



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:59 PM GMT

PDB ID : 3EE6  
Title : Crystal Structure Analysis of Tripeptidyl peptidase -I  
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Deposited on : 2008-09-04  
Resolution : 2.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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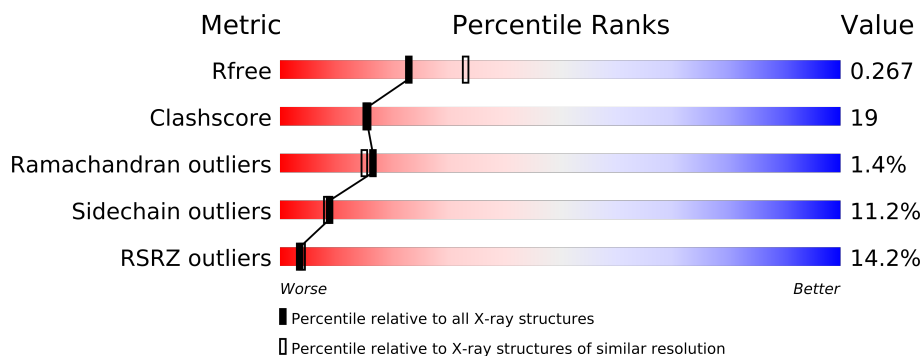
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	575	-	X
2	NAG	B	575	-	X
4	CL	A	580	-	X
6	SO4	A	582	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8361 atoms, of which 0 are hydrogen and 0 are deuterium.

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-peptidase1.

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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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 (three-letter code: ZN) (formula: Zn).

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

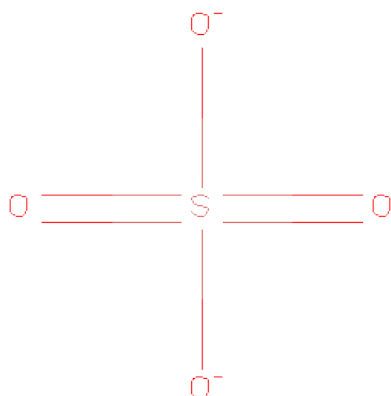
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is water.

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

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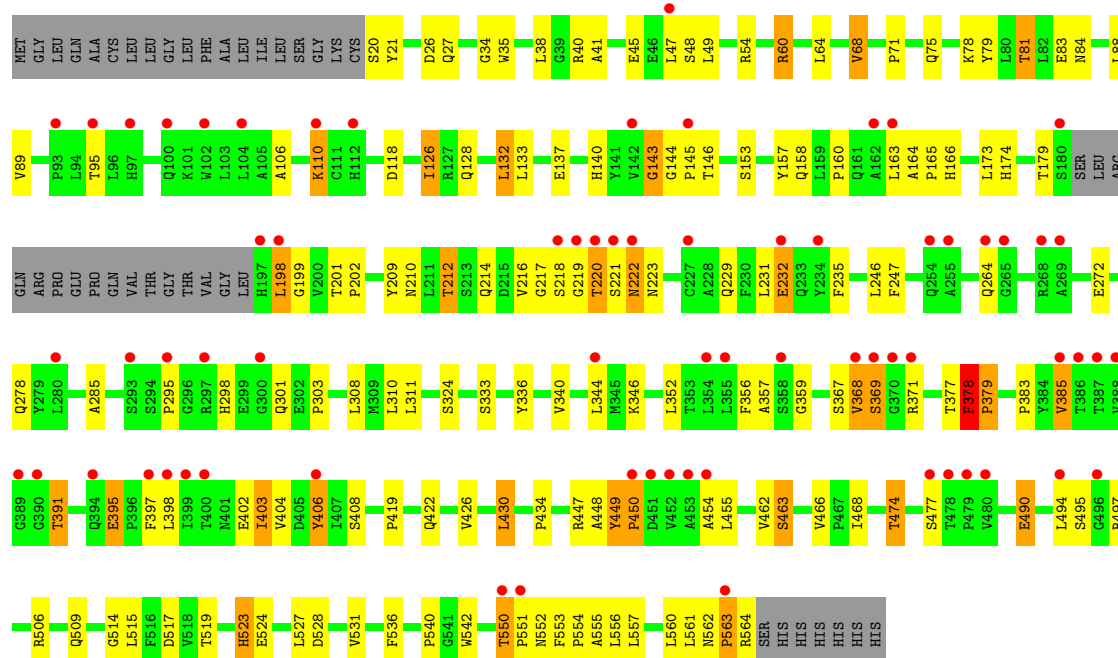
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	37	Total	O	0	0
			37	37		

