



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 01:27 pm BST

PDB ID : 4UYZ / pdb_00004uyz
Title : STRUCTURE OF THE WNT DEACYLASE NOTUM - CRYSTAL FORM II - 2.8Å
Authors : Zebisch, M.; Jones, E.Y.
Deposited on : 2014-09-03
Resolution : 2.80 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

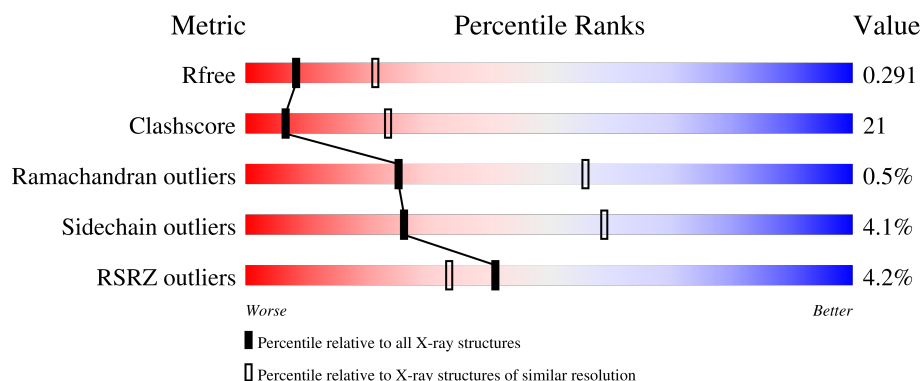
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	471	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>24%</div> <div>•</div> <div>27%</div> </div> </div>
1	B	471	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>22%</div> <div>•</div> <div>29%</div> </div> </div>
1	C	471	<div> <div>4%</div> <div> <div></div> <div>41%</div> <div>29%</div> <div>•</div> <div>28%</div> </div> </div>
1	D	471	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>25%</div> <div>•</div> <div>22%</div> </div> </div>
2	E	10	<div> <div>10%</div> <div> <div></div> <div>100%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	1452	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10991 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 PROTEIN NOTUM HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2730	1728	488	495	19			
1	B	335	Total	C	N	O	S	0	0	0
			2632	1671	468	474	19			
1	C	337	Total	C	N	O	S	0	0	0
			2676	1697	482	478	19			
1	D	369	Total	C	N	O	S	0	0	0
			2888	1828	519	519	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLU	-	expression tag	UNP Q6P988
A	36	THR	-	expression tag	UNP Q6P988
A	37	GLY	-	expression tag	UNP Q6P988
A	497	GLY	-	expression tag	UNP Q6P988
A	498	THR	-	expression tag	UNP Q6P988
A	499	LYS	-	expression tag	UNP Q6P988
A	500	HIS	-	expression tag	UNP Q6P988
A	501	HIS	-	expression tag	UNP Q6P988
A	502	HIS	-	expression tag	UNP Q6P988
A	503	HIS	-	expression tag	UNP Q6P988
A	504	HIS	-	expression tag	UNP Q6P988
A	505	HIS	-	expression tag	UNP Q6P988
B	35	GLU	-	expression tag	UNP Q6P988
B	36	THR	-	expression tag	UNP Q6P988
B	37	GLY	-	expression tag	UNP Q6P988
B	497	GLY	-	expression tag	UNP Q6P988
B	498	THR	-	expression tag	UNP Q6P988
B	499	LYS	-	expression tag	UNP Q6P988
B	500	HIS	-	expression tag	UNP Q6P988
B	501	HIS	-	expression tag	UNP Q6P988
B	502	HIS	-	expression tag	UNP Q6P988

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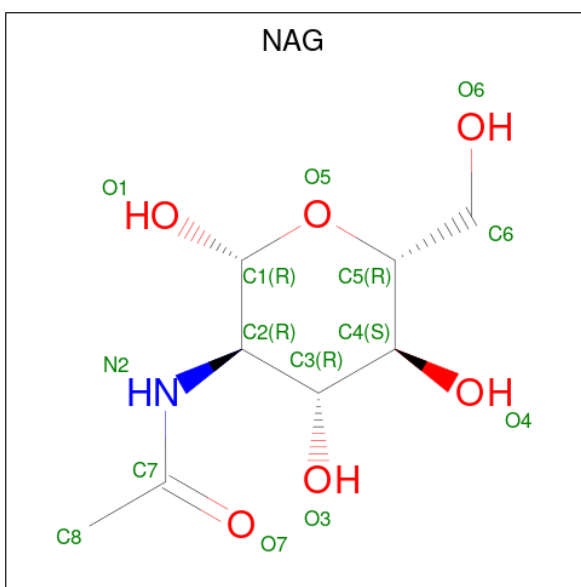
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Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP Q6P988
B	504	HIS	-	expression tag	UNP Q6P988
B	505	HIS	-	expression tag	UNP Q6P988
C	35	GLU	-	expression tag	UNP Q6P988
C	36	THR	-	expression tag	UNP Q6P988
C	37	GLY	-	expression tag	UNP Q6P988
C	497	GLY	-	expression tag	UNP Q6P988
C	498	THR	-	expression tag	UNP Q6P988
C	499	LYS	-	expression tag	UNP Q6P988
C	500	HIS	-	expression tag	UNP Q6P988
C	501	HIS	-	expression tag	UNP Q6P988
C	502	HIS	-	expression tag	UNP Q6P988
C	503	HIS	-	expression tag	UNP Q6P988
C	504	HIS	-	expression tag	UNP Q6P988
C	505	HIS	-	expression tag	UNP Q6P988
D	35	GLU	-	expression tag	UNP Q6P988
D	36	THR	-	expression tag	UNP Q6P988
D	37	GLY	-	expression tag	UNP Q6P988
D	497	GLY	-	expression tag	UNP Q6P988
D	498	THR	-	expression tag	UNP Q6P988
D	499	LYS	-	expression tag	UNP Q6P988
D	500	HIS	-	expression tag	UNP Q6P988
D	501	HIS	-	expression tag	UNP Q6P988
D	502	HIS	-	expression tag	UNP Q6P988
D	503	HIS	-	expression tag	UNP Q6P988
D	504	HIS	-	expression tag	UNP Q6P988
D	505	HIS	-	expression tag	UNP Q6P988

- Molecule 2 is a protein called POLY ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	0	0	0
			50	30	10	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

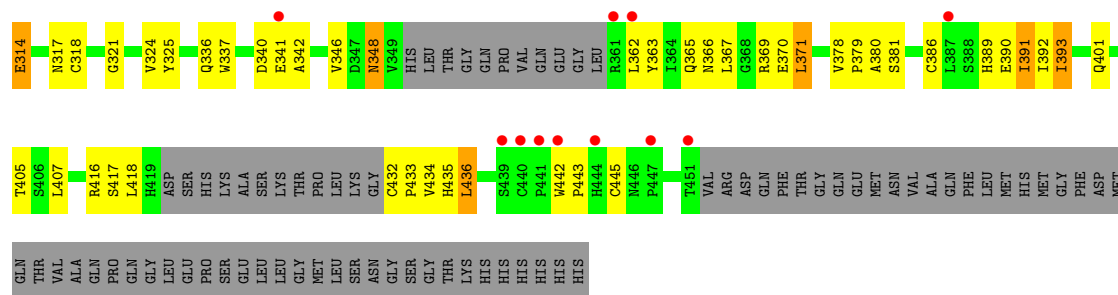
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

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.

