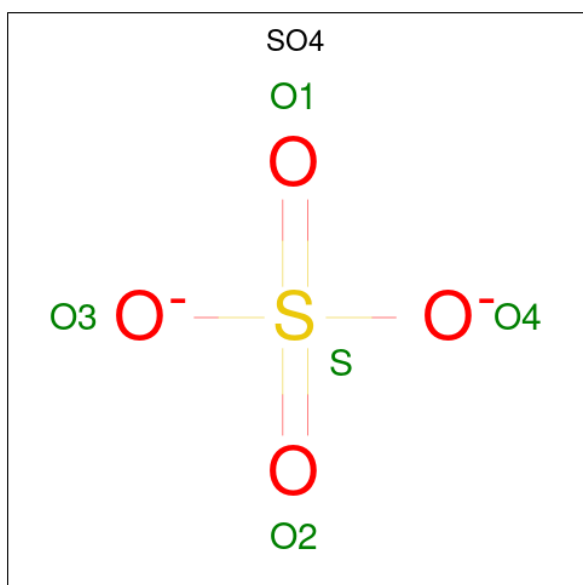
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	37	Total	O	0	0
			37	37		

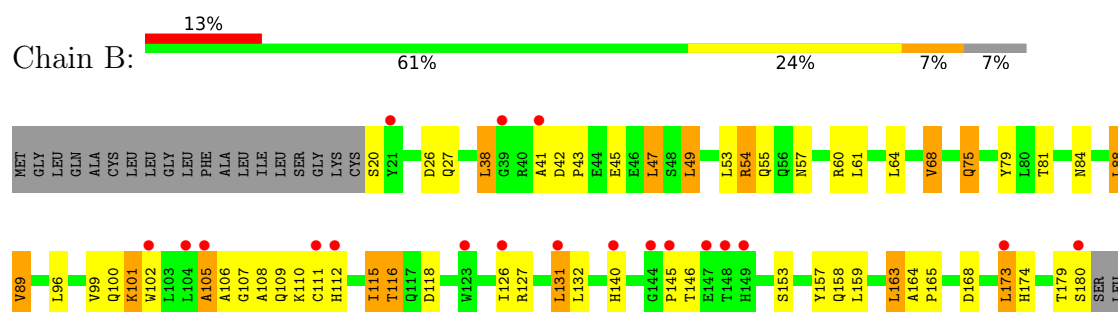
3 Residue-property plots [i](#)

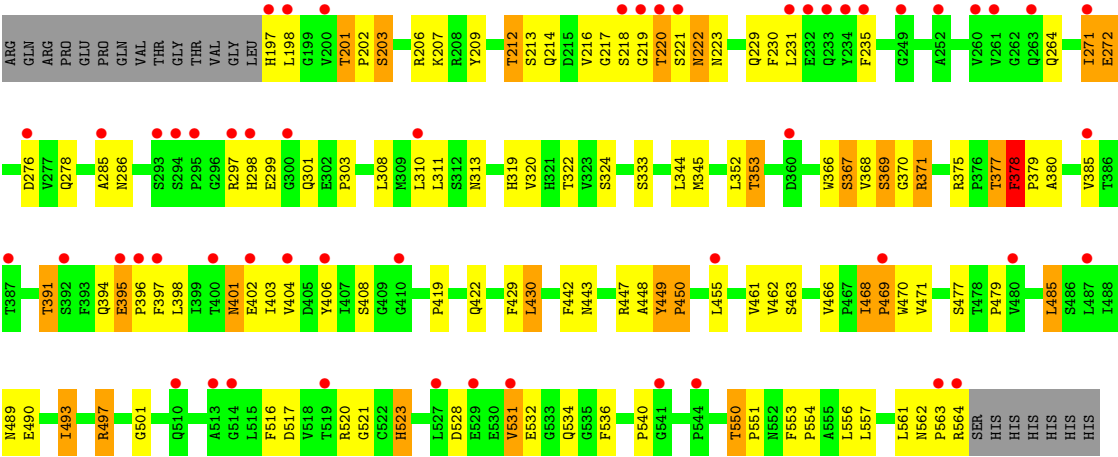
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Tripeptidyl-peptidase 1



• Molecule 1: Tripeptidyl-peptidase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.45Å 128.93Å 100.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 2.35 39.21 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.21-2.35) 99.5 (39.21-2.35)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.218 , 0.262 0.225 , 0.267	Depositor DCC
R_{free} test set	3150 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8361	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: ZN, SO4, CL, CA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/4204	1.01	8/5741 (0.1%)
1	B	0.65	0/4202	0.99	9/5739 (0.2%)
All	All	0.67	0/8406	1.00	17/11480 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	PHE	CA-C-N	9.89	132.20	119.84
1	B	378	PHE	C-N-CA	9.89	132.20	119.84
1	A	562	ASN	CA-C-N	9.60	131.84	119.84
1	A	562	ASN	C-N-CA	9.60	131.84	119.84
1	A	378	PHE	CA-C-N	7.94	129.77	119.84
1	A	378	PHE	C-N-CA	7.94	129.77	119.84
1	A	450	PRO	N-CA-C	-7.15	97.75	112.47
1	B	38	LEU	N-CA-C	-6.37	101.56	110.35
1	A	378	PHE	C-N-CD	-5.97	100.54	125.00
1	B	468	ILE	CA-C-N	5.89	127.20	119.84
1	B	468	ILE	C-N-CA	5.89	127.20	119.84
1	A	494	LEU	N-CA-C	-5.48	101.74	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	ALA	N-CA-C	-5.36	103.41	110.43
1	B	116	THR	N-CA-C	-5.30	106.77	113.18
1	B	442	PHE	N-CA-C	5.09	116.03	108.60
1	A	411	GLY	N-CA-C	5.04	116.83	110.38
1	B	378	PHE	C-N-CD	-5.02	104.42	125.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	PHE	Peptide
1	A	449	TYR	Peptide
1	B	378	PHE	Peptide
1	B	449	TYR	Peptide,Mainchain

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	4082	0	3900	148	0
1	B	4080	0	3901	167	0
2	A	52	0	44	0	0
2	B	52	0	44	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	36	0	0	0	0
7	B	37	0	0	2	0
All	All	8361	0	7889	314	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 19.