### 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.

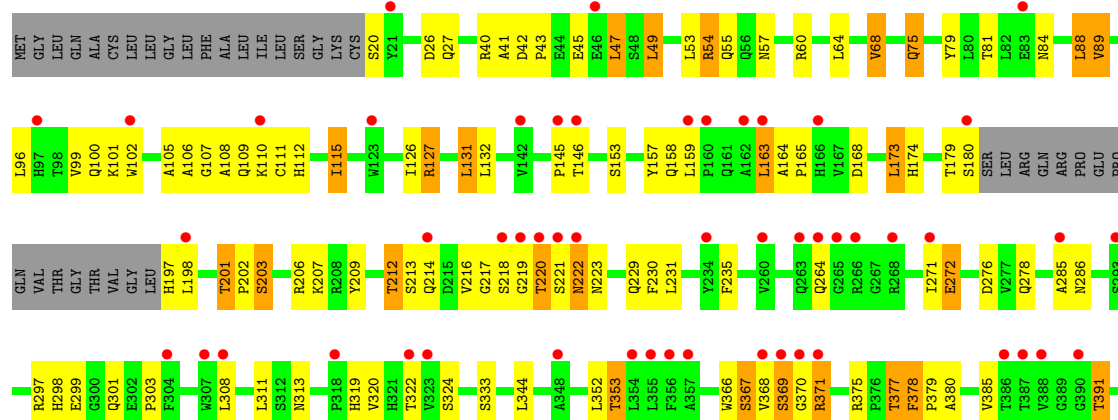
#### • Molecule 1: Tripeptidyl-peptidase1

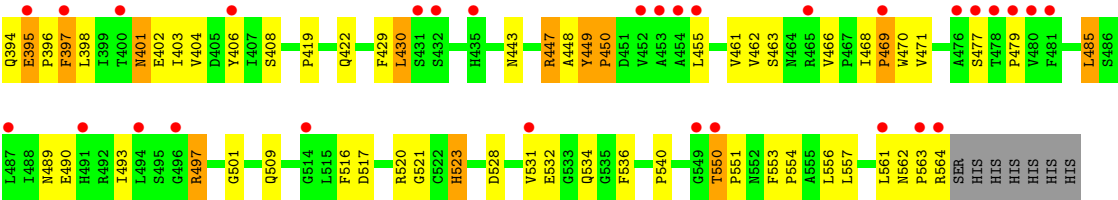
Chain A: 



#### • Molecule 1: Tripeptidyl-peptidase1

Chain B: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.6 (39.21-2.35)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 78.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61780 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.52	0/4204	0.75	2/5741 (0.0%)
1	B	0.48	0/4202	0.71	1/5739 (0.0%)
All	All	0.50	0/8406	0.73	3/11480 (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	A	0	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PHE	C-N-CD	-9.12	100.54	120.60
1	B	378	PHE	C-N-CD	-7.35	104.42	120.60
1	A	450	PRO	N-CA-C	-5.52	97.75	112.10