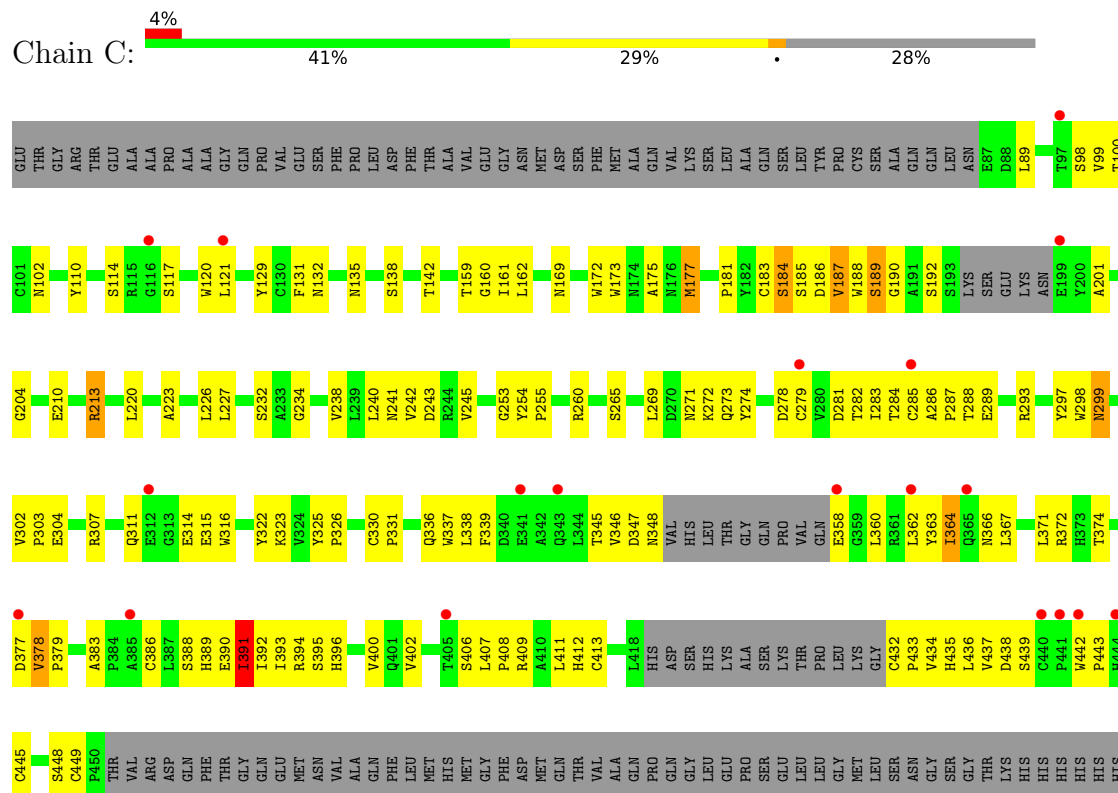
Chain A:

Chain B:

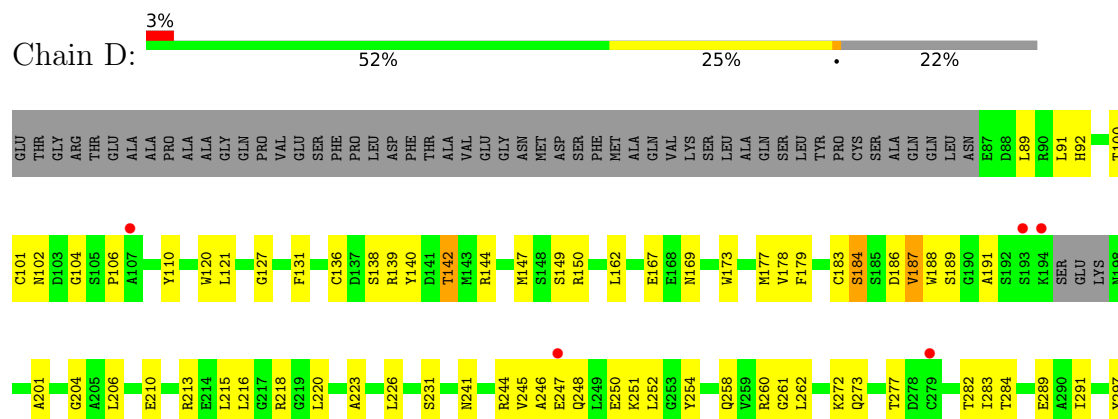
Position	Amino Acid	Frequency (%)
1	GLU	4.0
2	THR	0.0
3	GLY	0.0
4	ARG	0.0
5	THR	0.0
6	GLU	0.0
7	ALA	0.0
8	ALA	0.0
9	PRO	0.0
10	ALA	0.0
11	ALA	0.0
12	GLY	0.0
13	GLN	0.0
14	PRO	0.0
15	VAL	0.0
16	GLU	0.0
17	SER	0.0
18	PHE	0.0
19	PRO	0.0
20	LEU	0.0
21	ASP	0.0
22	PHE	0.0
23	THR	0.0
24	ALA	0.0
25	VAL	0.0
26	GLU	0.0
27	GLY	0.0
28	ASN	0.0
29	MET	0.0
30	ASP	0.0
31	SER	0.0
32	PHE	0.0
33	MET	0.0
34	ALA	0.0
35	GLN	0.0
36	SER	0.0
37	TYR	0.0
38	PRO	0.0
39	CYS	0.0
40	ALA	0.0
41	GLN	0.0
42	GLN	0.0
43	LEU	0.0
44	ASN	0.0
45	ASP	0.0
46	L91	0.0
47	H92	0.0
48	N96	0.0
49	T97	0.0
50	C98	0.0

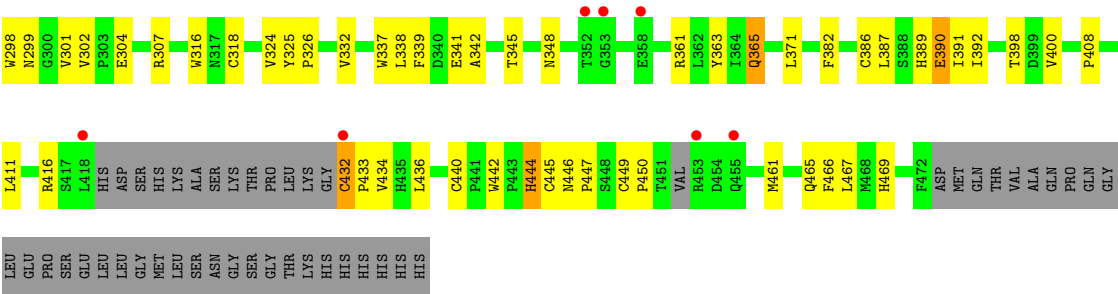


● Molecule 1: PROTEIN NOTUM HOMOLOG



● Molecule 1: PROTEIN NOTUM HOMOLOG





● Molecule 2: POLY ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.83Å 193.88Å 75.72Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	96.94 – 2.80 96.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (96.94-2.80) 88.9 (96.94-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.248 , 0.293 0.244 , 0.291	Depositor DCC
R_{free} test set	1143 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10991	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/2800	0.95	1/3810 (0.0%)
1	B	0.56	0/2703	0.95	2/3683 (0.1%)
1	C	0.55	0/2747	0.95	5/3735 (0.1%)
1	D	0.54	0/2963	0.93	2/4029 (0.0%)
2	E	0.63	0/49	0.85	0/67
All	All	0.55	0/11262	0.95	10/15324 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	VAL	CA-C-N	6.99	126.50	119.24
1	C	378	VAL	C-N-CA	6.99	126.50	119.24
1	D	184	SER	N-CA-C	6.51	119.69	111.69
1	C	449	CYS	N-CA-C	6.29	116.84	109.60
1	A	131	PHE	N-CA-C	5.98	120.60	112.88
1	D	142	THR	N-CA-C	5.54	117.40	111.36
1	C	395	SER	N-CA-C	5.48	117.34	111.36
1	B	152	TRP	CA-C-N	5.14	125.13	119.89
1	B	152	TRP	C-N-CA	5.14	125.13	119.89
1	C	184	SER	N-CA-C	5.09	117.95	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2730	0	2615	87	0
1	B	2632	0	2494	110	0
1	C	2676	0	2565	142	0
1	D	2888	0	2739	120	0
2	E	50	0	49	0	0
3	B	14	0	13	0	0
4	B	1	0	0	0	0
All	All	10991	0	10475	457	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 21.