All (314) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ASN:HB3	1:A:563:PRO:CD	1.57	1.33
1:A:95:THR:HG22	1:A:166:HIS:ND1	1.56	1.20
1:A:562:ASN:CB	1:A:563:PRO:HD3	1.69	1.20
1:A:20:SER:OG	1:A:158:GLN:NE2	1.78	1.17
1:B:368:VAL:HG12	1:B:369:SER:H	1.04	1.16
1:A:146:THR:CB	1:A:232:GLU:HG2	1.82	1.09
1:B:563:PRO:O	4:B:580:CL:CL	2.09	1.08
1:B:212:THR:HG22	1:B:214:GLN:H	1.19	1.03
1:A:497:ARG:NH1	1:A:561:LEU:O	1.92	1.03
1:B:101:LYS:HG3	1:B:102:TRP:N	1.71	1.02
1:B:368:VAL:HG12	1:B:369:SER:N	1.71	1.01
1:B:102:TRP:CZ3	1:B:163:LEU:HD11	1.99	0.97
1:B:371:ARG:HH11	1:B:371:ARG:CB	1.77	0.97
1:A:391:THR:HG22	1:A:455:LEU:HA	1.48	0.96
1:B:368:VAL:CG1	1:B:369:SER:H	1.77	0.96
1:A:357:ALA:HB1	1:A:474:THR:HG23	1.48	0.95
1:B:96:LEU:O	1:B:100:GLN:HG3	1.69	0.92
1:A:146:THR:CB	1:A:232:GLU:CG	2.49	0.90
1:B:102:TRP:CE3	1:B:163:LEU:HD11	2.07	0.89
1:A:34:GLY:O	1:A:143:GLY:O	1.90	0.89
1:A:463:SER:O	1:A:466:VAL:HG12	1.72	0.88
1:A:391:THR:HG21	1:A:402:GLU:OE1	1.72	0.87
1:A:562:ASN:HB3	1:A:563:PRO:HD3	0.87	0.87
1:A:368:VAL:HG12	1:A:369:SER:N	1.88	0.86
1:B:368:VAL:O	1:B:369:SER:C	2.18	0.86
1:B:422:GLN:HE22	1:B:448:ALA:H	1.23	0.85
1:B:371:ARG:HH11	1:B:371:ARG:HB3	1.41	0.84
1:A:41:ALA:HB1	1:A:126:ILE:HD13	1.60	0.83
1:B:391:THR:HG22	1:B:455:LEU:HA	1.58	0.83
1:A:81:THR:HG22	1:A:84:ASN:H	1.45	0.82
1:B:209:TYR:CE2	1:B:550:THR:HG23	2.15	0.81
1:B:404:VAL:HG22	1:B:521:GLY:HA3	1.60	0.81
1:B:497:ARG:NH1	1:B:561:LEU:HD22	1.96	0.81
1:B:102:TRP:CE3	1:B:163:LEU:CD1	2.63	0.81
1:B:209:TYR:HE2	1:B:550:THR:CG2	1.93	0.81
1:B:531:VAL:O	1:B:531:VAL:HG12	1.79	0.81
1:B:216:VAL:CG1	1:B:217:GLY:N	2.45	0.80
1:B:209:TYR:CE2	1:B:550:THR:CG2	2.66	0.79
1:A:41:ALA:HB1	1:A:126:ILE:CD1	2.13	0.79
1:B:105:ALA:O	1:B:106:ALA:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:THR:HG21	1:B:402:GLU:OE1	1.81	0.78
1:B:497:ARG:HH12	1:B:561:LEU:HD22	1.49	0.78
1:B:230:PHE:O	1:B:297:ARG:NH1	2.17	0.77
1:B:81:THR:HG23	1:B:84:ASN:H	1.48	0.77
1:A:216:VAL:CG1	1:A:217:GLY:N	2.48	0.77
1:A:357:ALA:HB1	1:A:474:THR:CG2	2.14	0.77
1:B:127:ARG:O	1:B:131:LEU:HD23	1.86	0.76
1:A:229:GLN:HE22	1:A:231:LEU:HB2	1.48	0.76
1:B:353:THR:HB	1:B:501:GLY:O	1.85	0.76
1:A:368:VAL:HG12	1:A:369:SER:H	1.48	0.76
1:A:41:ALA:CB	1:A:126:ILE:HD13	2.15	0.76
1:B:216:VAL:HG22	1:B:285:ALA:HB3	1.68	0.76
1:A:402:GLU:OE2	1:A:550:THR:HG21	1.85	0.76
1:B:216:VAL:HG12	1:B:217:GLY:N	1.99	0.75
1:B:563:PRO:O	1:B:564:ARG:HB2	1.86	0.75
1:A:517:ASP:OD2	1:A:540:PRO:O	2.04	0.75
1:B:497:ARG:NH2	1:B:561:LEU:O	2.21	0.74
1:B:550:THR:HG23	1:B:551:PRO:HD2	1.69	0.73
1:B:371:ARG:CB	1:B:371:ARG:NH1	2.51	0.73
1:B:497:ARG:HH21	1:B:563:PRO:HA	1.53	0.73
1:A:212:THR:HG23	1:A:214:GLN:H	1.54	0.72
1:B:229:GLN:HE22	1:B:231:LEU:HB2	1.54	0.72
1:A:422:GLN:HE22	1:A:448:ALA:H	1.34	0.72
1:B:101:LYS:HG3	1:B:102:TRP:H	1.54	0.72
1:A:562:ASN:CB	1:A:563:PRO:CD	2.38	0.72
1:B:109:GLN:O	1:B:111:CYS:SG	2.48	0.72
1:B:107:GLY:O	1:B:108:ALA:C	2.32	0.71
1:B:371:ARG:HH11	1:B:371:ARG:HB2	1.55	0.71
1:B:212:THR:CG2	1:B:214:GLN:H	1.99	0.70
1:B:371:ARG:NH1	1:B:371:ARG:HB2	2.05	0.70
1:A:157:TYR:CD2	1:A:173:LEU:HD23	2.25	0.70
1:A:391:THR:HG22	1:A:455:LEU:CA	2.20	0.70
1:A:527:LEU:HD22	1:B:406:TYR:OH	1.91	0.70
1:A:216:VAL:HG12	1:A:217:GLY:N	2.05	0.70
1:A:81:THR:HG23	1:A:83:GLU:H	1.55	0.70
1:A:198:LEU:HD23	1:A:199:GLY:H	1.57	0.70