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

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

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4082	0	3900	138	0
1	B	4080	0	3901	164	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	301	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (301) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:562:ASN:HB3	1:A:563:PRO:CD	1.57	1.33
1:A:562:ASN:CB	1:A:563:PRO:HD3	1.69	1.20
1:A:95:THR:HG22	1:A:166:HIS:ND1	1.56	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:368:VAL:O	1:B:369:SER:C	2.18	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:HG12	1:B:531:VAL:O	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:391:THR:HG21	1:B:402:GLU:OE1	1.81	0.78
1:B:105:ALA:O	1:B:106:ALA:HB3	1.83	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:357:ALA:HB1	1:A:474:THR:CG2	2.14	0.77
1:A:216:VAL:CG1	1:A:217:GLY:N	2.48	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:NH1	1:B:371:ARG:CB	2.51	0.73
1:B:497:ARG:HH21	1:B:563:PRO:HA	1.53	0.73
1:B:229:GLN:HE22	1:B:231:LEU:HB2	1.54	0.72
1:A:212:THR:HG23	1:A:214:GLN:H	1.54	0.72
1:B:101:LYS:HG3	1:B:102:TRP:H	1.54	0.72
1:A:422:GLN:HE22	1:A:448:ALA:H	1.34	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: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:391:THR:HG22	1:A:455:LEU:CA	2.20	0.70
1:A:157:TYR:CD2	1:A:173:LEU:HD23	2.25	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:B:102:TRP:CH2	1:B:163:LEU:HD11	2.29	0.68
1:A:223:ASN:HD22	1:A:490:GLU:HG3	1.59	0.68
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:107:GLY:O	1:B:108:ALA:C	2.32	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:OE1	1:B:299:GLU:N	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: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: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:CG1	1:B:531:VAL:O	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:132:LEU:C	1:A:133:LEU:HD23	2.24	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
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:CD2	1:A:298:HIS:H	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:368:VAL:CG1	1:A:369:SER:H	2.12	0.56
1:A:216:VAL:HG13	1:A:217:GLY:H	1.70	0.56
1:B:489:ASN:O	1:B:493:ILE:HG23	2.06	0.56
1:B:218:SER:O	1:B:220:THR:N	2.39	0.56
1:A:308:LEU:HD21	1:A:340:VAL:HG13	1.86	0.56
1:B:101:LYS:CG	1:B:102:TRP:N	2.56	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:144:GLY:C	1:A:146:THR:N	2.57	0.56
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:CE	1:A:110:LYS:HA	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:B:229:GLN:NE2	1:B:272:GLU:HG2	2.22	0.54
1:A:110:LYS:HE3	1:A:110:LYS:HA	1.89	0.54
1:B:102:TRP:CD2	1:B:163:LEU:CD1	2.90	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:216:VAL:HG22	1:B:285:ALA:CB	2.36	0.52
