



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:08 AM EDT

PDB ID : 9PR9 / pdb_00009pr9
Title : Crystal structure of the Clostridiodes difficile CspA homodimer
Authors : Heldwein, E.E.; Gonzalez-Del Pino, G.L.
Deposited on : 2025-07-23
Resolution : 3.26 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
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

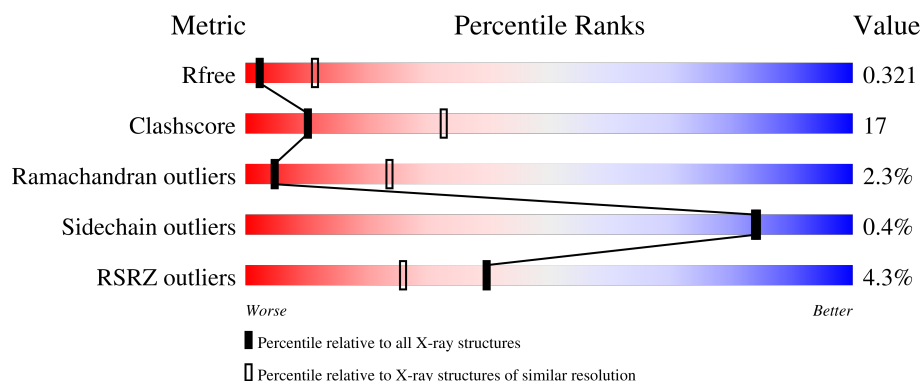
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	559	0% 60% 36% ..
1	B	559	3% 59% 29% 11%
1	C	559	4% 65% 30% ..
1	D	559	8% 62% 26% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15720 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 Germination-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4104	2604	690	799	11			
1	B	497	Total	C	N	O	S	0	0	0
			3739	2376	620	734	9			
1	C	542	Total	C	N	O	S	0	0	0
			4120	2618	687	804	11			
1	D	495	Total	C	N	O	S	0	0	0
			3757	2391	627	730	9			

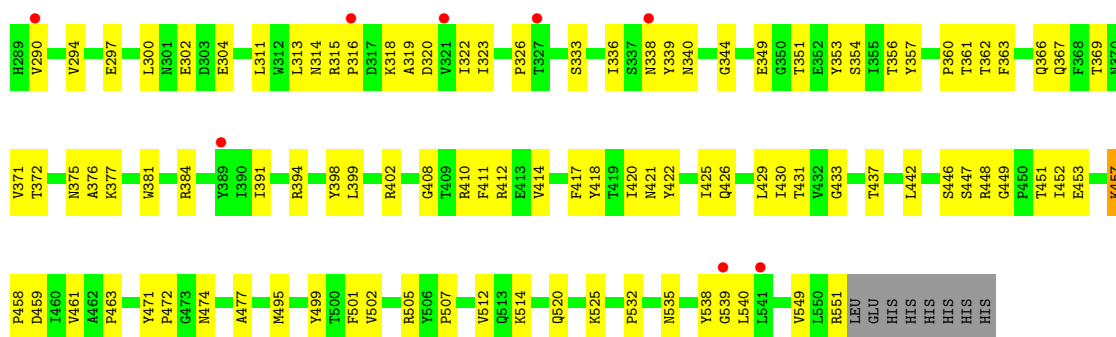
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A9R0BLF4
A	552	LEU	-	expression tag	UNP A0A9R0BLF4
A	553	GLU	-	expression tag	UNP A0A9R0BLF4
A	554	HIS	-	expression tag	UNP A0A9R0BLF4
A	555	HIS	-	expression tag	UNP A0A9R0BLF4
A	556	HIS	-	expression tag	UNP A0A9R0BLF4
A	557	HIS	-	expression tag	UNP A0A9R0BLF4
A	558	HIS	-	expression tag	UNP A0A9R0BLF4
A	559	HIS	-	expression tag	UNP A0A9R0BLF4
B	1	MET	-	initiating methionine	UNP A0A9R0BLF4
B	552	LEU	-	expression tag	UNP A0A9R0BLF4
B	553	GLU	-	expression tag	UNP A0A9R0BLF4
B	554	HIS	-	expression tag	UNP A0A9R0BLF4
B	555	HIS	-	expression tag	UNP A0A9R0BLF4
B	556	HIS	-	expression tag	UNP A0A9R0BLF4
B	557	HIS	-	expression tag	UNP A0A9R0BLF4
B	558	HIS	-	expression tag	UNP A0A9R0BLF4
B	559	HIS	-	expression tag	UNP A0A9R0BLF4
C	1	MET	-	initiating methionine	UNP A0A9R0BLF4
C	552	LEU	-	expression tag	UNP A0A9R0BLF4
C	553	GLU	-	expression tag	UNP A0A9R0BLF4

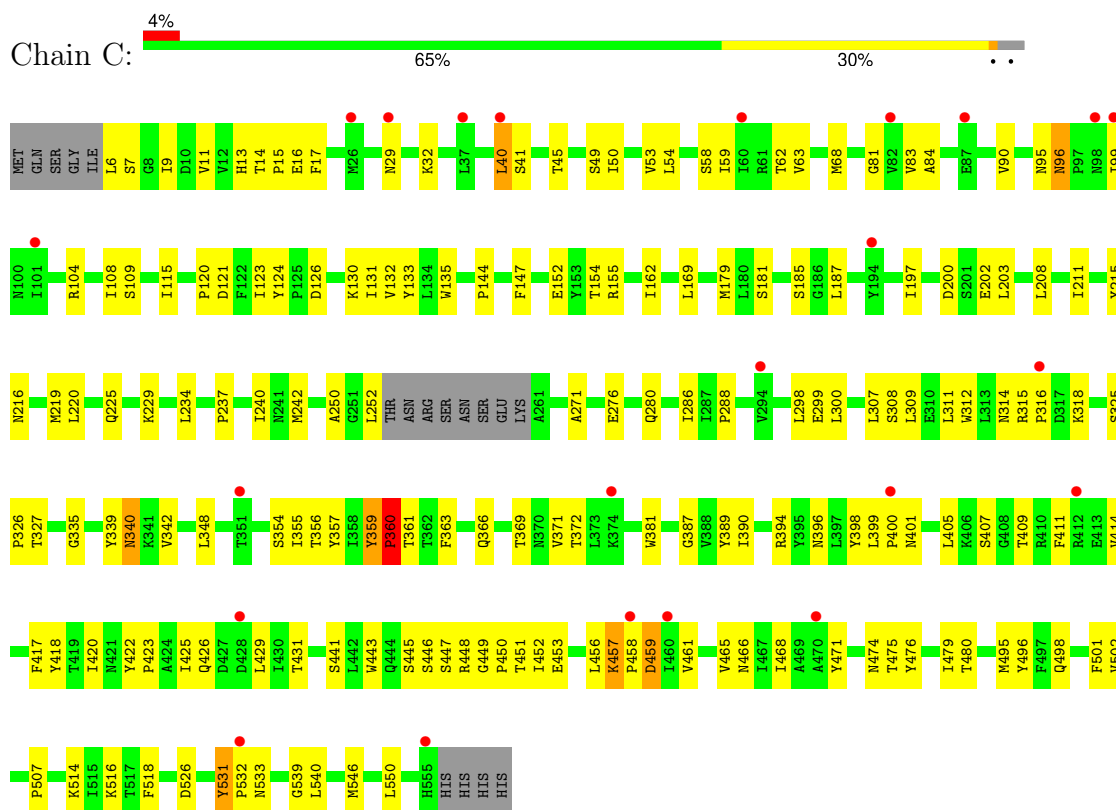
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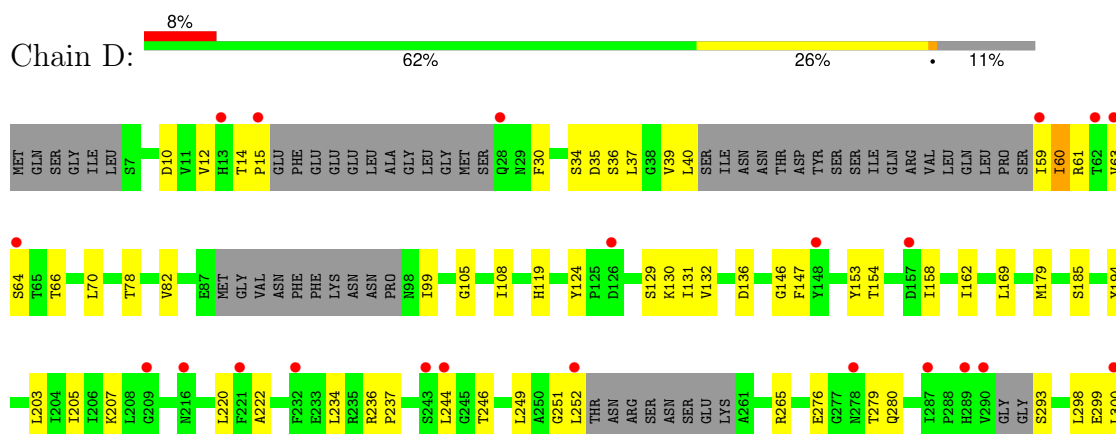
Chain	Residue	Modelled	Actual	Comment	Reference
C	554	HIS	-	expression tag	UNP A0A9R0BLF4
C	555	HIS	-	expression tag	UNP A0A9R0BLF4
C	556	HIS	-	expression tag	UNP A0A9R0BLF4
C	557	HIS	-	expression tag	UNP A0A9R0BLF4
C	558	HIS	-	expression tag	UNP A0A9R0BLF4
C	559	HIS	-	expression tag	UNP A0A9R0BLF4
D	1	MET	-	initiating methionine	UNP A0A9R0BLF4
D	552	LEU	-	expression tag	UNP A0A9R0BLF4
D	553	GLU	-	expression tag	UNP A0A9R0BLF4
D	554	HIS	-	expression tag	UNP A0A9R0BLF4
D	555	HIS	-	expression tag	UNP A0A9R0BLF4
D	556	HIS	-	expression tag	UNP A0A9R0BLF4
D	557	HIS	-	expression tag	UNP A0A9R0BLF4
D	558	HIS	-	expression tag	UNP A0A9R0BLF4
D	559	HIS	-	expression tag	UNP A0A9R0BLF4