All (457) 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:D:440:CYS:HB3	1:D:445:CYS:SG	1.57	1.42
1:B:132:ASN:OD1	1:B:135:ASN:HB2	1.32	1.24
1:C:271:ASN:HD21	1:C:347:ASP:CG	1.46	1.20
1:C:273:GLN:NE2	1:C:286:ALA:HB2	1.54	1.19
1:D:210:GLU:OE2	1:D:213:ARG:NE	1.77	1.18
1:B:416:ARG:NH2	1:B:432:CYS:SG	2.18	1.17
1:D:440:CYS:CB	1:D:445:CYS:SG	2.33	1.16
1:C:273:GLN:HE21	1:C:286:ALA:CB	1.59	1.14
1:C:132:ASN:CG	1:C:135:ASN:OD1	1.91	1.14
1:D:144:ARG:HH21	1:D:150:ARG:HD3	1.07	1.14
1:C:210:GLU:OE2	1:C:213:ARG:NH2	1.81	1.13
1:D:144:ARG:NH2	1:D:150:ARG:HD3	1.64	1.12
1:C:132:ASN:ND2	1:C:135:ASN:OD1	1.82	1.10
1:D:139:ARG:HG2	1:D:147:MET:HE2	1.23	1.10
1:D:444:HIS:CD2	1:D:449:CYS:SG	2.47	1.07
1:B:162:LEU:HA	1:B:177:MET:HE3	1.37	1.07
1:B:273:GLN:HE22	1:B:277:THR:HG22	1.21	1.05
1:B:162:LEU:HA	1:B:177:MET:CE	1.86	1.04
1:C:271:ASN:ND2	1:C:347:ASP:OD2	1.91	1.04
1:D:144:ARG:HH22	1:D:150:ARG:HB2	0.92	1.03
1:C:273:GLN:NE2	1:C:286:ALA:CB	2.20	1.02
1:D:144:ARG:NH2	1:D:150:ARG:HB2	1.76	1.01
1:B:433:PRO:O	1:B:436:LEU:HD21	1.61	1.01
1:C:287:PRO:HD3	1:C:346:VAL:HG12	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLU:OE2	1:C:213:ARG:CZ	2.10	0.99
1:C:413:CYS:SG	1:C:432:CYS:N	2.36	0.98
1:D:162:LEU:HA	1:D:177:MET:HE3	1.41	0.98
1:B:287:PRO:HD3	1:B:346:VAL:HG22	1.46	0.98
1:B:139:ARG:NH1	1:B:185:SER:OG	1.98	0.97
1:D:144:ARG:HH22	1:D:150:ARG:CB	1.78	0.96
1:D:140:TYR:HA	1:D:147:MET:HE3	1.46	0.96
1:C:339:PHE:CD2	1:C:443:PRO:HG3	2.02	0.93
1:A:311:GLN:HG2	1:A:312:GLU:N	1.83	0.93
1:C:121:LEU:HD12	1:C:177:MET:HE1	1.49	0.91
1:C:289:GLU:O	1:C:293:ARG:HG3	1.71	0.90
1:C:271:ASN:ND2	1:C:347:ASP:CG	2.28	0.90
1:D:304:GLU:HG3	1:D:307:ARG:HH21	1.37	0.89
1:B:435:HIS:C	1:B:436:LEU:HD23	1.96	0.89
1:D:139:ARG:CG	1:D:147:MET:HE2	2.03	0.89
1:C:288:THR:HG23	1:C:316:TRP:CZ3	2.07	0.88
1:C:172:TRP:HZ3	1:C:411:LEU:HD23	1.38	0.87
1:A:311:GLN:HG2	1:A:312:GLU:H	1.38	0.85
1:D:162:LEU:HA	1:D:177:MET:CE	2.07	0.85
1:B:132:ASN:OD1	1:B:135:ASN:CB	2.21	0.85
1:C:304:GLU:HG3	1:C:307:ARG:HH21	1.40	0.85
1:D:461:MET:HE1	1:D:469:HIS:CD2	2.12	0.84
1:C:186:ASP:O	1:C:189:SER:OG	1.94	0.84
1:A:184:SER:OG	1:A:186:ASP:OD1	1.95	0.84
1:B:186:ASP:O	1:B:189:SER:OG	1.95	0.84
1:C:132:ASN:OD1	1:C:135:ASN:OD1	1.94	0.84
1:D:140:TYR:CA	1:D:147:MET:HE3	2.08	0.83
1:D:138:SER:O	1:D:142:THR:HG22	1.78	0.83
1:D:291:ILE:HG22	1:D:316:TRP:HB2	1.59	0.83
1:B:273:GLN:NE2	1:B:277:THR:HG22	1.92	0.83
1:D:444:HIS:NE2	1:D:449:CYS:SG	2.53	0.82
1:D:186:ASP:O	1:D:189:SER:OG	1.98	0.82
1:A:231:SER:HB3	1:A:390:GLU:HG2	1.60	0.82
1:C:210:GLU:CD	1:C:213:ARG:HH21	1.88	0.81
1:C:271:ASN:ND2	1:C:347:ASP:OD1	2.14	0.81
1:C:432:CYS:HB2	1:C:433:PRO:HD2	1.63	0.80
1:B:162:LEU:CA	1:B:177:MET:CE	2.59	0.80
1:B:272:LYS:O	1:B:363:TYR:OH	1.98	0.80
1:B:366:ASN:O	1:B:370:GLU:HG3	1.81	0.80
1:C:210:GLU:OE2	1:C:213:ARG:NE	2.15	0.79
1:B:186:ASP:OD2	1:B:190:GLY:N	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:ARG:NH2	1:D:432:CYS:N	2.31	0.79
1:C:273:GLN:HE21	1:C:286:ALA:CA	1.95	0.78
1:D:398:THR:HG22	1:D:408:PRO:HG2	1.66	0.78
1:B:269:LEU:HD11	1:B:371:LEU:HG	1.64	0.78
1:C:273:GLN:NE2	1:C:286:ALA:CA	2.47	0.78
1:D:416:ARG:HH21	1:D:432:CYS:N	1.83	0.77
1:B:162:LEU:HD23	1:B:177:MET:HE3	1.67	0.76
1:C:162:LEU:HD12	1:C:393:ILE:HD11	1.67	0.76
1:D:140:TYR:N	1:D:147:MET:CE	2.50	0.75
1:A:409:ARG:HB2	1:B:167:GLU:OE2	1.86	0.75
1:C:281:ASP:O	1:C:284:THR:OG1	2.04	0.74
1:C:287:PRO:HD3	1:C:346:VAL:CG1	2.17	0.74
1:C:339:PHE:HD2	1:C:443:PRO:HG3	1.48	0.74
1:A:127:GLY:O	1:A:139:ARG:NH2	2.21	0.74
1:B:162:LEU:HD12	1:B:393:ILE:HD11	1.69	0.73
1:B:435:HIS:O	1:B:436:LEU:HD23	1.87	0.73
1:D:184:SER:HB3	1:D:186:ASP:CG	2.13	0.73
1:C:184:SER:HB3	1:C:186:ASP:OD1	1.88	0.73
1:D:136:CYS:O	1:D:147:MET:HE1	1.89	0.72
1:B:162:LEU:C	1:B:177:MET:HE2	2.15	0.72
1:B:391:ILE:HD13	1:B:407:LEU:CD2	2.20	0.72
1:C:339:PHE:HE2	1:C:443:PRO:CD	2.02	0.72
1:C:311:GLN:O	1:C:314:GLU:HB2	1.89	0.71
1:B:162:LEU:CA	1:B:177:MET:HE3	2.16	0.71
1:D:144:ARG:NH2	1:D:150:ARG:CD	2.50	0.71
1:B:380:ALA:HA	1:B:434:VAL:HG12	1.71	0.71
1:D:120:TRP:CD1	1:D:223:ALA:HB2	2.25	0.71
1:B:342:ALA:O	1:B:346:VAL:HG12	1.90	0.71
1:B:260:ARG:HD3	1:B:418:LEU:HD13	1.74	0.70
1:B:162:LEU:C	1:B:177:MET:CE	2.65	0.70
1:C:186:ASP:OD2	1:C:190:GLY:N	2.24	0.70
1:A:325:TYR:N	1:A:326:PRO:HD2	2.07	0.69
1:B:273:GLN:HE22	1:B:277:THR:CG2	2.03	0.69
1:B:162:LEU:O	1:B:177:MET:HE2	1.92	0.69
1:C:172:TRP:CZ3	1:C:411:LEU:HD23	2.27	0.69
1:D:244:ARG:O	1:D:248:GLN:HG3	1.91	0.69
1:A:175:ALA:O	1:A:177:MET:CE	2.40	0.69
1:A:205:ALA:O	1:A:209:GLN:HG3	1.93	0.69
1:C:175:ALA:HB3	1:C:177:MET:HE3	1.74	0.68
1:C:121:LEU:HD21	1:C:227:LEU:HD23	1.75	0.68
1:C:339:PHE:CE2	1:C:443:PRO:HD3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HB3	1:B:147:MET:SD	2.33	0.67
1:A:269:LEU:HD11	1:A:371:LEU:HD12	1.77	0.67
1:A:216:LEU:HA	1:A:220:LEU:HB3	1.76	0.67
1:C:210:GLU:CD	1:C:213:ARG:NH2	2.50	0.67
1:A:389:HIS:O	1:A:390:GLU:HB2	1.95	0.66
1:B:184:SER:OG	1:B:186:ASP:OD1	2.10	0.66
1:C:273:GLN:HB3	1:C:347:ASP:O	1.96	0.66
1:A:367:LEU:C	1:A:367:LEU:HD23	2.21	0.66
1:D:100:THR:HG22	1:D:101:CYS:O	1.94	0.66