1:B:497:ARG:NH1	1:B:561:LEU:CD2	2.56	0.69
1:A:562:ASN:HB3	1:A:563:PRO:HD2	1.72	0.69
1:B:212:THR:HG22	1:B:214:GLN:N	2.01	0.68
1:A:223:ASN:HD22	1:A:490:GLU:HG3	1.59	0.68
1:B:102:TRP:CH2	1:B:163:LEU:HD11	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:CE2	1:A:550:THR:HG23	2.29	0.68
1:B:402:GLU:OE2	1:B:550:THR:HG21	1.93	0.68
1:A:563:PRO:O	1:A:564:ARG:HG3	1.93	0.68
1:B:201:THR:HG23	1:B:202:PRO:HD2	1.76	0.68
1:B:115:ILE:HD13	1:B:313:ASN:OD1	1.93	0.67
1:A:132:LEU:HD13	1:A:133:LEU:HD21	1.75	0.67
1:B:100:GLN:O	1:B:101:LYS:CG	2.43	0.67
1:A:35:TRP:CZ3	1:A:143:GLY:HA2	2.31	0.66
1:A:81:THR:H	1:A:84:ASN:HD22	1.40	0.66
1:B:201:THR:HG22	1:B:203:SER:H	1.60	0.66
1:B:517:ASP:OD2	1:B:540:PRO:O	2.14	0.66
1:B:497:ARG:NH2	1:B:563:PRO:HA	2.10	0.66
1:B:209:TYR:HE2	1:B:550:THR:HG21	1.58	0.66
1:A:157:TYR:CD2	1:A:173:LEU:CD2	2.80	0.65
1:B:216:VAL:CG1	1:B:217:GLY:H	2.11	0.64
1:B:217:GLY:O	1:B:286:ASN:HB3	1.96	0.64
1:B:463:SER:O	1:B:466:VAL:HG12	1.97	0.64
1:A:359:GLY:H	1:A:474:THR:HG21	1.62	0.64
1:B:299:GLU:N	1:B:299:GLU:OE1	2.30	0.64
1:A:426:VAL:HG12	1:A:430:LEU:HD22	1.79	0.63
1:A:35:TRP:CE3	1:A:143:GLY:HA2	2.33	0.63
1:B:53:LEU:HD22	1:B:99:VAL:HG21	1.80	0.63
1:A:132:LEU:C	1:A:133:LEU:HD23	2.24	0.63
1:B:377:THR:HG22	1:B:380:ALA:HB3	1.81	0.62
1:B:449:TYR:HB2	1:B:450:PRO:HA	1.81	0.62
1:B:531:VAL:HG13	1:B:534:GLN:O	2.00	0.61
1:A:223:ASN:HD22	1:A:490:GLU:CG	2.13	0.61
1:B:497:ARG:HH21	1:B:563:PRO:CA	2.14	0.61
1:A:144:GLY:C	1:A:146:THR:N	2.57	0.60
1:B:497:ARG:NH2	1:B:562:ASN:O	2.35	0.60
1:A:132:LEU:HD13	1:A:133:LEU:CD2	2.31	0.60
1:B:531:VAL:O	1:B:531:VAL:CG1	2.47	0.60
1:B:100:GLN:O	1:B:102:TRP:N	2.28	0.59
1:B:367:SER:HA	1:B:371:ARG:O	2.03	0.59
1:B:368:VAL:CG1	1:B:369:SER:N	2.43	0.59
1:A:563:PRO:O	4:A:580:CL:CL	2.57	0.59
1:B:57:ASN:HB2	1:B:88:LEU:HD22	1.84	0.58
1:A:20:SER:OG	1:A:158:GLN:CD	2.46	0.58
1:A:563:PRO:O	1:A:564:ARG:CG	2.51	0.58
1:B:223:ASN:HD22	1:B:490:GLU:HG3	1.69	0.58
1:A:144:GLY:O	1:A:146:THR:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:VAL:HG13	1:B:217:GLY:H	1.67	0.58
1:A:216:VAL:CG1	1:A:217:GLY:H	2.15	0.57
1:A:298:HIS:H	1:A:298:HIS:CD2	2.21	0.57
1:B:197:HIS:HA	1:B:396:PRO:O	2.04	0.57
1:A:422:GLN:NE2	1:A:448:ALA:H	2.00	0.57
1:B:229:GLN:HE21	1:B:272:GLU:HG2	1.69	0.57
1:B:466:VAL:HG13	1:B:468:ILE:HD11	1.87	0.57
1:A:466:VAL:HG13	1:A:468:ILE:HD11	1.87	0.56
1:A:216:VAL:HG13	1:A:217:GLY:H	1.70	0.56
1:A:342:THR:HA	1:A:345:MET:HE3	1.87	0.56
1:A:368:VAL:CG1	1:A:369:SER:H	2.12	0.56
1:B:489:ASN:O	1:B:493:ILE:HG23	2.06	0.56
1:A:308:LEU:HD21	1:A:340:VAL:HG13	1.86	0.56
1:B:218:SER:O	1:B:220:THR:N	2.39	0.56
1:B:101:LYS:CG	1:B:102:TRP:N	2.56	0.56
1:B:102:TRP:CD2	1:B:163:LEU:HD11	2.40	0.56
1:B:391:THR:HG22	1:B:455:LEU:CA	2.33	0.56
1:B:61:LEU:HD23	1:B:345:MET:HE3	1.89	0.55
1:B:320:VAL:HG22	1:B:353:THR:HG23	1.88	0.55
1:A:45:GLU:HB3	1:A:126:ILE:HD12	1.88	0.55
1:A:110:LYS:HA	1:A:110:LYS:CE	2.37	0.55
1:B:201:THR:HG22	1:B:203:SER:N	2.22	0.54
1:B:20:SER:OG	1:B:158:GLN:NE2	2.41	0.54
1:B:212:THR:CG2	1:B:213:SER:N	2.70	0.54
1:A:216:VAL:HG22	1:A:285:ALA:HB3	1.90	0.54
1:A:95:THR:CG2	1:A:166:HIS:ND1	2.50	0.54
1:A:110:LYS:HA	1:A:110:LYS:HE3	1.89	0.54
1:B:229:GLN:NE2	1:B:272:GLU:HG2	2.22	0.54
1:B:102:TRP:CD2	1:B:163:LEU:CD1	2.90	0.53
1:B:397:PHE:C	1:B:398:LEU:HD22	2.33	0.53