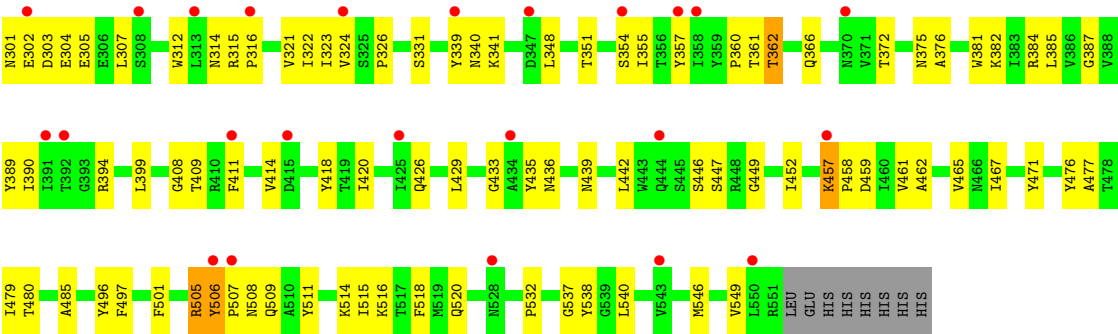


● Molecule 1: Germination-specific protease



● Molecule 1: Germination-specific protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.98Å 131.93Å 155.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.55 – 3.26 100.55 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.8 (100.55-3.26) 98.8 (100.55-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.279 , 0.322 0.280 , 0.321	Depositor DCC
R_{free} test set	1999 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15720	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8366e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.24	0/4188	0.56	0/5700
1	B	0.25	0/3811	0.58	0/5185
1	C	0.29	0/4205	0.59	0/5724
1	D	0.26	0/3829	0.60	0/5206
All	All	0.26	0/16033	0.58	0/21815

There are no bond length outliers.

There are no bond angle outliers.

