



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 PM UTC

PDB ID : 4AR2 / pdb_00004ar2
Title : Dodecahedron formed of penton base protein from adenovirus Ad3
Authors : Burmeister, W.P.; Szolajska, E.; Zochowska, M.; Nerlo, B.; Andreev, I.; Schoehn, G.; Andrieu, J.-P.; Fender, P.; Naskalska, A.; Zubieta, C.; Cusack, S.; Chroboczek, J.
Deposited on : 2012-04-20
Resolution : 3.80 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 Phenix2.0
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

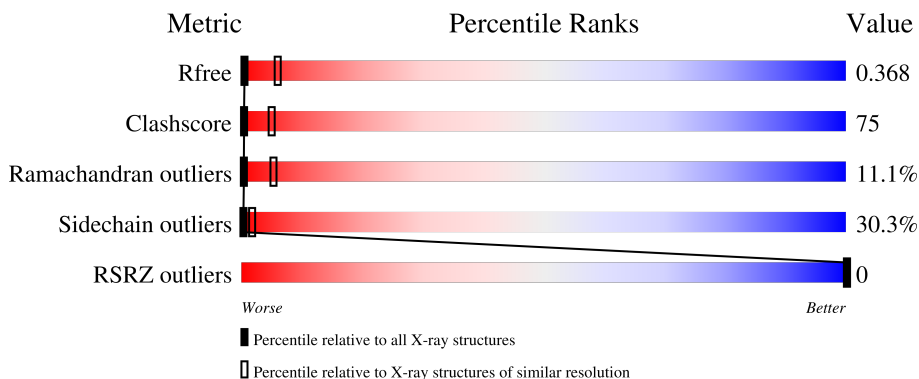
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	509	
2	P	21	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3757 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 L2 PROTEIN III (PENTON BASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3673	2324	629	706	14			

- Molecule 2 is a protein called FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	S	0	0	0
			83	53	11	18	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	21	CYS	-	expression tag	UNP P03275