1:B:404:VAL:CG2	1:B:521:GLY:HA3	2.37	0.53
1:B:550:THR:HG23	1:B:551:PRO:CD	2.38	0.53
1:A:550:THR:HG23	1:A:551:PRO:HD2	1.90	0.53
1:B:41:ALA:HB3	1:B:126:ILE:HD13	1.90	0.53
1:A:145:PRO:HD2	1:A:179:THR:HG23	1.91	0.52
1:B:216:VAL:HG13	1:B:286:ASN:H	1.75	0.52
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.74	0.52
1:B:100:GLN:C	1:B:102:TRP:N	2.67	0.52
1:B:216:VAL:HG22	1:B:285:ALA:CB	2.36	0.52
1:B:100:GLN:O	1:B:101:LYS:HG2	2.09	0.52
1:A:528:ASP:C	1:A:528:ASP:OD1	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLN:C	1:B:102:TRP:H	2.17	0.52
1:A:81:THR:HG23	1:A:83:GLU:N	2.24	0.52
1:A:160:PRO:HG2	1:A:163:LEU:HD23	1.92	0.52
1:A:40:ARG:CZ	1:A:137:GLU:HG3	2.40	0.52
1:A:201:THR:CG2	1:A:202:PRO:HD2	2.40	0.52
1:A:367:SER:HA	1:A:371:ARG:O	2.09	0.51
1:B:153:SER:O	1:B:174:HIS:HD2	1.92	0.51
1:A:209:TYR:CE2	1:A:550:THR:CG2	2.93	0.51
1:B:561:LEU:C	1:B:562:ASN:O	2.51	0.51
1:A:146:THR:CB	1:A:232:GLU:OE2	2.59	0.51
1:B:297:ARG:C	1:B:299:GLU:H	2.17	0.51
1:A:383:PRO:HB3	1:A:419:PRO:HG3	1.93	0.51
1:A:81:THR:HG22	1:A:84:ASN:N	2.21	0.51
1:A:556:LEU:HD22	1:A:560:LEU:HD12	1.92	0.50
1:B:109:GLN:O	1:B:110:LYS:C	2.55	0.50
1:A:494:LEU:O	1:A:495:SER:CB	2.60	0.50
1:B:562:ASN:O	1:B:563:PRO:C	2.54	0.50
1:A:218:SER:O	1:A:220:THR:N	2.44	0.49
1:B:102:TRP:CZ3	1:B:163:LEU:CD1	2.82	0.49
1:A:81:THR:H	1:A:84:ASN:ND2	2.08	0.49
1:A:336:TYR:O	1:A:340:VAL:HG23	2.12	0.49
1:A:71:PRO:HG2	1:A:509:GLN:NE2	2.28	0.49
1:A:359:GLY:N	1:A:474:THR:HG21	2.26	0.49
1:A:295:PRO:O	1:A:303:PRO:HA	2.13	0.49
1:B:27:GLN:HB2	1:B:333:SER:HB3	1.95	0.49
1:A:402:GLU:O	1:A:403:ILE:HD12	2.12	0.49
1:B:153:SER:O	1:B:174:HIS:CD2	2.66	0.49
1:A:449:TYR:CD1	1:A:449:TYR:C	2.90	0.48
1:B:298:HIS:HB3	1:B:299:GLU:OE1	2.13	0.48
1:B:395:GLU:CD	1:B:398:LEU:HB2	2.38	0.48
1:A:201:THR:HG23	1:A:202:PRO:HD2	1.95	0.48
1:A:278:GLN:HE22	1:A:462:VAL:H	1.59	0.48
1:A:27:GLN:HB2	1:A:333:SER:HB3	1.96	0.48
1:A:209:TYR:HE2	1:A:550:THR:CG2	2.27	0.48
1:A:514:GLY:HA2	1:A:555:ALA:HB1	1.96	0.48
1:B:404:VAL:HG21	1:B:521:GLY:C	2.38	0.48
1:A:146:THR:CB	1:A:232:GLU:CB	2.91	0.48
1:A:201:THR:HG22	1:A:202:PRO:N	2.29	0.48
1:B:297:ARG:C	1:B:299:GLU:N	2.68	0.48
1:B:408:SER:O	1:B:523:HIS:HD2	1.97	0.48
1:A:391:THR:HG23	1:A:455:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:THR:HG22	1:B:84:ASN:ND2	2.29	0.48
1:B:319:HIS:CD2	7:B:617:HOH:O	2.66	0.48
1:A:391:THR:CG2	1:A:455:LEU:HD23	2.44	0.47
1:B:398:LEU:HD22	1:B:398:LEU:N	2.28	0.47
1:B:497:ARG:NH2	1:B:562:ASN:C	2.72	0.47
1:B:516:PHE:N	1:B:550:THR:O	2.46	0.47
1:B:81:THR:HG22	1:B:84:ASN:CG	2.38	0.47
1:A:81:THR:CG2	1:A:84:ASN:H	2.23	0.47
1:B:54:ARG:NH1	1:B:168:ASP:OD1	2.48	0.47
1:A:356:PHE:CE2	1:A:385:VAL:HG21	2.50	0.47
1:B:47:LEU:HD22	1:B:49:LEU:HD13	1.96	0.47
1:B:447:ARG:NH1	1:B:448:ALA:O	2.44	0.47
1:B:497:ARG:NH2	1:B:563:PRO:CA	2.76	0.47
1:A:519:THR:O	1:A:519:THR:CG2	2.63	0.47
1:B:212:THR:HG23	1:B:213:SER:N	2.30	0.47
1:B:366:TRP:HB2	1:B:375:ARG:HB2	1.97	0.47
1:A:41:ALA:CB	1:A:126:ILE:CD1	2.86	0.47
1:A:221:SER:OG	1:A:222:ASN:N	2.48	0.46
1:A:378:PHE:CD1	1:A:379:PRO:HA	2.51	0.46
1:B:101:LYS:CG	1:B:102:TRP:H	2.27	0.46
1:A:201:THR:HG23	1:A:247:PHE:CD1	2.50	0.46
1:A:395:GLU:CD	1:A:398:LEU:HB2	2.40	0.46
1:B:42:ASP:O	1:B:43:PRO:C	2.58	0.46
1:B:216:VAL:CG1	1:B:286:ASN:HB2	2.45	0.46
1:B:561:LEU:O	1:B:562:ASN:C	2.55	0.46