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.74	0.52
1:B:100:GLN:O	1:B:101:LYS:HG2	2.09	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:201:THR:CG2	1:A:202:PRO:HD2	2.40	0.52
1:A:40:ARG:CZ	1:A:137:GLU:HG3	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:20:SER:OG	1:A:158:GLN:CD	2.46	0.51
1:A:209:TYR:CE2	1:A:550:THR:CG2	2.93	0.51
1:A:146:THR:CB	1:A:232:GLU:OE2	2.59	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:A:494:LEU:O	1:A:495:SER:CB	2.60	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:359:GLY:N	1:A:474:THR:HG21	2.26	0.49
1:A:71:PRO:HG2	1:A:509:GLN:NE2	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:397:PHE:C	1:B:398:LEU:HD22	2.33	0.49
1:B:27:GLN:HB2	1:B:333:SER:HB3	1.95	0.49
1:A:295:PRO:O	1:A:303:PRO:HA	2.13	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:B:298:HIS:HB3	1:B:299:GLU:OE1	2.13	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:209:TYR:HE2	1:A:550:THR:CG2	2.27	0.48
1:A:27:GLN:HB2	1:A:333:SER:HB3	1.96	0.48
1:A:514:GLY:HA2	1:A:555:ALA:HB1	1.96	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: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
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:N	1:B:398:LEU:HD22	2.28	0.47
1:B:516:PHE:N	1:B:550:THR:O	2.46	0.47
1:B:100:GLN:C	1:B:102:TRP:H	2.17	0.47
1:A:81:THR:CG2	1:A:84:ASN:H	2.23	0.47
1:A:528:ASP:C	1:A:528:ASP:OD1	2.52	0.47
1:B:54:ARG:NH1	1:B:168:ASP:OD1	2.48	0.47
1:B:497:ARG:NH2	1:B:563:PRO:CA	2.76	0.47
1:B:447:ARG:NH1	1:B:448:ALA:O	2.44	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:100:GLN:C	1:B:102:TRP:N	2.67	0.47
1:B:212:THR:HG23	1:B:213:SER:N	2.30	0.47
1:A:519:THR:CG2	1:A:519:THR:O	2.63	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:B:101:LYS:CG	1:B:102:TRP:H	2.27	0.46
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:216:VAL:CG1	1:B:286:ASN:HB2	2.45	0.46
1:B:297:ARG:C	1:B:299:GLU:H	2.17	0.46
1:A:201:THR:HG23	1:A:247:PHE:CD1	2.50	0.46
1:A:157:TYR:CE2	1:A:173:LEU:HD22	2.50	0.46
1:B:561:LEU:C	1:B:562:ASN:O	2.51	0.46
1:B:553:PHE:HB3	1:B:554:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:206:ARG:NH2	1:B:285:ALA:HB2	2.30	0.46
1:B:297:ARG:C	1:B:299:GLU:N	2.68	0.46
1:A:519:THR:HG22	1:A:519:THR:O	2.14	0.46
1:A:406:TYR:CZ	1:A:524:GLU:HB3	2.51	0.46
1:B:109:GLN:O	1:B:110:LYS:C	2.55	0.45
1:B:201:THR:HG23	1:B:202:PRO:CD	2.44	0.45
1:B:485:LEU:HA	1:B:485:LEU:HD12	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:B:301:GLN:O	1:B:303:PRO:HD3	2.16	0.45
1:B:271:ILE:HD12	1:B:471:VAL:CG2	2.47	0.45
1:A:398:LEU:N	1:A:398:LEU:HD22	2.31	0.45
1:B:562:ASN:O	1:B:563:PRO:C	2.54	0.45
1:A:68:VAL:HG13	1:A:79:TYR:CE1	2.52	0.45
1:B:102:TRP:CE2	1:B:132:LEU:HD21	2.52	0.45