1:B:243:ASP:O	1:B:247:GLU:HG3	1.96	0.65
1:B:161:ILE:HD11	1:B:172:TRP:CE3	2.31	0.65
1:C:400:VAL:HA	1:C:448:SER:HB3	1.78	0.65
1:C:438:ASP:OD1	1:C:439:SER:N	2.30	0.65
1:B:291:ILE:O	1:B:295:ILE:HG22	1.97	0.65
1:D:100:THR:CG2	1:D:104:GLY:HA2	2.26	0.65
1:C:220:LEU:HD11	1:C:226:LEU:HD12	1.78	0.65
1:C:339:PHE:CE2	1:C:443:PRO:CD	2.80	0.65
1:C:273:GLN:NE2	1:C:286:ALA:HA	2.12	0.65
1:A:162:LEU:HD23	1:A:177:MET:HG2	1.78	0.64
1:D:140:TYR:CA	1:D:147:MET:CE	2.74	0.64
1:D:318:CYS:O	1:D:324:VAL:HG21	1.97	0.64
1:C:121:LEU:HD23	1:C:227:LEU:HB3	1.80	0.64
1:B:391:ILE:HD13	1:B:407:LEU:HD22	1.80	0.64
1:A:367:LEU:O	1:A:371:LEU:HD13	1.98	0.63
1:A:175:ALA:O	1:A:177:MET:HE2	1.98	0.63
1:D:184:SER:CB	1:D:186:ASP:OD1	2.46	0.63
1:A:337:TRP:CE3	1:A:386:CYS:HB2	2.34	0.63
1:A:295:ILE:CD1	1:A:316:TRP:HA	2.30	0.62
1:C:364:ILE:N	1:C:364:ILE:HD13	2.15	0.62
1:A:162:LEU:HD12	1:A:393:ILE:CD1	2.29	0.62
1:C:367:LEU:HD23	1:C:367:LEU:C	2.25	0.62
1:D:342:ALA:HB2	1:D:389:HIS:CE1	2.34	0.62
1:B:401:GLN:HA	1:B:405:THR:O	1.98	0.62
1:C:409:ARG:HG2	1:D:167:GLU:OE2	2.00	0.62
1:A:287:PRO:O	1:A:291:ILE:HG12	2.00	0.61
1:C:272:LYS:O	1:C:363:TYR:OH	2.18	0.61
1:D:162:LEU:CA	1:D:177:MET:HE3	2.26	0.61
1:A:241:ASN:O	1:A:245:VAL:HG23	2.01	0.61
1:B:162:LEU:HA	1:B:177:MET:HE1	1.81	0.61
1:A:91:LEU:HB2	1:A:110:TYR:CE1	2.35	0.61
1:A:277:THR:HG21	1:A:348:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:VAL:HG13	1:C:243:ASP:N	2.15	0.60
1:C:339:PHE:HE2	1:C:443:PRO:HD3	1.64	0.60
1:D:140:TYR:N	1:D:147:MET:HE1	2.15	0.60
1:D:100:THR:HG21	1:D:104:GLY:HA2	1.82	0.60
1:D:231:SER:HB3	1:D:390:GLU:HG2	1.83	0.60
1:B:273:GLN:HE21	1:B:348:ASN:HB2	1.65	0.60
1:C:339:PHE:CE2	1:C:443:PRO:HG3	2.37	0.60
1:D:102:ASN:ND2	1:D:201:ALA:O	2.35	0.59
1:B:348:ASN:O	1:B:348:ASN:ND2	2.29	0.59
1:C:325:TYR:HB3	1:C:326:PRO:HD3	1.84	0.59
1:A:162:LEU:HD12	1:A:393:ILE:HD12	1.83	0.59
1:D:337:TRP:HZ2	1:D:391:ILE:HD13	1.68	0.59
1:A:402:VAL:HG12	1:A:403:LYS:HG3	1.84	0.59
1:C:315:GLU:N	1:C:315:GLU:OE1	2.35	0.59
1:D:283:ILE:HG23	1:D:345:THR:CG2	2.32	0.59
1:C:432:CYS:HB2	1:C:433:PRO:CD	2.30	0.59
1:C:232:SER:HA	1:C:265:SER:O	2.03	0.59
1:C:391:ILE:HG23	1:C:392:ILE:N	2.17	0.58
1:D:432:CYS:HB2	1:D:433:PRO:HD2	1.83	0.58
1:A:175:ALA:C	1:A:177:MET:HE2	2.27	0.58
1:A:191:ALA:HB2	1:A:301:VAL:CG2	2.33	0.58
1:A:311:GLN:CG	1:A:312:GLU:H	2.14	0.58
1:B:127:GLY:O	1:B:139:ARG:NH2	2.36	0.58
1:D:184:SER:HB2	1:D:186:ASP:OD1	2.03	0.58
1:D:210:GLU:OE2	1:D:213:ARG:CD	2.49	0.58
1:D:461:MET:HE1	1:D:469:HIS:HD2	1.65	0.58
1:D:187:VAL:HG12	1:D:187:VAL:O	2.03	0.58
1:C:132:ASN:OD1	1:C:135:ASN:CG	2.47	0.58
1:A:161:ILE:O	1:A:169:ASN:ND2	2.37	0.58
1:C:120:TRP:CD1	1:C:223:ALA:HB2	2.39	0.58
1:C:186:ASP:OD2	1:C:190:GLY:HA3	2.04	0.58
1:D:162:LEU:C	1:D:177:MET:HE2	2.28	0.58
1:B:161:ILE:HD11	1:B:172:TRP:CZ3	2.39	0.58
1:B:274:TYR:HD1	1:B:363:TYR:CD2	2.21	0.57
1:D:210:GLU:CD	1:D:213:ARG:HE	2.02	0.57
1:D:337:TRP:CZ2	1:D:391:ILE:HD13	2.39	0.57
1:C:406:SER:HB3	1:C:408:PRO:HD2	1.86	0.57
1:B:216:LEU:HD23	1:B:220:LEU:HD23	1.86	0.57
1:C:121:LEU:HD12	1:C:177:MET:CE	2.28	0.57
1:B:314:GLU:HG3	1:B:317:ASN:HD21	1.70	0.56
1:C:273:GLN:HE21	1:C:286:ALA:HA	1.65	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:TRP:HA	1:C:204:GLY:HA3	1.86	0.56
1:B:287:PRO:O	1:B:291:ILE:HG12	2.05	0.56
1:C:184:SER:O	1:C:185:SER:HB2	2.04	0.56
1:C:377:ASP:OD1	1:C:377:ASP:N	2.39	0.56
1:B:391:ILE:HD13	1:B:407:LEU:HD23	1.87	0.56
1:A:311:GLN:CG	1:A:312:GLU:N	2.62	0.56
1:A:304:GLU:HA	1:A:307:ARG:HB2	1.88	0.56
1:D:461:MET:HE2	1:D:466:PHE:N	2.21	0.56
1:A:295:ILE:HD11	1:A:316:TRP:HA	1.87	0.55
1:C:260:ARG:HG2	1:C:331:PRO:HG2	1.87	0.55
1:B:348:ASN:HD22	1:B:348:ASN:C	2.15	0.55
1:C:102:ASN:ND2	1:C:201:ALA:O	2.39	0.55
1:A:126:GLY:HA3	1:A:232:SER:HB3	1.88	0.55
1:C:435:HIS:C	1:C:436:LEU:HD22	2.31	0.55
1:D:184:SER:HB3	1:D:186:ASP:OD1	2.05	0.55
1:D:162:LEU:CA	1:D:177:MET:CE	2.81	0.55
1:B:186:ASP:OD2	1:B:190:GLY:CA	2.56	0.54
1:C:186:ASP:OD2	1:C:190:GLY:CA	2.56	0.54
1:C:187:VAL:HG12	1:C:187:VAL:O	2.07	0.54
1:A:191:ALA:HB2	1:A:301:VAL:HG22	1.89	0.54
1:A:152:TRP:CZ2	1:A:181:PRO:HB2	2.43	0.54
1:A:358:GLU:O	1:A:362:LEU:HD13	2.07	0.54
1:B:442:TRP:O	1:B:445:CYS:SG	2.66	0.54
1:B:187:VAL:HG12	1:B:187:VAL:O	2.09	0.53
1:B:365:GLN:O	1:B:369:ARG:HG3	2.08	0.53
1:C:442:TRP:O	1:C:445:CYS:SG	2.66	0.53
1:B:340:ASP:OD1	1:B:389:HIS:ND1	2.40	0.53
1:C:254:TYR:N	1:C:255:PRO:HD3	2.23	0.53
1:A:228:LEU:HG	1:A:238:VAL:HG22	1.89	0.53
1:A:442:TRP:O	1:A:445:CYS:SG	2.66	0.53
1:B:337:TRP:CE3	1:B:386:CYS:HB2	2.44	0.53
1:C:253:GLY:C	1:C:255:PRO:HD3	2.34	0.53
1:A:367:LEU:HD23	1:A:367:LEU:O	2.09	0.53
1:B:161:ILE:O	1:B:177:MET:HE1	2.08	0.53
1:C:389:HIS:O	1:C:390:GLU:HB2	2.08	0.53
1:D:186:ASP:OD2	1:D:204:GLY:N	2.41	0.53
1:A:260:ARG:HG2	1:A:331:PRO:HG2	1.91	0.53
1:B:220:LEU:HD11	1:B:226:LEU:HD12	1.90	0.53
1:C:407:LEU:HD12	1:C:407:LEU:O	2.09	0.53
1:B:260:ARG:CD	1:B:418:LEU:HD13	2.39	0.52
1:C:98:SER:O	1:C:100:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:TRP:O	1:D:445:CYS:SG	2.67	0.52
1:C:169:ASN:O	1:C:173:TRP:HB3	2.09	0.52
1:D:169:ASN:HB3	1:D:173:TRP:HB3	1.92	0.52
1:B:121:LEU:HD13	1:B:227:LEU:HD23	1.92	0.52