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	4104	0	3985	172	0
1	B	3739	0	3629	120	0
1	C	4120	0	4005	148	0
1	D	3757	0	3673	120	0
All	All	15720	0	15292	531	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (531) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:HG23	1:C:495:MET:HE1	1.16	1.15
1:C:90:VAL:HG23	1:C:495:MET:CE	1.85	1.05
1:A:514:LYS:HE3	1:B:362:THR:HG22	1.37	1.04
1:B:457:LYS:O	1:B:457:LYS:HD3	1.66	0.95
1:B:220:LEU:HD11	1:B:244:LEU:HD12	1.47	0.93
1:A:290:VAL:HA	1:A:390:ILE:HD13	1.54	0.89
1:A:194:TYR:HB2	1:A:476:TYR:HE2	1.36	0.88
1:D:194:TYR:HD2	1:D:476:TYR:HD2	1.20	0.88
1:A:88:MET:O	1:A:90:VAL:HG23	1.73	0.86
1:A:335:GLY:HA2	1:A:357:TYR:HE2	1.41	0.86
1:D:194:TYR:HD2	1:D:476:TYR:CD2	1.99	0.80
1:A:54:LEU:HA	1:A:59:ILE:HD13	1.63	0.79
1:A:498:GLN:HA	1:A:502:VAL:HG12	1.64	0.79
1:D:60:ILE:HG22	1:D:61:ARG:H	1.48	0.78
1:C:90:VAL:CG2	1:C:495:MET:HE1	2.08	0.77
1:A:360:PRO:HB2	1:B:514:LYS:HG2	1.65	0.77
1:B:446:SER:O	1:B:448:ARG:HG3	1.87	0.75
1:D:59:ILE:HG22	1:D:60:ILE:H	1.51	0.74
1:C:280:GLN:HG2	1:C:414:VAL:HG21	1.69	0.74
1:C:514:LYS:HG2	1:D:360:PRO:HG2	1.69	0.74
1:A:444:GLN:HA	1:A:448:ARG:HH22	1.53	0.74
1:C:514:LYS:HE3	1:D:362:THR:HG22	1.68	0.74
1:D:30:PHE:HD1	1:D:40:LEU:HB3	1.52	0.73
1:C:387:GLY:HA3	1:C:390:ILE:HD11	1.71	0.73
1:D:387:GLY:HA3	1:D:390:ILE:HD11	1.73	0.71
1:A:335:GLY:HA2	1:A:357:TYR:CE2	2.26	0.70
1:C:359:TYR:O	1:C:360:PRO:C	2.35	0.70
1:B:30:PHE:HD1	1:B:40:LEU:HB2	1.56	0.70
1:C:359:TYR:CG	1:C:360:PRO:HD3	2.27	0.70
1:A:465:VAL:HA	1:A:480:THR:HG23	1.74	0.69
1:D:194:TYR:CD2	1:D:476:TYR:HD2	2.08	0.69
1:A:194:TYR:HB2	1:A:476:TYR:CE2	2.25	0.69
1:C:286:ILE:HD13	1:C:394:ARG:HD2	1.75	0.68
1:A:119:HIS:CE1	1:A:476:TYR:HE1	2.11	0.68
1:B:431:THR:OG1	1:B:457:LYS:HD2	1.94	0.68
1:B:322:ILE:HD11	1:B:384:ARG:HE	1.59	0.67
1:B:280:GLN:HG3	1:B:414:VAL:HG21	1.74	0.67
1:C:475:THR:HG22	1:C:476:TYR:H	1.58	0.67
1:C:314:ASN:ND2	1:C:394:ARG:HB3	2.10	0.66
1:C:40:LEU:HD13	1:C:41:SER:H	1.61	0.66
1:C:360:PRO:HB3	1:D:514:LYS:HA	1.77	0.66
1:A:314:ASN:ND2	1:A:394:ARG:HB3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:C	1:A:59:ILE:HD13	2.21	0.66
1:A:360:PRO:O	1:B:514:LYS:HE2	1.96	0.66
1:B:314:ASN:ND2	1:B:394:ARG:HB3	2.11	0.66
1:A:54:LEU:CA	1:A:59:ILE:HD13	2.25	0.65
1:A:54:LEU:O	1:A:59:ILE:HD11	1.97	0.65
1:D:418:TYR:H	1:D:449:GLY:HA3	1.60	0.65
1:D:323:ILE:H	1:D:331:SER:HB3	1.62	0.64
1:A:54:LEU:C	1:A:59:ILE:CD1	2.70	0.64
1:B:250:ALA:O	1:B:452:ILE:HD13	1.97	0.64
1:C:286:ILE:CD1	1:C:394:ARG:HD2	2.27	0.64
1:A:108:ILE:HD13	1:A:184:CYS:SG	2.37	0.64
1:A:54:LEU:HD22	1:A:62:THR:HG21	1.80	0.64
1:B:116:ASP:OD2	1:B:119:HIS:HB2	1.98	0.63
1:B:417:PHE:HA	1:B:448:ARG:O	1.98	0.63
1:A:425:ILE:HD11	1:A:451:THR:HG23	1.80	0.63
1:C:155:ARG:HH21	1:C:202:GLU:HG2	1.64	0.63
1:C:400:PRO:HD2	1:C:405:LEU:HD11	1.80	0.63
1:D:420:ILE:HD13	1:D:447:SER:HB3	1.80	0.62
1:C:339:TYR:O	1:C:340:ASN:HB2	1.99	0.62
1:A:387:GLY:HA3	1:A:390:ILE:HD11	1.81	0.62
1:B:99:ILE:HD13	1:B:551:ARG:HH12	1.65	0.62
1:B:457:LYS:H	1:B:458:PRO:HD2	1.65	0.62
1:C:496:TYR:CD2	1:C:546:MET:HE2	2.35	0.62
1:D:304:GLU:HG2	1:D:307:LEU:HB2	1.82	0.62
1:A:237:PRO:HG3	1:A:501:PHE:CD2	2.33	0.62
1:B:216:ASN:HD21	1:B:218:ALA:HB3	1.63	0.62
1:B:237:PRO:HG3	1:B:501:PHE:CD2	2.35	0.62
1:B:420:ILE:HD13	1:B:447:SER:HB3	1.82	0.62
1:D:418:TYR:N	1:D:449:GLY:HA3	2.15	0.61
1:A:83:VAL:HG21	1:A:194:TYR:HD1	1.65	0.61
1:C:124:TYR:CZ	1:C:130:LYS:HG2	2.34	0.61
1:A:316:PRO:HG3	1:B:538:TYR:CE1	2.36	0.61
1:D:63:VAL:HG12	1:D:64:SER:H	1.65	0.61
1:A:418:TYR:CE1	1:A:450:PRO:HG2	2.35	0.61
1:C:11:VAL:HG11	1:C:17:PHE:HE2	1.66	0.61
1:C:452:ILE:HD12	1:C:452:ILE:H	1.65	0.61
1:C:516:LYS:HD2	1:D:315:ARG:HH22	1.65	0.60
1:D:465:VAL:HA	1:D:480:THR:HG23	1.83	0.60
1:B:304:GLU:HB2	1:B:376:ALA:HB3	1.83	0.60
1:C:121:ASP:OD2	1:C:476:TYR:OH	2.20	0.60
1:D:132:VAL:HG11	1:D:234:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LYS:NZ	1:C:185:SER:HB3	2.15	0.60
1:B:288:PRO:HD3	1:B:294:VAL:HG13	1.84	0.60
1:D:315:ARG:HB3	1:D:316:PRO:HD3	1.84	0.59
1:C:208:LEU:HD11	1:C:220:LEU:HD23	1.84	0.59
1:C:355:ILE:HG12	1:C:371:VAL:HG22	1.83	0.59
1:D:220:LEU:HD11	1:D:244:LEU:HB2	1.85	0.59
1:A:355:ILE:HG12	1:A:371:VAL:HG22	1.84	0.59
1:C:54:LEU:O	1:C:59:ILE:HD13	2.02	0.59
1:A:120:PRO:HD3	1:A:474:ASN:ND2	2.18	0.59
1:A:396:ASN:HB3	1:A:398:TYR:HE1	1.66	0.58
1:B:311:LEU:HB3	1:B:369:THR:OG1	2.03	0.58
1:C:496:TYR:HD2	1:C:546:MET:HE2	1.68	0.58
1:A:11:VAL:HG12	1:A:62:THR:HG22	1.84	0.58
1:A:225:GLN:O	1:A:229:LYS:HD3	2.02	0.58
1:D:251:GLY:HA2	1:D:452:ILE:HD11	1.85	0.58
1:C:11:VAL:HG22	1:C:62:THR:HG22	1.86	0.58
1:C:396:ASN:HD22	1:C:452:ILE:HG23	1.68	0.58
1:D:130:LYS:NZ	1:D:185:SER:HB3	2.17	0.58
1:A:120:PRO:HD3	1:A:474:ASN:HD22	1.67	0.58
1:A:155:ARG:NH2	1:A:202:GLU:HG2	2.19	0.58
1:B:499:TYR:CZ	1:B:505:ARG:HG2	2.39	0.58
1:B:12:VAL:HA	1:B:36:SER:O	2.04	0.57
1:B:287:ILE:HD12	1:B:313:LEU:HD11	1.86	0.57
1:A:63:VAL:HG12	1:A:64:SER:H	1.67	0.57
1:A:63:VAL:HG12	1:A:64:SER:N	2.18	0.57
1:A:116:ASP:OD2	1:A:472:PRO:HA	2.04	0.57
1:C:81:GLY:HA3	1:C:468:ILE:HD11	1.86	0.57
1:A:314:ASN:HD21	1:A:394:ARG:HB3	1.69	0.57
1:C:132:VAL:HG22	1:C:155:ARG:NH2	2.20	0.57
1:A:132:VAL:HG23	1:A:202:GLU:HB3	1.86	0.57
1:C:498:GLN:HA	1:C:502:VAL:HG12	1.86	0.57
1:A:60:ILE:HG22	1:A:61:ARG:HD2	1.85	0.57
1:C:179:MET:SD	1:C:479:ILE:HB	2.45	0.57
1:C:300:LEU:CD2	1:C:409:THR:HG23	2.35	0.56
1:B:130:LYS:HD2	1:B:187:LEU:HG	1.87	0.56
1:B:333:SER:OG	1:B:336:ILE:HG12	2.06	0.56
1:C:526:ASP:H	1:C:531:TYR:HE2	1.52	0.56
1:D:361:THR:HG23	1:D:366:GLN:O	2.04	0.56
1:A:422:TYR:O	1:A:425:ILE:HG22	2.05	0.56
1:B:398:TYR:OH	1:B:452:ILE:HD11	2.06	0.56
1:C:298:LEU:HD21	1:C:307:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ILE:HG12	1:B:525:LYS:NZ	2.21	0.56
1:C:315:ARG:HB3	1:C:316:PRO:HD3	1.88	0.56
1:D:179:MET:HE3	1:D:471:TYR:CD1	2.41	0.56
1:A:12:VAL:HG12	1:A:60:ILE:HD12	1.88	0.56
1:B:421:ASN:O	1:B:425:ILE:HG23	2.06	0.55