1:A:357:ALA:CB	1:A:474:THR:HG23	2.33	0.45
1:B:377:THR:HB	7:B:629:HOH:O	2.15	0.45
1:A:145:PRO:CD	1:A:179:THR:HG23	2.47	0.45
1:A:556:LEU:HD22	1:A:560:LEU:CD1	2.47	0.45
1:A:553:PHE:HB3	1:A:554:PRO:HD3	1.99	0.45
1:B:41:ALA:CB	1:B:126:ILE:HD13	2.47	0.44
1:A:408:SER:O	1:A:523:HIS:HD2	2.00	0.44
1:A:153:SER:O	1:A:174:HIS:HD2	2.00	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:B:419:PRO:HD2	1:B:422:GLN:NE2	2.33	0.44
1:B:395:GLU:CD	1:B:398:LEU:HB2	2.38	0.44
1:A:449:TYR:CD1	1:A:449:TYR:C	2.90	0.44
1:A:454:ALA:HB3	1:A:477:SER:HB2	1.99	0.44
1:B:369:SER:HB2	1:B:370:GLY:H	1.66	0.44
1:A:118:ASP:OD2	1:A:346:LYS:NZ	2.50	0.44
1:A:60:ARG:HD3	1:A:60:ARG:HA	1.74	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:528:ASP:O	1:B:532:GLU:HA	2.18	0.43
1:B:164:ALA:N	1:B:165:PRO:CD	2.81	0.43
1:B:563:PRO:O	1:B:564:ARG:CB	2.56	0.43
1:B:404:VAL:HG21	1:B:521:GLY:C	2.38	0.43
1:B:75:GLN:CA	1:B:75:GLN:HE21	2.31	0.43
1:B:20:SER:HB2	1:B:159:LEU:O	2.18	0.43
1:A:26:ASP:N	1:A:26:ASP:OD2	2.50	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:394:GLN:HE21	1:B:401:ASN:HB3	1.84	0.43
1:A:216:VAL:HG13	1:A:285:ALA:O	2.17	0.43
1:A:210:ASN:ND2	1:A:552:ASN:OD1	2.51	0.43
1:B:229:GLN:HG3	1:B:272:GLU:HG3	2.00	0.43
1:A:132:LEU:CD1	1:A:133:LEU:HD21	2.46	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:B:497:ARG:NH2	1:B:562:ASN:C	2.72	0.43
1:B:81:THR:HG22	1:B:84:ASN:CG	2.38	0.43
1:B:26:ASP:OD2	1:B:26:ASP:N	2.52	0.43
1:A:448:ALA:HB1	1:A:542:TRP:HH2	1.83	0.42
1:A:301:GLN:O	1:A:303:PRO:HD3	2.19	0.42
1:A:395:GLU:CD	1:A:398:LEU:HB2	2.40	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:21:TYR:O	1:A:158:GLN:CB	2.68	0.42
1:B:523:HIS:HE1	1:B:536:PHE:H	1.68	0.42
1:B:221:SER:OG	1:B:222:ASN:N	2.52	0.42
1:B:561:LEU:O	1:B:562:ASN:C	2.55	0.41
1:A:391:THR:HG22	1:A:455:LEU:N	2.34	0.41
1:B:42:ASP:O	1:B:43:PRO:C	2.58	0.41
1:A:298:HIS:N	1:A:298:HIS:CD2	2.85	0.41
1:B:198:LEU:HD11	1:B:397:PHE:O	2.21	0.41
1:A:515:LEU:HD23	1:A:551:PRO:HA	2.01	0.41
1:B:320:VAL:HG22	1:B:353:THR:CG2	2.50	0.41
1:B:45:GLU:O	1:B:126:ILE:HG23	2.19	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:B:297:ARG:O	1:B:299:GLU:N	2.54	0.41
1:A:144:GLY:O	1:A:146:THR:C	2.59	0.41
1:A:41:ALA:HA	1:A:140:HIS:CE1	2.56	0.41
1:B:201:THR:CG2	1:B:202:PRO:N	2.84	0.41
1:A:106:ALA:HB2	1:A:132:LEU:HD23	2.01	0.41
1:B:408:SER:O	1:B:523:HIS:CD2	2.74	0.41
1:B:55:GLN:HB3	1:B:89:VAL:HG22	2.02	0.41
1:B:229:GLN:HE21	1:B:231:LEU:HG	1.86	0.41
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:179:THR:O	1:B:180:SER:C	2.60	0.40
1:B:556:LEU:HA	1:B:556:LEU:HD23	1.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	525/571 (92%)	495 (94%)	21 (4%)	9 (2%)	14	11
1	B	525/571 (92%)	479 (91%)	40 (8%)	6 (1%)	21	21
All	All	1050/1142 (92%)	974 (93%)	61 (6%)	15 (1%)	16	15