1:D:92:HIS:NE2	1:D:218:ARG:NH1	2.58	0.52
1:D:440:CYS:HG	1:D:445:CYS:HG	1.54	0.52
1:C:337:TRP:CZ3	1:C:386:CYS:HB2	2.45	0.52
1:C:358:GLU:O	1:C:362:LEU:HG	2.09	0.52
1:A:207:ILE:O	1:A:211:VAL:HG23	2.09	0.52
1:B:321:GLY:HA2	1:B:324:VAL:HG12	1.92	0.52
1:B:321:GLY:HA2	1:B:324:VAL:CG1	2.40	0.52
1:C:432:CYS:CB	1:C:433:PRO:HD2	2.38	0.51
1:B:186:ASP:OD2	1:B:190:GLY:HA3	2.10	0.51
1:B:231:SER:HA	1:B:264:ASP:O	2.10	0.51
1:C:121:LEU:CD2	1:C:227:LEU:HD23	2.41	0.51
1:C:242:VAL:CG1	1:C:243:ASP:N	2.73	0.51
1:B:274:TYR:CD1	1:B:363:TYR:CD2	2.98	0.51
1:D:461:MET:HE2	1:D:465:GLN:C	2.36	0.51
1:D:298:TRP:O	1:D:299:ASN:HB2	2.10	0.51
1:B:91:LEU:HB2	1:B:110:TYR:CE2	2.46	0.51
1:D:162:LEU:C	1:D:177:MET:CE	2.83	0.51
1:B:162:LEU:HD12	1:B:393:ILE:CD1	2.40	0.51
1:D:241:ASN:O	1:D:245:VAL:HG23	2.11	0.51
1:D:272:LYS:O	1:D:363:TYR:OH	2.25	0.51
1:D:342:ALA:CB	1:D:389:HIS:CE1	2.94	0.50
1:C:172:TRP:CZ3	1:C:411:LEU:HB3	2.47	0.50
1:D:341:GLU:HB2	1:D:389:HIS:HB2	1.94	0.50
1:B:270:ASP:OD1	1:B:270:ASP:N	2.35	0.50
1:D:318:CYS:HA	1:D:324:VAL:HG22	1.93	0.50
1:D:391:ILE:HG23	1:D:392:ILE:N	2.27	0.50
1:B:184:SER:O	1:B:185:SER:HB2	2.11	0.50
1:B:433:PRO:C	1:B:436:LEU:HD21	2.35	0.50
1:A:187:VAL:HG12	1:A:187:VAL:O	2.10	0.50
1:B:391:ILE:HG23	1:B:392:ILE:N	2.27	0.50
1:C:138:SER:O	1:C:142:THR:HG22	2.11	0.50
1:D:162:LEU:O	1:D:177:MET:HE2	2.12	0.50
1:D:277:THR:HB	1:D:348:ASN:ND2	2.26	0.50
1:B:321:GLY:CA	1:B:324:VAL:HG12	2.42	0.50
1:C:367:LEU:HD23	1:C:367:LEU:O	2.12	0.49
1:B:389:HIS:O	1:B:390:GLU:HB2	2.12	0.49
1:C:304:GLU:HG3	1:C:307:ARG:NH2	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:TRP:CD1	1:C:388:SER:O	2.65	0.49
1:C:339:PHE:HE2	1:C:443:PRO:N	2.10	0.49
1:C:161:ILE:O	1:C:169:ASN:ND2	2.46	0.49
1:B:121:LEU:HD12	1:B:227:LEU:O	2.13	0.49
1:D:220:LEU:HD11	1:D:226:LEU:HD12	1.94	0.49
1:A:272:LYS:O	1:A:363:TYR:OH	2.23	0.49
1:C:131:PHE:O	1:C:297:TYR:CD2	2.66	0.49
1:C:271:ASN:CG	1:C:347:ASP:OD1	2.55	0.49
1:C:339:PHE:CE2	1:C:443:PRO:CG	2.96	0.49
1:D:440:CYS:CB	1:D:445:CYS:HG	2.02	0.49
1:D:461:MET:CE	1:D:469:HIS:CD2	2.92	0.49
1:B:139:ARG:HH11	1:B:185:SER:HG	1.56	0.49
1:C:241:ASN:O	1:C:245:VAL:HG23	2.12	0.49
1:D:289:GLU:HA	1:D:289:GLU:OE1	2.11	0.49
1:C:302:VAL:O	1:C:307:ARG:NH2	2.46	0.49
1:B:442:TRP:HD1	1:B:443:PRO:O	1.96	0.48
1:C:391:ILE:CG2	1:C:392:ILE:N	2.76	0.48
1:D:144:ARG:NH2	1:D:150:ARG:CB	2.55	0.48
1:B:435:HIS:O	1:B:436:LEU:CD2	2.61	0.48
1:D:273:GLN:HE22	1:D:277:THR:HG22	1.78	0.48
1:A:380:ALA:HA	1:A:434:VAL:HG12	1.95	0.48
1:C:102:ASN:OD1	1:C:185:SER:HB2	2.13	0.48
1:C:274:TYR:CE2	1:C:360:LEU:HD13	2.48	0.48
1:A:186:ASP:O	1:A:187:VAL:HB	2.13	0.48
1:A:392:ILE:HD13	1:A:407:LEU:HD21	1.96	0.48
1:B:314:GLU:HG3	1:B:317:ASN:ND2	2.28	0.48
1:C:269:LEU:HD21	1:C:374:THR:HG21	1.95	0.48
1:C:184:SER:CB	1:C:186:ASP:OD1	2.58	0.48
1:D:382:PHE:HA	1:D:436:LEU:O	2.14	0.48
1:A:102:ASN:ND2	1:A:201:ALA:O	2.47	0.48
1:B:232:SER:OG	1:B:233:ALA:N	2.46	0.48
1:D:361:ARG:O	1:D:365:GLN:HG2	2.14	0.48
1:C:394:ARG:CG	1:C:396:HIS:NE2	2.76	0.47
1:D:291:ILE:CG2	1:D:316:TRP:HB2	2.40	0.47
1:A:99:VAL:HG21	1:A:210:GLU:CG	2.44	0.47
1:B:216:LEU:CD2	1:B:220:LEU:HD23	2.44	0.47
1:C:192:SER:HB2	1:C:299:ASN:HB2	1.95	0.47
1:A:187:VAL:O	1:A:188:TRP:HB2	2.15	0.47
1:C:175:ALA:HB3	1:C:177:MET:CE	2.45	0.47
1:A:130:CYS:SG	1:A:136:CYS:N	2.87	0.47
1:A:188:TRP:HA	1:A:204:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:SER:HB3	1:A:408:PRO:HD2	1.95	0.47
1:D:261:GLY:HA3	1:D:332:VAL:HG22	1.97	0.47
1:B:393:ILE:HA	1:B:393:ILE:HD12	1.75	0.47
1:B:325:TYR:CE2	1:B:378:VAL:HG13	2.50	0.47
1:C:336:GLN:HG3	1:C:337:TRP:O	2.14	0.47
1:D:186:ASP:O	1:D:187:VAL:HB	2.14	0.47
1:B:362:LEU:O	1:B:366:ASN:HB2	2.15	0.46
1:B:442:TRP:CD1	1:B:443:PRO:O	2.69	0.46
1:C:159:THR:HG23	1:C:393:ILE:HG13	1.97	0.46
1:B:123:PHE:HE1	1:B:392:ILE:HD11	1.78	0.46
1:C:367:LEU:C	1:C:367:LEU:CD2	2.89	0.46
1:B:336:GLN:NE2	1:B:340:ASP:OD2	2.49	0.46
1:B:341:GLU:HB2	1:B:389:HIS:HB2	1.96	0.46
1:D:244:ARG:O	1:D:247:GLU:HB3	2.15	0.46
1:B:96:ASN:OD1	1:B:98:SER:OG	2.32	0.46
1:A:172:TRP:CZ3	1:A:411:LEU:HB3	2.51	0.46
1:A:99:VAL:HG21	1:A:210:GLU:HG3	1.98	0.46
1:A:169:ASN:HB3	1:A:173:TRP:HB3	1.96	0.46
1:C:383:ALA:HB3	1:C:437:VAL:HG13	1.98	0.46
1:D:283:ILE:HG23	1:D:345:THR:HG22	1.98	0.46
1:C:234:GLY:O	1:C:238:VAL:HG23	2.15	0.46
1:C:363:TYR:O	1:C:367:LEU:N	2.48	0.46
1:D:191:ALA:HA	1:D:206:LEU:HG	1.97	0.46
1:A:337:TRP:CD1	1:A:388:SER:O	2.68	0.46
1:C:406:SER:O	1:C:409:ARG:HB2	2.16	0.45
1:D:220:LEU:O	1:D:220:LEU:HD12	2.16	0.45
1:B:162:LEU:O	1:B:177:MET:CE	2.62	0.45
1:D:277:THR:HG21	1:D:284:THR:HB	1.98	0.45
1:D:389:HIS:O	1:D:390:GLU:HB2	2.17	0.45
1:B:246:ALA:O	1:B:250:GLU:HG3	2.15	0.45
1:D:91:LEU:HB2	1:D:110:TYR:CE2	2.51	0.45
1:C:337:TRP:CE3	1:C:386:CYS:HB2	2.51	0.45
1:A:213:ARG:HG2	1:A:252:LEU:HD11	1.99	0.45
1:D:106:PRO:O	1:D:149:SER:CB	2.64	0.45
1:C:347:ASP:O	1:C:348:ASN:HB3	2.17	0.45
1:D:110:TYR:HB2	1:D:179:PHE:HB3	1.99	0.45
1:D:89:LEU:HD21	1:D:177:MET:HB2	1.99	0.45
1:D:248:GLN:HA	1:D:251:LYS:HE3	1.99	0.45
1:D:446:ASN:OD1	1:D:447:PRO:HD2	2.17	0.45
1:A:114:SER:N	1:A:176:ASN:OD1	2.48	0.44