1:B:319:ALA:H	1:B:367:GLN:NE2	2.04	0.55
1:C:327:THR:HG21	1:C:348:LEU:HD22	1.89	0.55
1:C:418:TYR:CE1	1:C:450:PRO:HG2	2.41	0.55
1:A:208:LEU:HD11	1:A:220:LEU:HD13	1.89	0.55
1:A:391:ILE:HG12	1:B:525:LYS:HZ3	1.71	0.55
1:A:538:TYR:CE1	1:B:316:PRO:HG3	2.42	0.55
1:C:9:ILE:HD11	1:C:62:THR:HB	1.89	0.55
1:A:69:THR:HG21	1:A:401:ASN:HB2	1.87	0.55
1:C:451:THR:HG22	1:C:453:GLU:H	1.70	0.55
1:A:302:GLU:HB3	1:A:406:LYS:NZ	2.22	0.55
1:A:442:LEU:HD22	1:A:535:ASN:HB3	1.89	0.55
1:C:465:VAL:HA	1:C:480:THR:HG23	1.89	0.55
1:D:312:TRP:HE3	1:D:366:GLN:HE21	1.54	0.55
1:D:322:ILE:HD11	1:D:384:ARG:HE	1.72	0.55
1:A:436:ASN:HB3	1:A:439:ASN:OD1	2.07	0.55
1:C:342:VAL:O	1:C:354:SER:HA	2.07	0.55
1:C:514:LYS:CG	1:D:360:PRO:HG2	2.36	0.55
1:D:280:GLN:HG2	1:D:414:VAL:HG21	1.89	0.55
1:A:289:HIS:C	1:A:291:GLY:H	2.16	0.54
1:B:144:PRO:HG3	1:B:152:GLU:HB2	1.88	0.54
1:B:457:LYS:N	1:B:458:PRO:HD2	2.22	0.54
1:C:225:GLN:O	1:C:229:LYS:HG2	2.07	0.54
1:D:324:VAL:HB	1:D:382:LYS:HB2	1.87	0.54
1:A:21:LEU:HD22	1:A:26:MET:HB2	1.89	0.54
1:B:457:LYS:O	1:B:457:LYS:CD	2.50	0.54
1:D:82:VAL:HG23	1:D:467:ILE:HD13	1.88	0.54
1:A:331:SER:HB3	1:A:346:PHE:CZ	2.42	0.54
1:B:426:GLN:HB2	1:B:429:LEU:HD13	1.88	0.54
1:A:54:LEU:O	1:A:59:ILE:CD1	2.55	0.54
1:A:66:THR:HG21	1:A:249:LEU:HD13	1.88	0.54
1:A:334:VAL:HG12	1:A:357:TYR:HD2	1.73	0.54
1:B:129:SER:HB2	1:B:162:ILE:HD11	1.90	0.54
1:C:185:SER:HB2	1:C:203:LEU:HD11	1.89	0.54
1:A:399:LEU:HB3	1:A:405:LEU:HD11	1.89	0.54
1:C:420:ILE:HD13	1:C:447:SER:HB3	1.90	0.54
1:C:516:LYS:HD2	1:D:315:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:PRO:HG3	1:D:501:PHE:CD2	2.43	0.54
1:D:10:ASP:HA	1:D:39:VAL:HG22	1.89	0.54
1:D:203:LEU:HB3	1:D:205:ILE:HD11	1.88	0.54
1:A:387:GLY:C	1:A:390:ILE:HD11	2.34	0.53
1:A:37:LEU:HD23	1:A:222:ALA:HB2	1.91	0.53
1:D:12:VAL:HA	1:D:36:SER:O	2.08	0.53
1:A:354:SER:HB3	1:A:372:THR:OG1	2.08	0.53
1:A:357:TYR:HD1	1:A:358:ILE:N	2.06	0.53
1:B:300:LEU:HD11	1:B:304:GLU:HG2	1.90	0.53
1:B:315:ARG:HB3	1:B:316:PRO:HD3	1.89	0.53
1:D:131:ILE:HD12	1:D:205:ILE:HD13	1.89	0.53
1:A:315:ARG:HB3	1:A:316:PRO:HD3	1.89	0.53
1:A:442:LEU:HD23	1:A:448:ARG:HH21	1.73	0.53
1:B:532:PRO:HB3	1:B:538:TYR:CE1	2.44	0.53
1:A:457:LYS:H	1:A:458:PRO:HD2	1.74	0.53
1:C:130:LYS:HZ1	1:C:185:SER:HB3	1.73	0.53
1:A:297:GLU:HG2	1:A:382:LYS:HG2	1.90	0.53
1:A:324:VAL:HB	1:A:382:LYS:HB2	1.91	0.53
1:C:360:PRO:O	1:D:514:LYS:HE2	2.08	0.53
1:C:531:TYR:O	1:C:533:ASN:N	2.42	0.53
1:B:354:SER:HB3	1:B:372:THR:OG1	2.08	0.53
1:C:514:LYS:HE2	1:D:360:PRO:O	2.09	0.53
1:B:225:GLN:O	1:B:229:LYS:HG2	2.07	0.52
1:C:360:PRO:CB	1:D:514:LYS:HG2	2.39	0.52
1:A:197:ILE:O	1:A:495:MET:HE3	2.09	0.52
1:C:9:ILE:HG23	1:C:40:LEU:HB3	1.92	0.52
1:A:387:GLY:CA	1:A:390:ILE:HD11	2.40	0.52
1:A:515:ILE:HG23	1:A:546:MET:HE3	1.91	0.52
1:C:360:PRO:HG2	1:D:518:PHE:CE2	2.44	0.52
1:D:532:PRO:HB3	1:D:538:TYR:CE1	2.45	0.52
1:A:400:PRO:HD2	1:A:405:LEU:HD21	1.91	0.52
1:D:280:GLN:HA	1:D:414:VAL:HG11	1.92	0.52
1:D:321:VAL:HG12	1:D:385:LEU:HD23	1.91	0.52
1:A:108:ILE:HG21	1:A:184:CYS:SG	2.50	0.52
1:B:452:ILE:H	1:B:452:ILE:HD12	1.75	0.52
1:D:293:SER:HB2	1:D:385:LEU:O	2.10	0.52
1:D:326:PRO:HD3	1:D:381:TRP:CE2	2.45	0.51
1:A:356:THR:CG2	1:A:370:ASN:HB3	2.41	0.51
1:B:153:TYR:CE1	1:B:169:LEU:HD22	2.45	0.51
1:B:65:THR:HG23	1:B:216:ASN:OD1	2.10	0.51
1:C:132:VAL:HG11	1:C:234:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:TRP:HE3	1:C:366:GLN:HE21	1.57	0.51
1:A:54:LEU:C	1:A:59:ILE:HD11	2.35	0.51
1:A:356:THR:HG22	1:A:370:ASN:HB3	1.93	0.51
1:C:315:ARG:NH2	1:D:516:LYS:HD2	2.25	0.51
1:D:99:ILE:HG22	1:D:99:ILE:O	2.09	0.51
1:C:526:ASP:N	1:C:531:TYR:HE2	2.08	0.51
1:A:443:TRP:HB2	1:A:465:VAL:HG21	1.93	0.51
1:D:339:TYR:CG	1:D:340:ASN:N	2.79	0.51
1:C:318:LYS:HD2	1:C:359:TYR:CE2	2.46	0.51
1:C:359:TYR:CG	1:C:360:PRO:CD	2.94	0.51
1:A:27:SER:C	1:A:29:ASN:H	2.19	0.50
1:B:37:LEU:HD23	1:B:222:ALA:HB2	1.94	0.50
1:B:418:TYR:H	1:B:449:GLY:HA3	1.76	0.50
1:C:276:GLU:OE2	1:C:401:ASN:HB3	2.12	0.50
1:D:37:LEU:HD23	1:D:222:ALA:HB2	1.92	0.50
1:A:305:GLU:O	1:A:374:LYS:HD3	2.11	0.50
1:C:309:LEU:HD21	1:C:399:LEU:HD23	1.94	0.50
1:D:314:ASN:ND2	1:D:394:ARG:HB3	2.26	0.50
1:B:138:THR:HG22	1:B:209:GLY:HA2	1.93	0.50
1:B:442:LEU:HD22	1:B:535:ASN:HB3	1.94	0.50
1:D:435:TYR:CG	1:D:540:LEU:HD11	2.47	0.50
1:D:505:ARG:O	1:D:506:TYR:C	2.53	0.50
1:A:326:PRO:HD3	1:A:381:TRP:CD2	2.47	0.50
1:B:422:TYR:O	1:B:425:ILE:HG12	2.11	0.50
1:A:312:TRP:HE3	1:A:366:GLN:HE21	1.57	0.50
1:A:431:THR:OG1	1:A:457:LYS:HE3	2.12	0.50
1:C:115:ILE:HD13	1:C:131:ILE:HD11	1.94	0.50
1:D:124:TYR:CZ	1:D:130:LYS:HG2	2.47	0.50
1:A:389:TYR:CZ	1:B:549:VAL:HG22	2.47	0.50
1:C:300:LEU:HD22	1:C:409:THR:HG23	1.93	0.50
1:C:123:ILE:HG12	1:C:162:ILE:HD13	1.92	0.49
1:C:531:TYR:CE1	1:C:539:GLY:HA2	2.48	0.49
1:B:351:THR:HG22	1:B:375:ASN:O	2.13	0.49
1:C:132:VAL:HG23	1:C:202:GLU:HB3	1.95	0.49
1:C:250:ALA:HB1	1:C:452:ILE:HD13	1.94	0.49
1:A:361:THR:HG23	1:A:366:GLN:O	2.12	0.49
1:A:13:HIS:CD2	1:A:17:PHE:HB3	2.48	0.49
1:A:448:ARG:O	1:A:448:ARG:HG3	2.12	0.49
1:C:425:ILE:HD11	1:C:451:THR:HG23	1.95	0.49
1:A:66:THR:CG2	1:A:249:LEU:HD13	2.42	0.49
1:A:475:THR:O	1:A:476:TYR:HD1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LEU:HG	1:B:540:LEU:O	2.13	0.49
1:D:34:SER:O	1:D:36:SER:N	2.46	0.49
1:A:13:HIS:HB2	1:A:17:PHE:HB2	1.95	0.48
1:A:17:PHE:CZ	1:A:21:LEU:HG	2.48	0.48
1:A:132:VAL:HG22	1:A:155:ARG:NH2	2.27	0.48
1:B:322:ILE:CG2	1:B:333:SER:HB3	2.43	0.48
1:C:311:LEU:HB3	1:C:369:THR:OG1	2.12	0.48
1:C:179:MET:HE3	1:C:471:TYR:CD1	2.48	0.48
1:D:302:GLU:HG3	1:D:303:ASP:H	1.78	0.48
1:B:451:THR:HG22	1:B:453:GLU:H	1.78	0.48
1:C:431:THR:OG1	1:C:457:LYS:HE3	2.13	0.48
1:D:60:ILE:HG22	1:D:61:ARG:N	2.22	0.48
1:A:59:ILE:O	1:A:59:ILE:HG13	2.14	0.48
1:A:443:TRP:CE2	1:A:445:SER:HB2	2.49	0.48
1:C:120:PRO:HD3	1:C:474:ASN:OD1	2.13	0.48
1:C:299:GLU:O	1:C:300:LEU:HD23	2.14	0.48
1:B:408:GLY:O	1:B:410:ARG:HG3	2.14	0.48
1:D:301:ASN:HB2	1:D:408:GLY:HA3	1.96	0.48