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%)	396 (89%)	47 (11%)	10	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	443/479 (92%)	391 (88%)	52 (12%)	8 7
All	All	886/958 (92%)	787 (89%)	99 (11%)	9 8

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
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	212	THR
1	A	220	THR
1	A	222	ASN
1	A	232	GLU
1	A	235	PHE
1	A	246	LEU
1	A	264	GLN
1	A	272	GLU
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	397	PHE
1	A	403	ILE

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Mol	Chain	Res	Type
1	A	404	VAL
1	A	430	LEU
1	A	447	ARG
1	A	463	SER
1	A	474	THR
1	A	490	GLU
1	A	506	ARG
1	A	523	HIS
1	A	531	VAL
1	A	550	THR
1	A	557	LEU
1	B	40	ARG
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	112	HIS
1	B	115	ILE
1	B	127	ARG
1	B	131	LEU
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	272	GLU
1	B	276	ASP
1	B	308	LEU
1	B	311	LEU
1	B	324	SER
1	B	344	LEU

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Mol	Chain	Res	Type
1	B	352	LEU
1	B	353	THR
1	B	367	SER
1	B	371	ARG
1	B	377	THR
1	B	385	VAL
1	B	391	THR
1	B	395	GLU
1	B	397	PHE
1	B	401	ASN
1	B	430	LEU
1	B	443	ASN
1	B	447	ARG
1	B	461	VAL
1	B	477	SER
1	B	485	LEU
1	B	497	ARG
1	B	509	GLN
1	B	523	HIS
1	B	550	THR
1	B	557	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	75	GLN
1	A	84	ASN
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	504	ASN
1	A	509	GLN
1	A	523	HIS

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Mol	Chain	Res	Type
1	B	56	GLN
1	B	57	ASN
1	B	75	GLN
1	B	100	GLN
1	B	158	GLN
1	B	174	HIS
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	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 chains 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 carbohydrates 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	11,13,15	1.13	1 (9%)	9,17,21	0.79	0
2	NAG	A	573	1	11,13,15	1.30	1 (9%)	9,17,21	1.94	3 (33%)
2	NAG	A	574	1	11,13,15	0.95	1 (9%)	9,17,21	1.30	2 (22%)
2	NAG	A	575	1	11,13,15	0.88	1 (9%)	9,17,21	0.72	0
6	SO4	A	582	-	4,4,4	0.15	0	6,6,6	0.25	0
2	NAG	B	572	1	11,13,15	1.02	1 (9%)	9,17,21	1.51	1 (11%)
2	NAG	B	573	1	11,13,15	1.02	1 (9%)	9,17,21	1.37	1 (11%)
2	NAG	B	574	1	11,13,15	1.07	1 (9%)	9,17,21	1.30	1 (11%)
2	NAG	B	575	1	11,13,15	1.02	1 (9%)	9,17,21	0.96	0
6	SO4	B	582	-	4,4,4	0.17	0	6,6,6	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	572	1	-	1/6/19/26	0/1/1/1
2	NAG	A	573	1	-	0/6/19/26	0/1/1/1
2	NAG	A	574	1	-	0/6/19/26	0/1/1/1
2	NAG	A	575	1	-	0/6/19/26	0/1/1/1
6	SO4	A	582	-	-	0/0/0/0	0/0/0/0
2	NAG	B	572	1	-	0/6/19/26	0/1/1/1
2	NAG	B	573	1	-	0/6/19/26	0/1/1/1
2	NAG	B	574	1	-	0/6/19/26	0/1/1/1
2	NAG	B	575	1	-	0/6/19/26	0/1/1/1
6	SO4	B	582	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	572	NAG	C6-C5	3.08	1.55	1.50
2	A	573	NAG	C2-C3	3.03	1.56	1.53
2	B	575	NAG	C6-C5	2.79	1.54	1.50
2	B	573	NAG	C6-C5	2.70	1.54	1.50
2	B	574	NAG	C6-C5	2.67	1.54	1.50
2	B	572	NAG	C6-C5	2.59	1.54	1.50
2	A	574	NAG	C6-C5	2.39	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	575	NAG	C6-C5	2.30	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	572	NAG	O3-C3-C2	-3.95	105.13	111.85
2	B	574	NAG	O3-C3-C2	-3.34	106.16	111.85
2	B	573	NAG	O3-C3-C2	-3.20	106.39	111.85
2	A	573	NAG	O3-C3-C2	-3.12	106.53	111.85
2	A	574	NAG	O3-C3-C2	-3.01	106.73	111.85
2	A	573	NAG	C2-N2-C7	2.80	127.79	123.09
2	A	573	NAG	O7-C7-C8	-2.27	117.62	122.04
2	A	574	NAG	O6-C6-C5	-2.13	109.26	112.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	572	NAG	C1-C2-N2-C7