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	346.04Å 348.55Å 372.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	258.20 – 3.80 254.63 – 3.80	Depositor EDS
% Data completeness (in resolution range)	56.8 (258.20-3.80) 47.7 (254.63-3.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.6.0114	Depositor
R, R_{free}	0.280 , 0.278 0.371 , 0.368	Depositor DCC
R_{free} test set	5040 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	101.2	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.065 for k,h,-l	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	3757	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.88	3/3758 (0.1%)	1.56	100/5103 (2.0%)
2	P	0.56	0/86	0.84	0/119
All	All	0.88	3/3844 (0.1%)	1.55	100/5222 (1.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ILE	CA-CB	10.02	1.68	1.54
1	A	80	ALA	N-CA	-8.70	1.35	1.46
1	A	79	ILE	C-N	-5.95	1.26	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	N-CA-C	-15.22	92.75	112.24
1	A	158	THR	N-CA-C	12.46	126.42	108.86
1	A	469	PHE	N-CA-C	-12.37	89.08	109.24
1	A	414	LEU	N-CA-C	-11.96	94.83	110.39
1	A	51	GLY	N-CA-C	11.90	129.11	110.90
1	A	157	VAL	N-CA-C	11.82	133.92	109.34
1	A	155	GLU	N-CA-C	11.78	131.63	113.72
1	A	111	ILE	N-CA-C	-10.78	94.67	108.89
1	A	414	LEU	CA-C-N	-9.88	107.50	119.84
1	A	414	LEU	C-N-CA	-9.88	107.50	119.84
1	A	387	ASN	N-CA-C	9.35	130.46	109.81
1	A	281	LYS	N-CA-C	-9.34	94.88	109.07
1	A	197	ILE	N-CA-C	-9.32	101.70	111.58
1	A	461	GLN	N-CA-C	-9.22	102.16	113.50
1	A	63	LEU	N-CA-C	9.03	123.85	110.48
1	A	279	GLY	N-CA-C	-8.63	92.72	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	GLU	CA-C-N	-8.55	113.34	121.46
1	A	50	GLU	C-N-CA	-8.55	113.34	121.46
1	A	305	LYS	N-CA-C	-8.40	92.92	110.80
1	A	451	GLU	N-CA-C	8.33	122.79	110.30
1	A	280	PHE	N-CA-C	8.30	122.96	108.52
1	A	195	ASN	N-CA-C	-8.29	98.99	111.34
1	A	140	SER	N-CA-C	-8.25	99.11	111.81
1	A	178	ILE	N-CA-C	8.23	121.95	109.20
1	A	433	TYR	N-CA-C	8.13	127.77	109.81
1	A	459	LEU	N-CA-C	-8.10	102.71	112.59
1	A	231	GLU	N-CA-C	7.88	119.50	111.07
1	A	95	VAL	N-CA-C	-7.86	103.55	113.22
1	A	83	ASN	N-CA-C	7.76	122.50	112.26
1	A	384	ASN	N-CA-C	7.72	119.48	111.14
1	A	540	SER	CB-CA-C	-7.64	107.75	116.54
1	A	94	THR	N-CA-C	-7.56	97.73	109.76
1	A	52	ARG	N-CA-C	-7.56	101.17	110.61
1	A	159	VAL	N-CA-C	7.51	124.96	109.34
1	A	124	LYS	N-CA-C	-7.46	98.86	110.42
1	A	115	GLU	N-CA-C	7.39	126.53	110.80
1	A	50	GLU	N-CA-C	-7.32	98.00	109.72
1	A	200	ASN	N-CA-C	-7.14	103.43	112.93
1	A	215	ILE	N-CA-C	-7.10	103.74	110.42
1	A	82	LEU	CA-C-N	-7.09	112.01	122.86
1	A	82	LEU	C-N-CA	-7.09	112.01	122.86
1	A	102	THR	N-CA-C	-7.07	100.85	109.83
1	A	216	GLY	N-CA-C	7.03	124.35	115.21
1	A	114	ASP	N-CA-C	6.96	120.00	109.63
1	A	351	LEU	N-CA-C	6.87	125.42	110.80
1	A	53	ASN	N-CA-C	-6.85	100.14	110.28
1	A	520	ARG	N-CA-C	-6.74	104.95	112.57
1	A	79	ILE	CA-C-N	-6.71	111.29	120.28
1	A	79	ILE	C-N-CA	-6.71	111.29	120.28
1	A	540	SER	N-CA-C	6.69	118.47	108.31
1	A	404	THR	N-CA-C	-6.68	104.02	111.71
1	A	87	ASP	N-CA-C	6.68	125.03	110.80
1	A	233	LYS	N-CA-C	-6.67	104.45	112.58
1	A	168	ASP	N-CA-C	6.65	122.89	114.31
1	A	240	TYR	N-CA-C	-6.63	95.91	108.17
1	A	184	PHE	N-CA-C	6.62	120.31	109.85
1	A	439	GLU	N-CA-C	-6.61	99.03	109.07
1	A	76	SER	N-CA-C	6.60	124.86	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	TYR	N-CA-C	-6.41	105.76	113.97
1	A	393	ARG	N-CA-C	-6.40	105.33	113.01
1	A	80	ALA	N-CA-C	6.36	118.21	111.28
1	A	407	ALA	N-CA-C	-6.25	100.16	109.15
1	A	416	ASP	N-CA-C	-6.14	105.66	113.02
1	A	212	GLU	N-CA-C	-6.03	104.78	111.71
1	A	193	MET	N-CA-C	-5.96	104.36	111.69
1	A	274	HIS	CA-C-N	5.91	127.23	119.84
1	A	274	HIS	C-N-CA	5.91	127.23	119.84
1	A	423	THR	N-CA-C	5.90	123.36	110.80
1	A	62	PRO	N-CA-C	-5.77	100.58	112.47
1	A	110	THR	N-CA-C	5.75	118.84	109.59
1	A	224	PHE	N-CA-C	-5.66	101.92	110.24
1	A	113	PHE	CA-C-N	-5.65	110.84	122.82
1	A	113	PHE	C-N-CA	-5.65	110.84	122.82
1	A	101	PHE	N-CA-C	5.61	118.24	108.76
1	A	219	PHE	N-CA-C	-5.57	102.65	110.50
1	A	483	ALA	N-CA-C	-5.57	102.11	110.24
1	A	456	SER	N-CA-C	-5.55	105.23	112.23
1	A	79	ILE	CA-CB-CG2	5.53	119.90	110.50
1	A	82	LEU	N-CA-C	5.53	121.90	113.61
1	A	157	VAL	CB-CA-C	-5.51	102.26	111.29
1	A	531	LEU	CA-C-N	-5.49	117.03	122.36
1	A	531	LEU	C-N-CA	-5.49	117.03	122.36
1	A	116	ARG	CA-CB-CG	5.47	125.04	114.10
1	A	386	GLY	N-CA-C	5.41	125.99	113.18
1	A	445	SER	N-CA-C	5.36	117.64	108.90
1	A	306	LYS	N-CA-C	5.32	120.05	113.50
1	A	450	ASN	N-CA-C	-5.28	101.83	109.59
1	A	83	ASN	CB-CA-C	5.23	119.55	111.13
1	A	378	SER	N-CA-C	5.20	117.38	108.90
1	A	489	VAL	N-CA-C	5.17	115.57	108.12
1	A	251	LEU	N-CA-C	5.16	117.51	109.52
1	A	486	ILE	N-CA-C	5.15	115.26	107.75
1	A	479	ILE	N-CA-C	5.12	116.12	108.54
1	A	229	ASP	N-CA-C	-5.11	101.52	108.11
1	A	385	TYR	N-CA-C	5.11	119.59	112.90
1	A	80	ALA	N-CA-CB	-5.10	102.62	110.12
1	A	100	ASP	N-CA-C	-5.05	106.96	113.02
1	A	467	HIS	N-CA-C	-5.04	100.06	110.80
1	A	262	SER	N-CA-C	5.03	116.71	109.07
1	A	505	ARG	N-CA-C	-5.01	103.92	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3673	0	3600	556	0
2	P	83	0	68	3	0
3	A	1	0	0	0	0
All	All	3757	0	3668	557	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 75.