1:B:418:TYR:N	1:B:449:GLY:HA3	2.29	0.47
1:C:96:ASN:HD22	1:C:99:ILE:HG23	1.78	0.47
1:D:130:LYS:HZ3	1:D:185:SER:HB3	1.78	0.47
1:D:194:TYR:HB2	1:D:476:TYR:CE2	2.48	0.47
1:A:471:TYR:CD1	1:A:472:PRO:HD2	2.49	0.47
1:C:396:ASN:ND2	1:C:452:ILE:HG23	2.29	0.47
1:D:321:VAL:HG12	1:D:385:LEU:CD2	2.44	0.47
1:D:496:TYR:HD2	1:D:546:MET:HE2	1.78	0.47
1:A:119:HIS:CE1	1:A:476:TYR:CE1	2.99	0.47
1:B:132:VAL:HG23	1:B:202:GLU:HB3	1.96	0.47
1:B:457:LYS:HE2	1:B:457:LYS:HA	1.95	0.47
1:C:360:PRO:HB3	1:D:514:LYS:HG2	1.96	0.47
1:C:13:HIS:HB2	1:C:17:PHE:HB3	1.96	0.47
1:C:104:ARG:HA	1:C:200:ASP:O	2.15	0.47
1:A:119:HIS:HE1	1:A:476:TYR:HE1	1.57	0.47
1:A:475:THR:C	1:A:476:TYR:HD1	2.21	0.47
1:C:426:GLN:O	1:C:457:LYS:HE2	2.13	0.47
1:A:351:THR:HG22	1:A:375:ASN:O	2.15	0.47
1:A:448:ARG:HD3	1:A:535:ASN:OD1	2.14	0.47
1:C:14:THR:C	1:C:16:GLU:H	2.22	0.47
1:C:68:MET:O	1:C:215:TYR:HB2	2.15	0.47
1:C:216:ASN:HD21	1:C:219:MET:HG3	1.80	0.47
1:C:316:PRO:HG3	1:D:538:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:HG	1:B:302:GLU:O	2.15	0.47
1:C:237:PRO:HG3	1:C:501:PHE:CD1	2.49	0.47
1:C:326:PRO:HD3	1:C:381:TRP:CD2	2.50	0.47
1:D:203:LEU:HB3	1:D:205:ILE:CD1	2.45	0.47
1:C:280:GLN:HA	1:C:414:VAL:HG11	1.97	0.46
1:A:136:ASP:OD1	1:A:207:LYS:HD3	2.15	0.46
1:C:325:SER:HA	1:C:381:TRP:CE3	2.50	0.46
1:D:14:THR:HG23	1:D:60:ILE:HG13	1.97	0.46
1:A:248:SER:HA	1:A:310:GLU:OE1	2.15	0.46
1:A:271:ALA:HB2	1:A:429:LEU:HD23	1.96	0.46
1:C:417:PHE:HA	1:C:448:ARG:O	2.16	0.46
1:D:457:LYS:HD2	1:D:457:LYS:HA	1.47	0.46
1:A:452:ILE:HD12	1:A:452:ILE:H	1.81	0.46
1:D:249:LEU:C	1:D:251:GLY:H	2.23	0.46
1:A:124:TYR:CZ	1:A:130:LYS:HG2	2.51	0.46
1:C:181:SER:OG	1:C:203:LEU:HD13	2.15	0.46
1:C:354:SER:HB3	1:C:372:THR:CG2	2.46	0.46
1:D:34:SER:HA	1:D:147:PHE:HA	1.98	0.46
1:B:108:ILE:HB	1:B:203:LEU:HD23	1.98	0.46
1:B:270:THR:HG22	1:B:430:ILE:HB	1.98	0.46
1:D:276:GLU:HG2	1:D:279:THR:OG1	2.16	0.46
1:A:280:GLN:HG2	1:A:414:VAL:HG21	1.98	0.46
1:A:417:PHE:HA	1:A:448:ARG:O	2.15	0.46
1:C:130:LYS:HD2	1:C:187:LEU:HG	1.98	0.46
1:C:396:ASN:HB3	1:C:398:TYR:HE1	1.81	0.46
1:D:462:ALA:HB3	1:D:485:ALA:HB1	1.97	0.46
1:D:70:LEU:HD23	1:D:244:LEU:HD21	1.98	0.45
1:D:194:TYR:CD2	1:D:476:TYR:CD2	2.91	0.45
1:A:500:THR:HG22	1:A:506:TYR:HB2	1.98	0.45
1:B:344:GLY:HA3	1:B:353:TYR:CE1	2.51	0.45
1:D:136:ASP:OD1	1:D:207:LYS:HD3	2.16	0.45
1:C:418:TYR:H	1:C:449:GLY:HA3	1.82	0.45
1:C:220:LEU:HD11	1:C:242:MET:SD	2.57	0.45
1:A:68:MET:HB3	1:A:244:LEU:HB3	1.98	0.45
1:A:84:ALA:C	1:A:86:GLU:H	2.25	0.45
1:B:136:ASP:OD1	1:B:207:LYS:HD3	2.17	0.45
1:C:144:PRO:HA	1:C:152:GLU:OE1	2.17	0.45
1:A:155:ARG:HH21	1:A:202:GLU:HG2	1.81	0.45
1:B:179:MET:HE2	1:B:477:ALA:HB3	1.99	0.45
1:B:297:GLU:OE1	1:B:412:ARG:HD2	2.17	0.45
1:B:322:ILE:HG13	1:B:384:ARG:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLU:HG3	1:B:377:LYS:HD3	1.98	0.45
1:C:356:THR:O	1:C:369:THR:HA	2.16	0.45
1:D:78:THR:HG21	1:D:194:TYR:CE2	2.52	0.45
1:A:518:PHE:CE2	1:A:550:LEU:HD13	2.52	0.45
1:A:519:MET:O	1:A:523:ALA:HB2	2.17	0.45
1:B:216:ASN:ND2	1:B:218:ALA:HB3	2.30	0.45
1:B:461:VAL:O	1:B:540:LEU:HD12	2.16	0.45
1:C:335:GLY:HA2	1:C:357:TYR:CE2	2.52	0.45
1:A:357:TYR:CD1	1:A:358:ILE:N	2.84	0.45
1:A:465:VAL:O	1:A:466:ASN:HB2	2.17	0.45
1:D:129:SER:OG	1:D:131:ILE:HG12	2.17	0.45
1:A:144:PRO:HG3	1:A:152:GLU:HB2	2.00	0.44
1:A:399:LEU:HG	1:A:411:PHE:CE2	2.52	0.44
1:B:107:LEU:HD23	1:B:202:GLU:HB2	1.98	0.44
1:D:66:THR:HG21	1:D:246:THR:HG21	1.99	0.44
1:D:129:SER:HB2	1:D:162:ILE:HD11	1.99	0.44
1:A:37:LEU:HD22	1:A:221:PHE:HD2	1.83	0.44
1:A:293:SER:HB2	1:A:384:ARG:NH1	2.32	0.44
1:B:280:GLN:HG2	1:B:410:ARG:HB2	1.99	0.44
1:C:29:ASN:O	1:C:40:LEU:HD22	2.16	0.44
1:C:124:TYR:CE2	1:C:130:LYS:HG2	2.52	0.44
1:C:456:LEU:HD22	1:C:458:PRO:HD2	1.98	0.44
1:B:326:PRO:HD3	1:B:381:TRP:CD2	2.53	0.44
1:A:77:GLY:O	1:A:477:ALA:HA	2.17	0.44
1:A:300:LEU:O	1:A:378:ARG:HA	2.17	0.44
1:B:357:TYR:CD1	1:B:369:THR:HG22	2.51	0.44
1:C:308:SER:HA	1:C:372:THR:HA	2.00	0.44
1:D:179:MET:HE3	1:D:471:TYR:HD1	1.81	0.44
1:A:136:ASP:HA	1:A:207:LYS:HB3	2.00	0.44
1:A:304:GLU:OE1	1:A:307:LEU:HD21	2.17	0.44
1:A:457:LYS:HD2	1:A:457:LYS:HA	1.60	0.44
1:A:496:TYR:CD2	1:A:546:MET:HE2	2.52	0.44
1:A:496:TYR:CE1	1:A:500:THR:HG21	2.52	0.44
1:C:13:HIS:HB2	1:C:17:PHE:CB	2.48	0.44
1:D:299:GLU:O	1:D:300:LEU:HD23	2.18	0.44
1:B:237:PRO:HG2	1:B:502:VAL:HG23	1.99	0.44
1:B:433:GLY:HA3	1:B:461:VAL:HG12	1.99	0.44
1:C:326:PRO:HD3	1:C:381:TRP:CE2	2.52	0.44
1:C:422:TYR:O	1:C:425:ILE:HG22	2.18	0.44
1:D:348:LEU:HD23	1:D:348:LEU:O	2.18	0.44
1:A:138:THR:HG22	1:A:209:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:THR:O	1:B:369:THR:HA	2.18	0.44
1:B:505:ARG:HA	1:B:505:ARG:HD3	1.67	0.44
1:A:42:ILE:HG23	1:A:50:ILE:HD13	2.00	0.44
1:C:498:GLN:HA	1:C:502:VAL:CG1	2.48	0.44
1:D:205:ILE:N	1:D:205:ILE:HD12	2.32	0.44
1:A:317:ASP:HA	1:A:389:TYR:O	2.18	0.43
1:B:107:LEU:HD13	1:B:204:ILE:HD11	2.00	0.43
1:B:318:LYS:HG3	1:B:357:TYR:OH	2.18	0.43
1:D:119:HIS:CE1	1:D:476:TYR:HE1	2.36	0.43
1:A:104:ARG:HA	1:A:200:ASP:O	2.17	0.43
1:A:283:THR:HG21	1:A:296:VAL:HG11	1.99	0.43
1:D:354:SER:HB3	1:D:372:THR:HB	2.00	0.43
1:C:95:ASN:O	1:C:96:ASN:C	2.61	0.43
1:C:359:TYR:HB3	1:C:360:PRO:HD2	1.99	0.43
1:C:518:PHE:CE2	1:C:550:LEU:HD13	2.54	0.43
1:C:526:ASP:N	1:C:531:TYR:CE2	2.83	0.43
1:C:422:TYR:HB3	1:C:423:PRO:HD3	1.99	0.43
1:B:399:LEU:HG	1:B:411:PHE:CE2	2.53	0.43
1:C:431:THR:O	1:C:459:ASP:HB2	2.17	0.43
1:C:443:TRP:HB2	1:C:465:VAL:CG2	2.48	0.43
1:D:497:PHE:CE1	1:D:515:ILE:HD11	2.54	0.43
1:B:99:ILE:HG22	1:B:101:ILE:HG13	1.99	0.43
1:C:32:LYS:O	1:C:32:LYS:HG3	2.16	0.43
1:C:109:SER:HB3	1:C:240:ILE:HA	2.01	0.43
1:C:446:SER:O	1:C:448:ARG:HG3	2.18	0.43
1:D:265:ARG:HE	1:D:265:ARG:HB3	1.61	0.43
1:A:299:GLU:C	1:A:300:LEU:HD12	2.44	0.43
1:C:211:ILE:HD12	1:C:216:ASN:HD22	1.84	0.43
1:C:418:TYR:N	1:C:449:GLY:HA3	2.33	0.43
1:D:496:TYR:CD2	1:D:546:MET:HE2	2.53	0.43
1:B:251:GLY:O	1:B:363:PHE:HE2	2.02	0.43