1:A:157:TYR:CE2	1:A:173:LEU:HD22	2.50	0.46
1:B:553:PHE:HB3	1:B:554:PRO:HD3	1.97	0.46
1:B:206:ARG:NH2	1:B:285:ALA:HB2	2.30	0.46
1:A:406:TYR:CZ	1:A:524:GLU:HB3	2.51	0.46
1:A:519:THR:O	1:A:519:THR:HG22	2.14	0.46
1:A:144:GLY:O	1:A:146:THR:C	2.59	0.45
1:B:201:THR:HG23	1:B:202:PRO:CD	2.44	0.45
1:B:485:LEU:HD12	1:B:485:LEU:HA	1.85	0.45
1:A:368:VAL:CG1	1:A:369:SER:N	2.57	0.45
1:B:105:ALA:O	1:B:106:ALA:CB	2.50	0.45
1:A:398:LEU:N	1:A:398:LEU:HD22	2.31	0.45
1:B:179:THR:O	1:B:180:SER:C	2.60	0.45
1:B:271:ILE:HD12	1:B:471:VAL:CG2	2.47	0.45
1:B:301:GLN:O	1:B:303:PRO:HD3	2.16	0.45
1:A:68:VAL:HG13	1:A:79:TYR:CE1	2.52	0.45
1:A:145:PRO:CD	1:A:179:THR:HG23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ALA:CB	1:A:474:THR:HG23	2.33	0.45
1:A:556:LEU:HD22	1:A:560:LEU:CD1	2.47	0.45
1:B:102:TRP:CE2	1:B:132:LEU:HD21	2.52	0.45
1:B:377:THR:HB	7:B:629:HOH:O	2.15	0.45
1:A:553:PHE:HB3	1:A:554:PRO:HD3	1.99	0.45
1:A:408:SER:O	1:A:523:HIS:HD2	2.00	0.44
1:B:41:ALA:CB	1:B:126:ILE:HD13	2.47	0.44
1:A:153:SER:O	1:A:174:HIS:HD2	2.00	0.44
1:B:105:ALA:C	1:B:107:GLY:H	2.25	0.44
1:A:514:GLY:HA2	1:A:555:ALA:CB	2.47	0.44
1:A:41:ALA:HB3	1:A:126:ILE:HD13	1.96	0.44
1:A:523:HIS:HE1	1:A:536:PHE:H	1.64	0.44
1:A:454:ALA:HB3	1:A:477:SER:HB2	1.99	0.44
1:B:419:PRO:HD2	1:B:422:GLN:NE2	2.33	0.44
1:A:60:ARG:HA	1:A:60:ARG:HD3	1.74	0.44
1:A:118:ASP:OD2	1:A:346:LYS:NZ	2.50	0.44
1:B:369:SER:HB2	1:B:370:GLY:H	1.66	0.44
1:B:278:GLN:HE22	1:B:462:VAL:H	1.65	0.44
1:B:157:TYR:CD2	1:B:173:LEU:HD22	2.53	0.43
1:B:164:ALA:N	1:B:165:PRO:CD	2.81	0.43
1:B:528:ASP:O	1:B:532:GLU:HA	2.18	0.43
1:B:75:GLN:HE21	1:B:75:GLN:CA	2.31	0.43
1:A:26:ASP:OD2	1:A:26:ASP:N	2.50	0.43
1:B:20:SER:HB2	1:B:159:LEU:O	2.18	0.43
1:B:116:THR:OG1	1:B:118:ASP:OD1	2.31	0.43
1:B:394:GLN:HE21	1:B:401:ASN:HB3	1.84	0.43
1:A:210:ASN:ND2	1:A:552:ASN:OD1	2.51	0.43
1:A:216:VAL:HG13	1:A:285:ALA:O	2.17	0.43
1:A:132:LEU:CD1	1:A:133:LEU:HD21	2.46	0.43
1:B:229:GLN:HG3	1:B:272:GLU:HG3	2.00	0.43
1:B:469:PRO:HB2	1:B:470:TRP:CD1	2.54	0.43
1:A:128:GLN:O	1:A:132:LEU:HB2	2.19	0.43
1:A:146:THR:CB	1:A:232:GLU:CD	2.92	0.43
1:B:26:ASP:OD2	1:B:26:ASP:N	2.52	0.43
1:A:144:GLY:O	1:A:145:PRO:C	2.62	0.42
1:A:301:GLN:O	1:A:303:PRO:HD3	2.19	0.42
1:A:448:ALA:HB1	1:A:542:TRP:HH2	1.83	0.42
1:B:68:VAL:HG13	1:B:79:TYR:CE1	2.55	0.42
1:B:429:PHE:HD2	1:B:430:LEU:HD13	1.84	0.42
1:A:131:LEU:O	1:A:132:LEU:C	2.63	0.42
1:A:21:TYR:O	1:A:158:GLN:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:CD	1:A:270:GLY:HA3	2.45	0.42
1:B:221:SER:OG	1:B:222:ASN:N	2.52	0.42
1:B:523:HIS:HE1	1:B:536:PHE:H	1.68	0.42
1:A:169:PHE:CD1	1:A:169:PHE:C	2.96	0.41
1:A:391:THR:HG22	1:A:455:LEU:N	2.34	0.41
1:A:298:HIS:CD2	1:A:298:HIS:N	2.85	0.41
1:B:198:LEU:HD11	1:B:397:PHE:O	2.21	0.41
1:A:144:GLY:C	1:A:146:THR:H	2.28	0.41
1:A:515:LEU:HD23	1:A:551:PRO:HA	2.01	0.41
1:B:45:GLU:O	1:B:126:ILE:HG23	2.19	0.41
1:B:320:VAL:HG22	1:B:353:THR:CG2	2.50	0.41
1:B:403:ILE:HG13	1:B:520:ARG:HB3	2.03	0.41
1:A:21:TYR:O	1:A:158:GLN:HB2	2.20	0.41
1:A:164:ALA:N	1:A:165:PRO:CD	2.84	0.41
1:A:293:SER:O	1:A:294:SER:C	2.63	0.41
1:B:297:ARG:O	1:B:299:GLU:N	2.54	0.41
1:A:41:ALA:HA	1:A:140:HIS:CE1	2.56	0.41
1:B:378:PHE:CD2	1:B:378:PHE:C	2.98	0.41
1:A:106:ALA:HB2	1:A:132:LEU:HD23	2.01	0.41
1:B:55:GLN:HB3	1:B:89:VAL:HG22	2.02	0.41