1:B:285:CYS:HB3	1:B:290:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:HD23	1:C:303:PRO:HD2	1.98	0.44
1:C:288:THR:CG2	1:C:316:TRP:CZ3	2.93	0.44
1:C:394:ARG:HG3	1:C:396:HIS:NE2	2.32	0.44
1:D:291:ILE:HG22	1:D:316:TRP:CB	2.40	0.44
1:B:216:LEU:HD23	1:B:220:LEU:HB3	1.97	0.44
1:B:241:ASN:O	1:B:245:VAL:HG23	2.17	0.44
1:C:271:ASN:OD1	1:C:347:ASP:OD1	2.36	0.44
1:C:160:GLY:HA3	1:C:392:ILE:O	2.17	0.44
1:A:407:LEU:HB3	1:A:408:PRO:HD3	2.00	0.44
1:C:409:ARG:O	1:C:412:HIS:N	2.51	0.44
1:D:213:ARG:HA	1:D:216:LEU:HD12	2.00	0.44
1:C:102:ASN:ND2	1:C:184:SER:O	2.48	0.44
1:A:191:ALA:HB2	1:A:301:VAL:HG21	1.99	0.44
1:A:262:LEU:HD22	1:A:411:LEU:HD21	1.98	0.44
1:B:401:GLN:CA	1:B:405:THR:O	2.63	0.44
1:A:295:ILE:HD11	1:A:319:PHE:CE1	2.53	0.44
1:B:98:SER:O	1:B:100:THR:HG23	2.17	0.44
1:B:378:VAL:HA	1:B:379:PRO:HD3	1.88	0.44
1:A:322:TYR:OH	1:A:323:LYS:HE3	2.17	0.44
1:D:188:TRP:HA	1:D:204:GLY:HA3	2.00	0.44
1:D:338:LEU:O	1:D:371:LEU:HD12	2.17	0.44
1:A:348:ASN:O	1:A:348:ASN:ND2	2.49	0.43
1:D:187:VAL:O	1:D:188:TRP:HB2	2.18	0.43
1:B:216:LEU:HA	1:B:220:LEU:HB3	2.00	0.43
1:C:298:TRP:O	1:C:299:ASN:HB2	2.18	0.43
1:A:336:GLN:O	1:A:383:ALA:HA	2.19	0.43
1:D:449:CYS:SG	1:D:450:PRO:HD2	2.59	0.43
1:A:103:ASP:OD2	1:A:148:SER:OG	2.34	0.43
1:A:378:VAL:O	1:A:435:HIS:CD2	2.72	0.43
1:C:110:TYR:HE1	1:C:181:PRO:HG3	1.83	0.43
1:C:114:SER:HB3	1:C:117:SER:HB3	2.00	0.43
1:D:339:PHE:O	1:D:387:LEU:HA	2.18	0.43
1:A:162:LEU:CD1	1:A:393:ILE:CD1	2.97	0.43
1:B:325:TYR:CD1	1:B:325:TYR:C	2.96	0.43
1:C:238:VAL:O	1:C:242:VAL:HB	2.19	0.43
1:D:262:LEU:HD21	1:D:392:ILE:HD13	2.00	0.43
1:D:461:MET:CE	1:D:469:HIS:HD2	2.28	0.43
1:A:91:LEU:HD12	1:A:92:HIS:N	2.34	0.43
1:B:92:HIS:CD2	1:B:218:ARG:NH2	2.87	0.43
1:A:387:LEU:C	1:A:387:LEU:HD23	2.43	0.42
1:D:89:LEU:HB3	1:D:110:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TRP:CH2	1:A:411:LEU:HB3	2.54	0.42
1:C:435:HIS:O	1:C:436:LEU:HD13	2.19	0.42
1:D:391:ILE:CG2	1:D:392:ILE:N	2.82	0.42
1:C:330:CYS:HA	1:C:331:PRO:HD2	1.86	0.42
1:D:246:ALA:O	1:D:250:GLU:HG2	2.19	0.42
1:B:302:VAL:HG11	1:B:318:CYS:HB2	2.00	0.42
1:D:337:TRP:HB3	1:D:386:CYS:O	2.20	0.42
1:A:132:ASN:OD1	1:A:135:ASN:HB2	2.19	0.42
1:A:325:TYR:N	1:A:326:PRO:CD	2.80	0.42
1:D:252:LEU:O	1:D:254:TYR:CD2	2.73	0.42
1:A:392:ILE:CD1	1:A:407:LEU:HD21	2.50	0.42
1:D:247:GLU:HG2	1:D:251:LYS:HE2	2.02	0.42
1:A:193:SER:HA	1:A:203:MET:HE3	2.02	0.42
1:B:162:LEU:CD2	1:B:177:MET:HB3	2.50	0.42
1:B:314:GLU:OE1	1:B:314:GLU:HA	2.19	0.42
1:D:131:PHE:C	1:D:297:TYR:CD2	2.98	0.42
1:D:258:GLN:OE1	1:D:260:ARG:NH2	2.44	0.42
1:A:110:TYR:HB2	1:A:179:PHE:HB3	2.01	0.41
1:A:311:GLN:O	1:A:314:GLU:HB2	2.20	0.41
1:C:129:TYR:O	1:C:282:THR:HG21	2.20	0.41
1:C:322:TYR:OH	1:C:323:LYS:HE3	2.19	0.41
1:C:363:TYR:HB3	1:C:364:ILE:HD13	2.02	0.41
1:C:378:VAL:HA	1:C:379:PRO:HD2	1.78	0.41
1:C:394:ARG:HG2	1:C:396:HIS:NE2	2.34	0.41
1:B:304:GLU:HG3	1:B:307:ARG:HH21	1.83	0.41
1:B:380:ALA:HA	1:B:434:VAL:CG1	2.44	0.41
1:D:102:ASN:ND2	1:D:184:SER:O	2.46	0.41
1:C:283:ILE:HG23	1:C:345:THR:CG2	2.50	0.41
1:C:363:TYR:O	1:C:366:ASN:HB3	2.20	0.41
1:D:139:ARG:C	1:D:147:MET:CE	2.92	0.41
1:A:180:ILE:HG22	1:A:188:TRP:HH2	1.85	0.41
1:D:139:ARG:CB	1:D:147:MET:HE2	2.51	0.41
1:A:152:TRP:HA	1:A:153:PRO:HD3	1.88	0.41
1:B:442:TRP:O	1:B:445:CYS:HB3	2.21	0.41
1:C:172:TRP:CH2	1:C:411:LEU:HB3	2.56	0.41
1:A:99:VAL:HA	1:A:203:MET:CE	2.51	0.41
1:A:288:THR:O	1:A:292:ARG:HG3	2.20	0.41
1:A:401:GLN:HA	1:A:405:THR:O	2.21	0.41
1:A:302:VAL:HG23	1:A:307:ARG:HG3	2.02	0.41
1:B:108:GLY:O	1:B:181:PRO:HD2	2.21	0.41
1:B:274:TYR:CD1	1:B:363:TYR:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ASP:O	1:C:187:VAL:HB	2.21	0.41
1:D:434:VAL:HG12	1:D:434:VAL:O	2.19	0.41
1:C:89:LEU:HB3	1:C:110:TYR:HB3	2.03	0.41
1:C:338:LEU:O	1:C:371:LEU:HD12	2.21	0.41
1:D:178:VAL:HG21	1:D:215:LEU:HD11	2.03	0.41
1:D:325:TYR:N	1:D:326:PRO:HD2	2.36	0.41
1:A:184:SER:O	1:A:185:SER:HB2	2.21	0.41
1:A:367:LEU:C	1:A:367:LEU:CD2	2.90	0.41
1:B:111:LEU:HD21	1:B:113:GLU:HG3	2.03	0.41
1:B:405:THR:CG2	1:B:436:LEU:CD1	2.99	0.41
1:B:405:THR:HG21	1:B:436:LEU:CD1	2.51	0.41
1:C:281:ASP:N	1:C:284:THR:OG1	2.51	0.41
1:C:162:LEU:CD1	1:C:393:ILE:HD11	2.45	0.40
1:C:278:ASP:OD1	1:C:279:CYS:N	2.53	0.40
1:B:159:THR:O	1:B:160:GLY:C	2.64	0.40
1:C:339:PHE:CD2	1:C:443:PRO:CG	2.91	0.40
1:D:210:GLU:HA	1:D:213:ARG:HG2	2.03	0.40
1:B:143:MET:HE2	1:B:143:MET:HA	2.02	0.40
1:D:302:VAL:O	1:D:307:ARG:NH2	2.54	0.40
1:A:130:CYS:HB2	1:A:139:ARG:HD2	2.03	0.40
1:A:165:GLN:O	1:A:168:GLU:N	2.52	0.40
1:C:159:THR:HG23	1:C:393:ILE:O	2.22	0.40
1:D:127:GLY:O	1:D:139:ARG:NH2	2.54	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	337/471 (72%)	324 (96%)	11 (3%)	2 (1%)	22 51
1	B	327/471 (69%)	312 (95%)	14 (4%)	1 (0%)	37 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	329/471 (70%)	308 (94%)	19 (6%)	2 (1%)	22	51
1	D	361/471 (77%)	340 (94%)	19 (5%)	2 (1%)	22	51
2	E	8/10 (80%)	8 (100%)	0	0	100	100
All	All	1362/1894 (72%)	1292 (95%)	63 (5%)	7 (0%)	25	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	390	GLU
1	A	390	GLU
1	A	187	VAL
1	C	187	VAL
1	D	187	VAL
1	B	187	VAL
1	C	391	ILE