1:B:282:HIS:HD2	1:B:398:TYR:CE1	2.37	0.43
1:D:179:MET:HE2	1:D:477:ALA:HB3	2.00	0.43
1:D:426:GLN:HB2	1:D:429:LEU:HD13	2.01	0.43
1:A:268:CYS:HA	1:A:512:VAL:HG22	2.01	0.43
1:A:317:ASP:O	1:A:359:TYR:HE1	2.01	0.43
1:A:522:GLY:HA3	1:A:545:GLY:C	2.44	0.43
1:A:523:ALA:HB1	1:A:540:LEU:O	2.19	0.43
1:A:554:HIS:HD2	1:B:338:ASN:HA	1.84	0.43
1:B:116:ASP:C	1:B:118:LEU:H	2.27	0.43
1:C:13:HIS:CB	1:C:17:PHE:HD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:PHE:HB2	1:C:58:SER:HB2	2.00	0.43
1:D:63:VAL:HG12	1:D:64:SER:N	2.32	0.43
1:D:251:GLY:O	1:D:252:LEU:HB2	2.18	0.43
1:A:300:LEU:HD13	1:A:381:TRP:CD1	2.55	0.42
1:A:331:SER:HB3	1:A:346:PHE:HZ	1.83	0.42
1:B:316:PRO:HB2	1:B:391:ILE:HD12	2.01	0.42
1:C:135:TRP:CH2	1:C:147:PHE:HD2	2.37	0.42
1:C:359:TYR:CB	1:C:360:PRO:CD	2.96	0.42
1:D:307:LEU:HD11	1:D:399:LEU:HD22	2.00	0.42
1:A:156:GLU:O	1:A:160:ARG:HG3	2.19	0.42
1:A:347:ASP:C	1:A:349:GLU:H	2.27	0.42
1:A:525:LYS:HB3	1:A:531:TYR:CD2	2.54	0.42
1:B:132:VAL:HG11	1:B:234:LEU:HD11	2.01	0.42
1:C:389:TYR:CE2	1:D:549:VAL:HG22	2.54	0.42
1:C:443:TRP:CE2	1:C:445:SER:HB2	2.54	0.42
1:A:532:PRO:HA	1:A:537:GLY:O	2.18	0.42
1:B:101:ILE:HD11	1:B:551:ARG:NH2	2.34	0.42
1:C:40:LEU:HD22	1:C:40:LEU:HA	1.87	0.42
1:C:318:LYS:HG3	1:C:357:TYR:OH	2.20	0.42
1:A:302:GLU:HB3	1:A:406:LYS:HZ1	1.83	0.42
1:C:271:ALA:HB2	1:C:429:LEU:HD23	2.01	0.42
1:C:360:PRO:HB2	1:D:514:LYS:HG2	2.01	0.42
1:D:34:SER:HB2	1:D:147:PHE:CD1	2.55	0.42
1:D:341:LYS:HA	1:D:355:ILE:O	2.20	0.42
1:D:433:GLY:HA3	1:D:461:VAL:HG12	2.02	0.42
1:A:421:ASN:O	1:A:425:ILE:HB	2.20	0.42
1:B:179:MET:CE	1:B:477:ALA:HB3	2.50	0.42
1:A:211:ILE:HB	1:A:216:ASN:HD22	1.85	0.42
1:A:458:PRO:O	1:A:537:GLY:HA3	2.20	0.42
1:A:514:LYS:CE	1:B:362:THR:HG22	2.27	0.42
1:B:66:THR:HG21	1:B:249:LEU:HD13	2.01	0.42
1:B:110:ILE:HD11	1:B:184:CYS:SG	2.59	0.42
1:B:120:PRO:HD3	1:B:474:ASN:OD1	2.19	0.42
1:B:202:GLU:HG3	1:B:236:ARG:NH1	2.34	0.42
1:C:40:LEU:HD13	1:C:41:SER:N	2.32	0.42
1:D:351:THR:HG21	1:D:376:ALA:HA	2.02	0.42
1:D:507:PRO:C	1:D:509:GLN:H	2.28	0.42
1:B:167:PRO:C	1:B:169:LEU:H	2.28	0.42
1:B:320:ASP:OD2	1:B:333:SER:HB2	2.19	0.42
1:C:45:THR:OG1	1:C:50:ILE:HD11	2.20	0.42
1:C:63:VAL:HG11	1:C:252:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:THR:HB	1:C:363:PHE:CE1	2.55	0.42
1:D:234:LEU:O	1:D:236:ARG:HG3	2.18	0.42
1:D:351:THR:HG22	1:D:375:ASN:O	2.20	0.42
1:A:47:TYR:O	1:A:51:GLN:HG2	2.20	0.42
1:B:505:ARG:O	1:B:507:PRO:HD3	2.19	0.42
1:C:90:VAL:HG23	1:C:495:MET:HE3	1.89	0.42
1:D:300:LEU:CD2	1:D:409:THR:HG23	2.49	0.42
1:D:459:ASP:HB3	1:D:520:GLN:HE21	1.84	0.42
1:D:509:GLN:HA	1:D:514:LYS:HD3	2.00	0.42
1:A:40:LEU:HD13	1:A:41:SER:N	2.35	0.41
1:A:262:PHE:HE1	1:A:428:ASP:HA	1.84	0.41
1:A:325:SER:HA	1:A:381:TRP:CE3	2.55	0.41
1:A:326:PRO:HD3	1:A:381:TRP:CE2	2.55	0.41
1:A:357:TYR:CE1	1:A:367:GLN:HG3	2.55	0.41
1:A:390:ILE:N	1:A:390:ILE:HD12	2.35	0.41
1:A:556:HIS:HA	1:B:339:TYR:CE1	2.55	0.41
1:B:197:ILE:O	1:B:495:MET:HE3	2.20	0.41
1:C:359:TYR:CD2	1:C:360:PRO:HD3	2.55	0.41
1:D:304:GLU:HG3	1:D:305:GLU:N	2.35	0.41
1:C:49:SER:O	1:C:53:VAL:HG23	2.20	0.41
1:D:59:ILE:C	1:D:60:ILE:HG12	2.46	0.41
1:D:442:LEU:HD21	1:D:446:SER:HB3	2.02	0.41
1:A:116:ASP:C	1:A:118:LEU:H	2.29	0.41
1:B:402:ARG:HH22	1:B:410:ARG:HB3	1.85	0.41
1:C:50:ILE:O	1:C:54:LEU:HG	2.20	0.41
1:D:265:ARG:HB2	1:D:511:TYR:CZ	2.56	0.41
1:D:298:LEU:HD13	1:D:411:PHE:CD1	2.55	0.41
1:A:124:TYR:C	1:A:126:ASP:H	2.29	0.41
1:A:292:GLY:O	1:A:386:VAL:HA	2.20	0.41
1:A:526:ASP:H	1:A:531:TYR:HE2	1.67	0.41
1:B:124:TYR:CZ	1:B:130:LYS:HG2	2.55	0.41
1:B:339:TYR:CG	1:B:340:ASN:N	2.88	0.41
1:C:399:LEU:HG	1:C:411:PHE:CE2	2.55	0.41
1:D:14:THR:HA	1:D:15:PRO:HD3	1.94	0.41
1:D:108:ILE:HB	1:D:203:LEU:HD23	2.02	0.41
1:D:146:GLY:C	1:D:147:PHE:HD1	2.27	0.41
1:A:496:TYR:HB2	1:A:546:MET:HE2	2.01	0.41
1:B:268:CYS:HA	1:B:512:VAL:HG22	2.02	0.41
1:A:194:TYR:CB	1:A:476:TYR:CE2	3.00	0.41
1:A:532:PRO:HB3	1:A:538:TYR:CE1	2.55	0.41
1:B:437:THR:HG21	1:B:463:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:HIS:HA	1:B:339:TYR:HE1	1.86	0.41
1:B:323:ILE:HD11	1:B:371:VAL:HG13	2.02	0.41
1:A:69:THR:CG2	1:A:404:LEU:HG	2.51	0.41
1:A:116:ASP:HB2	1:A:472:PRO:HG3	2.02	0.41
1:A:315:ARG:HD3	1:B:520:GLN:OE1	2.21	0.41
1:A:349:GLU:HB3	1:A:377:LYS:HD3	2.03	0.41
1:B:202:GLU:HG3	1:B:236:ARG:HH12	1.85	0.41
1:D:298:LEU:HD13	1:D:411:PHE:CE1	2.55	0.41
1:A:197:ILE:HD11	1:A:488:HIS:ND1	2.36	0.41
1:B:288:PRO:CD	1:B:294:VAL:HG13	2.49	0.41
1:D:154:THR:O	1:D:158:ILE:HG12	2.21	0.41
1:D:436:ASN:HB3	1:D:439:ASN:OD1	2.21	0.41
1:D:458:PRO:O	1:D:537:GLY:HA3	2.21	0.41
1:A:514:LYS:HG2	1:B:360:PRO:HB2	2.03	0.40
1:C:354:SER:HB3	1:C:372:THR:HG22	2.02	0.40
1:C:465:VAL:O	1:C:466:ASN:HB2	2.20	0.40
1:D:179:MET:SD	1:D:479:ILE:HB	2.61	0.40
1:B:155:ARG:HG2	1:B:159:ASN:ND2	2.37	0.40
1:A:26:MET:SD	1:A:49:SER:HB3	2.62	0.40
1:B:68:MET:HE2	1:B:220:LEU:HD22	2.03	0.40
1:B:471:TYR:CD1	1:B:472:PRO:HD2	2.56	0.40
1:C:6:LEU:HB3	1:C:7:SER:H	1.64	0.40
1:C:461:VAL:O	1:C:540:LEU:HD12	2.21	0.40
1:A:146:GLY:C	1:A:147:PHE:HD1	2.29	0.40
1:A:265:ARG:HD2	1:A:507:PRO:O	2.21	0.40
1:B:361:THR:HG23	1:B:366:GLN:O	2.22	0.40
1:C:108:ILE:HB	1:C:203:LEU:HD23	2.04	0.40
1:C:133:TYR:CE1	1:C:154:THR:HG22	2.57	0.40
1:D:60:ILE:HD12	1:D:60:ILE:HG23	1.81	0.40
1:D:105:GLY:O	1:D:237:PRO:HD2	2.21	0.40
1:A:138:THR:CG2	1:A:209:GLY:HA2	2.52	0.40
1:A:144:PRO:HA	1:A:152:GLU:OE1	2.21	0.40
1:B:116:ASP:O	1:B:118:LEU:N	2.54	0.40
1:B:251:GLY:C	1:B:252:LEU:HD12	2.47	0.40
1:B:300:LEU:HD23	1:B:377:LYS:O	2.21	0.40
1:C:121:ASP:OD2	1:C:476:TYR:CZ	2.74	0.40
1:C:197:ILE:O	1:C:495:MET:HE3	2.22	0.40
1:D:153:TYR:CE1	1:D:169:LEU:HD22	2.56	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	538/559 (96%)	468 (87%)	56 (10%)	14 (3%)	4	21
1	B	487/559 (87%)	430 (88%)	45 (9%)	12 (2%)	4	22
1	C	538/559 (96%)	471 (88%)	52 (10%)	15 (3%)	4	20
1	D	483/559 (86%)	426 (88%)	50 (10%)	7 (1%)	9	33
All	All	2046/2236 (92%)	1795 (88%)	203 (10%)	48 (2%)	5	24