1:B:201:THR:CG2	1:B:202:PRO:N	2.84	0.41
1:B:408:SER:O	1:B:523:HIS:CD2	2.74	0.41
1:A:511:HIS:C	1:A:513:ALA:H	2.29	0.41
1:B:229:GLN:HE21	1:B:231:LEU:HG	1.86	0.41
1:A:397:PHE:C	1:A:398:LEU:HD22	2.46	0.40
1:A:463:SER:O	1:A:466:VAL:CG1	2.56	0.40
1:B:322:THR:HG21	1:B:479:PRO:HA	2.02	0.40
1:B:556:LEU:HD23	1:B:556:LEU:HA	1.94	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	525/571 (92%)	495 (94%)	21 (4%)	9 (2%)	7	6
1	B	525/571 (92%)	479 (91%)	40 (8%)	6 (1%)	11	11
All	All	1050/1142 (92%)	974 (93%)	61 (6%)	15 (1%)	9	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLY
1	A	368	VAL
1	B	219	GLY
1	B	369	SER
1	A	406	TYR
1	A	450	PRO
1	A	563	PRO
1	B	379	PRO
1	A	369	SER
1	B	450	PRO
1	A	379	PRO
1	A	434	PRO
1	B	145	PRO
1	A	143	GLY
1	B	469	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	443/479 (92%)	395 (89%)	48 (11%)	6	5
1	B	443/479 (92%)	389 (88%)	54 (12%)	5	4
All	All	886/958 (92%)	784 (88%)	102 (12%)	5	5

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU

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Mol	Chain	Res	Type
1	A	40	ARG
1	A	47	LEU
1	A	48	SER
1	A	49	LEU
1	A	54	ARG
1	A	60	ARG
1	A	64	LEU
1	A	68	VAL
1	A	75	GLN
1	A	78	LYS
1	A	81	THR
1	A	88	LEU
1	A	89	VAL
1	A	110	LYS
1	A	126	ILE
1	A	132	LEU
1	A	198	LEU
1	A	207	LYS
1	A	212	THR
1	A	220	THR
1	A	222	ASN
1	A	232	GLU
1	A	246	LEU
1	A	264	GLN
1	A	272	GLU
1	A	298	HIS
1	A	310	LEU
1	A	311	LEU
1	A	324	SER
1	A	344	LEU
1	A	352	LEU
1	A	377	THR
1	A	385	VAL
1	A	391	THR
1	A	395	GLU
1	A	401	ASN
1	A	403	ILE
1	A	404	VAL
1	A	430	LEU
1	A	463	SER
1	A	474	THR
1	A	485	LEU

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Mol	Chain	Res	Type
1	A	490	GLU
1	A	523	HIS
1	A	531	VAL
1	A	550	THR
1	A	557	LEU
1	B	38	LEU
1	B	47	LEU
1	B	49	LEU
1	B	54	ARG
1	B	60	ARG
1	B	64	LEU
1	B	68	VAL
1	B	75	GLN
1	B	88	LEU
1	B	89	VAL
1	B	101	LYS
1	B	112	HIS
1	B	115	ILE
1	B	131	LEU
1	B	140	HIS
1	B	146	THR
1	B	163	LEU
1	B	173	LEU
1	B	201	THR
1	B	203	SER
1	B	207	LYS
1	B	212	THR
1	B	220	THR
1	B	222	ASN
1	B	235	PHE
1	B	264	GLN
1	B	271	ILE
1	B	272	GLU
1	B	276	ASP
1	B	308	LEU
1	B	310	LEU
1	B	311	LEU
1	B	324	SER
1	B	344	LEU
1	B	352	LEU
1	B	353	THR
1	B	367	SER

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Mol	Chain	Res	Type
1	B	371	ARG
1	B	377	THR
1	B	385	VAL
1	B	391	THR
1	B	395	GLU
1	B	401	ASN
1	B	430	LEU
1	B	443	ASN
1	B	461	VAL
1	B	477	SER
1	B	485	LEU
1	B	493	ILE
1	B	497	ARG
1	B	523	HIS
1	B	531	VAL
1	B	550	THR
1	B	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	84	ASN
1	A	155	HIS
1	A	158	GLN
1	A	161	GLN
1	A	174	HIS
1	A	223	ASN
1	A	225	GLN
1	A	229	GLN
1	A	278	GLN
1	A	298	HIS
1	A	321	HIS
1	A	394	GLN
1	A	422	GLN
1	A	435	HIS
1	A	504	ASN
1	A	509	GLN
1	A	523	HIS
1	B	56	GLN
1	B	57	ASN
1	B	75	GLN

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Mol	Chain	Res	Type
1	B	84	ASN
1	B	100	GLN
1	B	158	GLN
1	B	174	HIS
1	B	214	GLN
1	B	222	ASN
1	B	223	ASN
1	B	225	GLN
1	B	229	GLN
1	B	254	GLN
1	B	264	GLN
1	B	278	GLN
1	B	394	GLN
1	B	401	ASN
1	B	422	GLN
1	B	504	ASN
1	B	509	GLN
1	B	523	HIS
1	B	552	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 12 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	$\# Z > 2$
2	NAG	A	572	1	13,13,15	1.01	0	12,17,21	1.11	1 (8%)
2	NAG	A	575	1	13,13,15	0.75	0	12,17,21	1.05	0
2	NAG	B	574	1	13,13,15	1.19	2 (15%)	12,17,21	1.45	1 (8%)