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	529/571 (92%)	0.70	69 (13%) 4 5	49, 67, 79, 88	0
1	B	529/571 (92%)	0.82	82 (15%) 3 3	60, 67, 79, 91	0
All	All	1058/1142 (92%)	0.76	151 (14%) 3 4	49, 67, 79, 91	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	THR	13.4
1	A	220	THR	10.0
1	A	255	ALA	8.0
1	A	198	LEU	7.7
1	A	388	VAL	6.4
1	B	355	LEU	6.1
1	B	369	SER	6.0
1	A	399	ILE	5.7
1	B	395	GLU	5.6
1	A	265	GLY	5.5
1	B	265	GLY	5.3
1	A	369	SER	5.2
1	B	368	VAL	5.2
1	B	123	TRP	4.9
1	A	368	VAL	4.7
1	B	480	VAL	4.5
1	A	400	THR	4.4
1	A	452	VAL	4.4
1	B	531	VAL	4.2
1	A	496	GLY	4.2
1	A	355	LEU	4.2
1	A	264	GLN	4.1
1	B	102	TRP	4.1
1	B	264	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	453	ALA	4.0
1	A	180	SER	4.0
1	A	354	LEU	4.0
1	B	110	LYS	3.9
1	A	454	ALA	3.9
1	A	163	LEU	3.9
1	B	371	ARG	3.8
1	B	221	SER	3.8
1	A	551	PRO	3.8
1	A	563	PRO	3.7
1	B	564	ARG	3.7
1	B	388	VAL	3.6
1	B	266	ARG	3.5
1	B	145	PRO	3.5
1	B	234	TYR	3.5
1	B	496	GLY	3.4
1	A	387	THR	3.4
1	B	180	SER	3.4
1	B	477	SER	3.4
1	B	163	LEU	3.4
1	A	145	PRO	3.3
1	B	370	GLY	3.3
1	B	397	PHE	3.3
1	B	387	THR	3.2
1	B	268	ARG	3.2
1	A	197	HIS	3.2
1	B	214	GLN	3.2
1	B	219	GLY	3.2
1	A	398	LEU	3.1
1	B	400	THR	3.1
1	B	356	PHE	3.1
1	A	453	ALA	3.1
1	B	263	GLN	3.1
1	A	295	PRO	3.1
1	B	307	TRP	3.0
1	B	308	LEU	3.0
1	B	293	SER	3.0
1	A	477	SER	3.0
1	B	563	PRO	3.0
1	A	47	LEU	3.0
1	A	451	ASP	3.0
1	A	222	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	370	GLY	2.9
1	B	386	THR	2.9
1	A	110	LYS	2.9
1	B	142	VAL	2.9
1	A	397	PHE	2.9
1	A	219	GLY	2.9
1	B	323	VAL	2.9
1	B	198	LEU	2.8
1	A	386	THR	2.8
1	B	354	LEU	2.8
1	B	479	PRO	2.8
1	A	102	TRP	2.8
1	A	300	GLY	2.8
1	A	389	GLY	2.8
1	A	227	CYS	2.8
1	B	159	LEU	2.8
1	A	97	HIS	2.7
1	A	95	THR	2.7
1	B	218	SER	2.7
1	B	406	TYR	2.7
1	A	221	SER	2.6
1	B	348	ALA	2.6
1	B	454	ALA	2.6
1	A	142	VAL	2.6
1	B	322	THR	2.6
1	B	561	LEU	2.6
1	B	166	HIS	2.6
1	B	160	PRO	2.6
1	B	97	HIS	2.6
1	A	232	GLU	2.6
1	A	104	LEU	2.6
1	A	269	ALA	2.5
1	B	514	GLY	2.5
1	A	550	THR	2.5