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	THR
1	A	288	PRO
1	B	117	TYR
1	B	290	VAL
1	C	340	ASN
1	C	359	TYR
1	D	35	ASP
1	D	60	ILE
1	D	505	ARG
1	A	89	GLY
1	A	99	ILE
1	A	336	ILE
1	B	60	ILE
1	B	98	ASN
1	B	167	PRO
1	B	459	ASP
1	C	407	SER
1	A	251	GLY
1	A	290	VAL
1	B	84	ALA
1	C	169	LEU
1	C	360	PRO

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Mol	Chain	Res	Type
1	C	459	ASP
1	C	532	PRO
1	A	169	LEU
1	A	466	ASN
1	B	14	THR
1	B	539	GLY
1	C	84	ALA
1	C	96	ASN
1	C	126	ASP
1	C	288	PRO
1	C	457	LYS
1	D	508	ASN
1	B	13	HIS
1	C	441	SER
1	C	507	PRO
1	D	362	THR
1	A	15	PRO
1	A	96	ASN
1	C	15	PRO
1	A	335	GLY
1	D	506	TYR
1	A	458	PRO
1	A	457	LYS
1	B	251	GLY
1	B	457	LYS
1	D	457	LYS

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	433/468 (92%)	432 (100%)	1 (0%)	87	87
1	B	391/468 (84%)	391 (100%)	0	100	100
1	C	437/468 (93%)	433 (99%)	4 (1%)	70	76
1	D	396/468 (85%)	394 (100%)	2 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1657/1872 (88%)	1650 (100%)	7 (0%)	84 84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	C	40	LEU
1	C	83	VAL
1	C	360	PRO
1	C	531	TYR
1	D	357	TYR
1	D	389	TYR