6	SO4	B	582	-	4,4,4	0.26	0	6,6,6	0.19	0
2	NAG	A	573	1	13,13,15	1.57	2 (15%)	12,17,21	2.29	6 (50%)
2	NAG	B	573	1	13,13,15	0.98	0	12,17,21	1.34	3 (25%)
6	SO4	A	582	-	4,4,4	0.26	0	6,6,6	0.20	0
2	NAG	A	574	1	13,13,15	0.88	0	12,17,21	1.38	1 (8%)
2	NAG	B	575	1	13,13,15	0.95	0	12,17,21	1.10	1 (8%)
2	NAG	B	572	1	13,13,15	0.95	0	12,17,21	1.64	3 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	572	1	-	4/6/19/26	1/1/1/1
2	NAG	A	575	1	-	4/6/19/26	0/1/1/1
2	NAG	B	574	1	-	2/6/19/26	0/1/1/1
2	NAG	A	573	1	-	5/6/19/26	0/1/1/1
2	NAG	B	573	1	-	5/6/19/26	0/1/1/1
2	NAG	A	574	1	-	3/6/19/26	0/1/1/1
2	NAG	B	575	1	-	5/6/19/26	0/1/1/1
2	NAG	B	572	1	-	2/6/19/26	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	573	NAG	C3-C2	4.02	1.56	1.52
2	A	573	NAG	C4-C3	2.60	1.57	1.52
2	B	574	NAG	C4-C3	2.41	1.57	1.52
2	B	574	NAG	C3-C2	2.05	1.54	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	573	NAG	C3-C4-C5	-4.70	103.25	111.19
2	A	574	NAG	O5-C1-C2	-3.72	105.53	111.29
2	A	573	NAG	C2-N2-C7	3.65	127.79	122.90
2	B	574	NAG	O5-C1-C2	-3.51	105.87	111.29
2	B	572	NAG	O5-C1-C2	-3.08	106.52	111.29
2	B	572	NAG	C3-C4-C5	-2.84	106.38	111.19
2	A	573	NAG	O5-C5-C4	2.52	115.12	110.26
2	A	573	NAG	O7-C7-C8	-2.49	117.62	122.05
2	B	575	NAG	O5-C1-C2	-2.30	107.73	111.29
2	B	572	NAG	O3-C3-C2	-2.25	105.13	109.88
2	B	573	NAG	O5-C1-C2	-2.20	107.89	111.29
2	A	572	NAG	C4-C5-C6	2.18	116.53	112.50
2	A	573	NAG	O5-C1-C2	-2.12	108.02	111.29
2	A	573	NAG	O7-C7-N2	2.09	125.68	121.98
2	B	573	NAG	C3-C4-C5	-2.04	107.75	111.19
2	B	573	NAG	C4-C5-C6	2.01	116.22	112.50

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	572	NAG	C1-C2-N2-C7
2	A	572	NAG	C4-C5-C6-O6
2	A	572	NAG	C8-C7-N2-C2
2	A	572	NAG	O7-C7-N2-C2
2	A	573	NAG	C4-C5-C6-O6
2	A	573	NAG	O5-C5-C6-O6
2	A	574	NAG	C1-C2-N2-C7
2	B	573	NAG	C4-C5-C6-O6
2	B	573	NAG	O5-C5-C6-O6
2	B	574	NAG	C4-C5-C6-O6
2	B	574	NAG	O5-C5-C6-O6
2	B	575	NAG	C3-C2-N2-C7
2	B	575	NAG	C4-C5-C6-O6
2	B	575	NAG	O5-C5-C6-O6
2	B	575	NAG	C8-C7-N2-C2
2	B	575	NAG	O7-C7-N2-C2
2	A	573	NAG	C8-C7-N2-C2
2	A	573	NAG	O7-C7-N2-C2
2	A	575	NAG	O7-C7-N2-C2
2	A	575	NAG	C8-C7-N2-C2
2	B	572	NAG	C8-C7-N2-C2
2	A	574	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	574	NAG	O7-C7-N2-C2
2	B	572	NAG	O7-C7-N2-C2
2	B	573	NAG	C8-C7-N2-C2
2	A	575	NAG	O5-C5-C6-O6
2	B	573	NAG	O7-C7-N2-C2
2	A	575	NAG	C4-C5-C6-O6
2	A	573	NAG	C1-C2-N2-C7
2	B	573	NAG	C1-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	572	NAG	C1-C2-C3-C4-C5-O5
2	A	572	NAG	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	529/571 (92%)	1.20	85 (16%) 4 5	49, 67, 79, 88	0
1	B	529/571 (92%)	1.10	73 (13%) 6 7	60, 67, 79, 91	0
All	All	1058/1142 (92%)	1.15	158 (14%) 5 6	49, 67, 79, 91	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	THR	7.1
1	A	198	LEU	7.1
1	A	399	ILE	6.6
1	A	300	GLY	5.4
1	B	395	GLU	5.4
1	A	220	THR	5.0
1	B	293	SER	4.7
1	A	219	GLY	4.5
1	B	219	GLY	4.5
1	B	514	GLY	4.4
1	A	295	PRO	4.3
1	A	563	PRO	4.3
1	B	513	ALA	4.2
1	A	47	LEU	4.1
1	B	285	ALA	4.0
1	B	406	TYR	4.0
1	B	564	ARG	3.9
1	A	298	HIS	3.8
1	A	393	PHE	3.7
1	A	297	ARG	3.7
1	B	295	PRO	3.4
1	B	198	LEU	3.4
1	B	563	PRO	3.4
1	A	293	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	531	VAL	3.4
1	B	123	TRP	3.3
1	B	397	PHE	3.3
1	A	234	TYR	3.3
1	B	234	TYR	3.3