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	293/405 (72%)	285 (97%)	8 (3%)	40	74
1	B	278/405 (69%)	261 (94%)	17 (6%)	15	43
1	C	285/405 (70%)	273 (96%)	12 (4%)	25	58
1	D	303/405 (75%)	293 (97%)	10 (3%)	33	67
All	All	1159/1620 (72%)	1112 (96%)	47 (4%)	26	59

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	177	MET
1	A	183	CYS
1	A	283	ILE

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Mol	Chain	Res	Type
1	A	291	ILE
1	A	348	ASN
1	A	356	VAL
1	A	448	SER
1	B	139	ARG
1	B	189	SER
1	B	203	MET
1	B	212	VAL
1	B	282	THR
1	B	285	CYS
1	B	308	ARG
1	B	309	GLN
1	B	314	GLU
1	B	348	ASN
1	B	367	LEU
1	B	371	LEU
1	B	381	SER
1	B	391	ILE
1	B	393	ILE
1	B	417	SER
1	B	436	LEU
1	C	99	VAL
1	C	177	MET
1	C	183	CYS
1	C	189	SER
1	C	213	ARG
1	C	285	CYS
1	C	299	ASN
1	C	364	ILE
1	C	372	ARG
1	C	391	ILE
1	C	402	VAL
1	C	434	VAL
1	D	121	LEU
1	D	183	CYS
1	D	282	THR
1	D	301	VAL
1	D	365	GLN
1	D	400	VAL
1	D	411	LEU
1	D	432	CYS
1	D	444	HIS