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	44	ASN
1	A	51	GLN
1	A	225	GLN
1	A	289	HIS
1	A	474	ASN
1	A	528	ASN
1	B	367	GLN
1	B	375	ASN
1	C	51	GLN
1	C	96	ASN
1	C	396	ASN
1	C	426	GLN
1	D	119	HIS
1	D	508	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	542/559 (96%)	0.34	3 (0%) 85 73	51, 68, 89, 104	0
1	B	497/559 (88%)	0.32	17 (3%) 48 32	46, 61, 80, 95	0
1	C	542/559 (96%)	0.61	23 (4%) 40 26	49, 68, 87, 104	0
1	D	495/559 (88%)	0.83	46 (9%) 14 11	53, 70, 91, 107	0
All	All	2076/2236 (92%)	0.52	89 (4%) 40 26	46, 67, 88, 107	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	MET	4.4
1	B	221	PHE	3.8
1	D	157	ASP	3.7
1	C	40	LEU	3.7
1	C	555	HIS	3.6
1	D	216	ASN	3.5
1	D	316	PRO	3.4
1	D	62	THR	3.2
1	C	316	PRO	3.2
1	D	415	ASP	3.2
1	D	244	LEU	3.1
1	D	63	VAL	3.0
1	B	97	PRO	2.9
1	D	15	PRO	2.9
1	D	232	PHE	2.9
1	D	209	GLY	2.9
1	D	252	LEU	2.9
1	D	357	TYR	2.8
1	D	278	ASN	2.7
1	B	116	ASP	2.7
1	C	60	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	532	PRO	2.6
1	D	290	VAL	2.6
1	D	28	GLN	2.6
1	D	308	SER	2.6
1	B	192	SER	2.5
1	D	300	LEU	2.5
1	D	126	ASP	2.5
1	C	458	PRO	2.5
1	D	347	ASP	2.5
1	C	37	LEU	2.5
1	D	339	TYR	2.5
1	B	39	VAL	2.5
1	D	324	VAL	2.4
1	D	354	SER	2.4
1	D	506	TYR	2.4
1	D	302	GLU	2.4
1	D	528	ASN	2.4
1	D	434	ALA	2.4
1	B	539	GLY	2.3
1	D	13	HIS	2.3
1	B	10	ASP	2.3
1	B	541	LEU	2.3
1	D	550	LEU	2.3
1	C	400	PRO	2.3
1	D	392	THR	2.3
1	D	457	LYS	2.3
1	B	149	ILE	2.3
1	B	327	THR	2.3
1	C	470	ALA	2.2
1	C	194	TYR	2.2
1	D	59	ILE	2.2
1	D	425	ILE	2.2
1	C	412	ARG	2.2
1	C	82	VAL	2.2
1	D	370	ASN	2.2
1	D	358	ILE	2.2
1	D	313	LEU	2.2
1	B	253	THR	2.2
1	B	290	VAL	2.2
1	D	289	HIS	2.2
1	C	99	ILE	2.2
1	D	243	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	287	ILE	2.2
1	B	338	ASN	2.2
1	D	221	PHE	2.2
1	D	411	PHE	2.2
1	C	460	ILE	2.1
1	A	307	LEU	2.1
1	D	64	SER	2.1
1	C	29	ASN	2.1
1	D	444	GLN	2.1
1	B	202	GLU	2.1
1	C	294	VAL	2.1
1	C	26	MET	2.1
1	B	316	PRO	2.1
1	D	391	ILE	2.1
1	A	422	TYR	2.1
1	C	87	GLU	2.1
1	B	321	VAL	2.0
1	D	543	VAL	2.0
1	C	351	THR	2.0
1	C	428	ASP	2.0
1	D	148	TYR	2.0
1	C	98	ASN	2.0
1	B	389	TYR	2.0
1	C	374	LYS	2.0
1	D	507	PRO	2.0
1	C	101	ILE	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.