1	A	512	GLY	3.3
1	A	396	PRO	3.3
1	A	95	THR	3.3
1	A	162	ALA	3.2
1	A	255	ALA	3.2
1	A	237	ASP	3.2
1	A	265	GLY	3.2
1	B	145	PRO	3.1
1	A	140	HIS	3.0
1	B	180	SER	3.0
1	A	296	GLY	3.0
1	B	469	PRO	3.0
1	A	398	LEU	3.0
1	A	264	GLN	3.0
1	A	397	PHE	2.9
1	A	163	LEU	2.9
1	B	271	ILE	2.9
1	B	544	PRO	2.9
1	B	149	HIS	2.9
1	A	102	TRP	2.8
1	B	102	TRP	2.8
1	A	143	GLY	2.8
1	A	197	HIS	2.8
1	B	294	SER	2.8
1	A	232	GLU	2.8
1	A	537	CYS	2.8
1	A	406	TYR	2.8
1	B	310	LEU	2.8
1	A	294	SER	2.7
1	A	536	PHE	2.7
1	A	99	VAL	2.7
1	A	400	THR	2.7
1	A	545	VAL	2.6
1	B	400	THR	2.6
1	A	319	HIS	2.6
1	B	276	ASP	2.6
1	A	434	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	211	LEU	2.6
1	B	261	VAL	2.6
1	B	111	CYS	2.5
1	A	180	SER	2.5
1	A	233	GLN	2.5
1	B	260	VAL	2.5
1	B	480	VAL	2.5
1	B	21	TYR	2.5
1	A	250	ASN	2.5
1	A	551	PRO	2.5
1	B	39	GLY	2.5
1	A	41	ALA	2.5
1	B	232	GLU	2.4
1	B	519	THR	2.4
1	B	218	SER	2.4
1	A	136	ALA	2.4
1	B	148	THR	2.4
1	A	124	LEU	2.4
1	B	487	LEU	2.4
1	B	298	HIS	2.4
1	A	235	PHE	2.4
1	A	218	SER	2.4
1	A	151	VAL	2.4
1	B	300	GLY	2.3
1	A	487	LEU	2.3
1	A	59	GLU	2.3
1	B	147	GLU	2.3
1	A	540	PRO	2.3
1	A	144	GLY	2.3
1	A	564	ARG	2.3
1	A	36	VAL	2.3
1	A	310	LEU	2.3
1	A	269	ALA	2.3
1	B	297	ARG	2.3
1	B	140	HIS	2.3
1	A	142	VAL	2.3
1	A	60	ARG	2.3
1	A	441	TYR	2.3
1	B	126	ILE	2.3
1	B	385	VAL	2.3
1	B	404	VAL	2.3
1	B	396	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	39	GLY	2.2
1	A	199	GLY	2.2
1	A	421	TYR	2.2
1	B	197	HIS	2.2
1	A	374	PHE	2.2
1	B	235	PHE	2.2
1	A	210	ASN	2.2
1	A	521	GLY	2.2
1	A	83	GLU	2.2
1	A	123	TRP	2.2
1	B	173	LEU	2.2
1	B	231	LEU	2.2
1	A	251	PHE	2.2
1	B	105	ALA	2.2
1	B	527	LEU	2.2
1	A	122	CYS	2.2
1	B	221	SER	2.2
1	A	53	LEU	2.1
1	A	254	GLN	2.1
1	B	112	HIS	2.1
1	A	496	GLY	2.1
1	B	387	THR	2.1
1	B	131	LEU	2.1
1	B	233	GLN	2.1
1	B	249	GLY	2.1
1	B	252	ALA	2.1
1	B	200	VAL	2.1
1	A	176	PHE	2.1
1	B	410	GLY	2.1
1	A	22	SER	2.1
1	B	392	SER	2.1
1	B	41	ALA	2.1
1	A	149	HIS	2.1
1	A	534	GLN	2.1
1	B	455	LEU	2.1
1	B	360	ASP	2.1
1	B	510	GLN	2.1
1	A	145	PRO	2.1
1	A	146	THR	2.0
1	A	444	ALA	2.0
1	B	402	GLU	2.0
1	B	104	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	150	VAL	2.0
1	A	261	VAL	2.0
1	B	144	GLY	2.0
1	B	541	GLY	2.0
1	B	529	GLU	2.0
1	A	229	GLN	2.0
1	B	263	GLN	2.0
1	A	110	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	575	13/15	0.37	0.24	87,88,90,91	0
6	SO4	A	582	5/5	0.39	0.18	112,112,112,112	0
2	NAG	B	575	13/15	0.45	0.22	88,90,93,93	0
2	NAG	A	572	13/15	0.50	0.22	82,85,89,90	0
2	NAG	B	574	13/15	0.59	0.17	81,83,85,85	0
2	NAG	A	573	13/15	0.65	0.18	68,72,79,80	0
6	SO4	B	582	5/5	0.67	0.14	104,104,105,105	0
2	NAG	A	574	13/15	0.73	0.16	80,81,84,85	0
2	NAG	B	573	13/15	0.74	0.17	69,74,79,80	0
2	NAG	B	572	13/15	0.80	0.17	72,73,77,78	0
4	CL	B	580	1/1	0.81	0.29	112,112,112,112	0
3	ZN	B	579	1/1	0.85	0.16	116,116,116,116	0
4	CL	A	580	1/1	0.90	0.40	98,98,98,98	0
3	ZN	A	579	1/1	0.91	0.11	114,114,114,114	0
3	ZN	B	576	1/1	0.95	0.11	87,87,87,87	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	577	1/1	0.96	0.10	94,94,94,94	0
3	ZN	A	578	1/1	0.96	0.18	83,83,83,83	0
3	ZN	B	578	1/1	0.97	0.10	90,90,90,90	0
3	ZN	A	576	1/1	0.97	0.11	91,91,91,91	0
3	ZN	A	577	1/1	0.97	0.08	71,71,71,71	1
5	CA	B	581	1/1	0.98	0.14	61,61,61,61	0
5	CA	A	581	1/1	0.99	0.13	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.