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Mol	Chain	Res	Type
1	D	467	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	ASN
1	A	412	HIS
1	B	174	ASN
1	B	209	GLN
1	B	273	GLN
1	B	396	HIS
1	B	435	HIS
1	C	96	ASN
1	C	273	GLN
1	D	174	ASN
1	D	276	HIS
1	D	365	GLN
1	D	412	HIS
1	D	469	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	NAG	B	1452	1	14,14,15	0.97	1 (7%)	17,19,21	1.95	6 (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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1452	1	1/1/5/7	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1452	NAG	C1-C2	2.63	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1452	NAG	O5-C1-C2	-4.36	104.40	111.29
3	B	1452	NAG	C1-C2-N2	3.14	115.85	110.49
3	B	1452	NAG	O5-C5-C4	-2.80	104.01	110.83
3	B	1452	NAG	C2-N2-C7	2.73	126.78	122.90
3	B	1452	NAG	C3-C4-C5	-2.60	105.60	110.24
3	B	1452	NAG	O6-C6-C5	-2.01	104.38	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1452	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1452	NAG	O5-C5-C6-O6
3	B	1452	NAG	C4-C5-C6-O6
3	B	1452	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	1452	NAG	C3-C2-N2-C7

There are no ring outliers.

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	345/471 (73%)	0.25	9 (2%) 57 49	28, 43, 68, 84	0
1	B	335/471 (71%)	0.32	17 (5%) 34 27	25, 42, 88, 108	0
1	C	337/471 (71%)	0.38	19 (5%) 31 24	25, 45, 92, 130	0
1	D	369/471 (78%)	0.26	12 (3%) 49 41	26, 44, 67, 84	0
2	E	10/10 (100%)	1.23	1 (10%) 14 11	50, 62, 69, 71	0
All	All	1396/1894 (73%)	0.31	58 (4%) 41 33	25, 44, 79, 130	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	353	GLY	6.3
1	C	442	TRP	4.4
1	B	387	LEU	4.3
1	B	441	PRO	3.8
1	B	439	SER	3.5
1	B	279	CYS	3.4
1	B	444	HIS	3.2
1	B	341	GLU	3.1
1	B	361	ARG	3.0
2	E	7	ALA	3.0
1	A	116	GLY	3.0
1	B	442	TRP	2.8
1	A	452	VAL	2.8
1	C	97	THR	2.8
1	C	312	GLU	2.8
1	C	341	GLU	2.8
1	D	358	GLU	2.8
1	C	279	CYS	2.7
1	A	247	GLU	2.7
1	C	199	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	441	PRO	2.6
1	B	362	LEU	2.6
1	C	285	CYS	2.5
1	B	447	PRO	2.4
1	C	440	CYS	2.4
1	A	403	LYS	2.4
1	D	193	SER	2.4
1	D	455	GLN	2.4
1	A	448	SER	2.4
1	C	405	THR	2.4
1	C	444	HIS	2.3
1	D	194	LYS	2.3
1	B	98	SER	2.3
1	D	247	GLU	2.3
1	C	121	LEU	2.3
1	B	440	CYS	2.3
1	A	213	ARG	2.3
1	C	116	GLY	2.2
1	D	352	THR	2.2
1	D	279	CYS	2.2
1	D	418	LEU	2.2
1	B	278	ASP	2.2
1	D	453	ARG	2.2
1	C	365	GLN	2.2
1	B	274	TYR	2.2
1	C	362	LEU	2.1
1	A	281	ASP	2.1
1	C	343	GLN	2.1
1	B	285	CYS	2.1
1	C	385	ALA	2.1
1	C	358	GLU	2.1
1	B	172	TRP	2.1
1	A	402	VAL	2.1
1	A	282	THR	2.1
1	D	107	ALA	2.1
1	B	451	THR	2.0
1	D	432	CYS	2.0
1	C	377	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	B	1452	14/15	0.44	0.20	60,62,66,67	0
4	CL	B	1453	1/1	0.91	0.10	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.