1	B	550	THR	2.5
1	A	479	PRO	2.5
1	A	494	LEU	2.5
1	B	146	THR	2.5
1	B	21	TYR	2.4
1	A	385	VAL	2.4
1	A	480	VAL	2.4
1	A	218	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	222	ASN	2.4
1	A	234	TYR	2.4
1	A	93	PRO	2.4
1	A	450	PRO	2.4
1	B	455	LEU	2.4
1	B	46	GLU	2.4
1	B	452	VAL	2.3
1	A	478	THR	2.3
1	B	304	PHE	2.3
1	B	494	LEU	2.3
1	A	112	HIS	2.3
1	B	357	ALA	2.3
1	A	268	ARG	2.3
1	A	162	ALA	2.3
1	B	476	ALA	2.3
1	A	254	GLN	2.3
1	B	162	ALA	2.2
1	B	285	ALA	2.2
1	A	406	TYR	2.2
1	B	260	VAL	2.2
1	A	344	LEU	2.2
1	A	390	GLY	2.2
1	B	432	SER	2.2
1	A	297	ARG	2.2
1	B	491	HIS	2.2
1	A	358	SER	2.2
1	A	100	GLN	2.2
1	B	478	THR	2.2
1	B	549	GLY	2.1
1	B	431	SER	2.1
1	B	271	ILE	2.1
1	B	481	PHE	2.1
1	A	293	SER	2.1
1	A	280	LEU	2.1
1	A	371	ARG	2.1
1	B	465	ARG	2.1
1	B	469	PRO	2.1
1	B	487	LEU	2.1
1	B	390	GLY	2.0
1	A	394	GLN	2.0
1	B	83	GLU	2.0
1	B	435	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	318	PRO	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	575	13/15	0.37	4.99	87,88,90,91	0
2	NAG	B	575	13/15	0.34	3.33	88,90,93,93	0
4	CL	A	580	1/1	0.38	2.62	98,98,98,98	0
6	SO4	A	582	5/5	0.28	2.56	112,112,112,112	0
6	SO4	B	582	5/5	0.19	1.42	104,104,105,105	0
3	ZN	A	577	1/1	0.12	1.41	71,71,71,71	1
4	CL	B	580	1/1	0.33	1.03	112,112,112,112	0
2	NAG	B	574	13/15	0.18	-0.15	81,83,85,85	0
2	NAG	B	572	13/15	0.11	-0.63	72,73,77,78	0
2	NAG	A	573	13/15	0.12	-0.71	68,72,79,80	0
2	NAG	A	574	13/15	0.10	-0.74	80,81,84,85	0
2	NAG	B	573	13/15	0.12	-0.76	69,74,79,80	0
2	NAG	A	572	13/15	0.12	-0.83	82,85,89,90	0
5	CA	B	581	1/1	0.09	-1.36	61,61,61,61	0
3	ZN	B	576	1/1	0.07	-1.44	87,87,87,87	1
5	CA	A	581	1/1	0.09	-1.50	66,66,66,66	0
3	ZN	A	579	1/1	0.07	-1.54	114,114,114,114	0
3	ZN	A	576	1/1	0.06	-1.91	91,91,91,91	0
3	ZN	B	577	1/1	0.07	-2.34	94,94,94,94	0
3	ZN	A	578	1/1	0.04	-2.34	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	578	1/1	0.04	-2.68	90,90,90,90	0
3	ZN	B	579	1/1	0.10	-58.33	116,116,116,116	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.