All (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:SER:CB	1:A:351:LEU:HB3	1.65	1.24
1:A:114:ASP:CG	1:A:115:GLU:H	1.49	1.13
1:A:131:MET:H	1:A:492:ASN:ND2	1.46	1.12
1:A:431:ASN:O	1:A:521:ARG:HD3	1.52	1.09
1:A:304:SER:HB3	1:A:351:LEU:HB3	1.12	1.08
1:A:259:PHE:HB2	1:A:280:PHE:HE1	1.16	1.08
1:A:501:THR:HG21	1:A:537:ARG:HH21	1.15	1.07
1:A:235:ILE:HG12	1:A:295:LEU:HA	1.34	1.06
1:A:129:THR:OG1	1:A:442:PRO:HG2	1.54	1.06
1:A:381:LEU:HD12	1:A:381:LEU:H	1.15	1.04
1:A:178:ILE:HD13	1:A:178:ILE:H	1.23	1.02
1:A:105:GLU:O	1:A:108:THR:HG22	1.58	1.01
1:A:132:PRO:HD2	1:A:526:TYR:CE2	1.97	1.00
1:A:351:LEU:O	1:A:352:LYS:HB3	1.59	1.00
1:A:132:PRO:HD2	1:A:526:TYR:HE2	1.27	0.98
1:A:301:TYR:HD2	1:A:352:LYS:HD2	1.28	0.97
1:A:131:MET:N	1:A:492:ASN:HD21	1.64	0.95
1:A:293:PRO:O	1:A:373:ASN:HA	1.67	0.94
1:A:517:THR:HG21	1:A:521:ARG:HG3	1.50	0.94
1:A:235:ILE:CG1	1:A:295:LEU:HA	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLN:HA	1:A:429:GLN:HE21	1.33	0.92
1:A:403:VAL:CG2	1:A:488:THR:HB	2.00	0.91
1:A:259:PHE:HB2	1:A:280:PHE:CE1	2.06	0.91
1:A:501:THR:HG21	1:A:537:ARG:NH2	1.83	0.90
1:A:114:ASP:CG	1:A:115:GLU:N	2.26	0.88
1:A:304:SER:CB	1:A:351:LEU:CB	2.52	0.88
1:A:435:VAL:HG23	1:A:521:ARG:HH22	1.39	0.87
1:A:413:SER:HB3	1:A:435:VAL:HA	1.57	0.87
1:A:381:LEU:H	1:A:381:LEU:CD1	1.87	0.87
1:A:131:MET:H	1:A:492:ASN:HD21	0.86	0.86
1:A:263:ARG:HD2	1:A:406:GLY:HA3	1.57	0.86
1:A:131:MET:HE1	1:A:138:MET:CG	2.05	0.85
1:A:221:THR:O	1:A:222:ARG:HB2	1.75	0.85
1:A:226:LEU:HD23	1:A:227:GLY:H	1.41	0.85
1:A:159:VAL:HA	1:A:162:THR:HB	1.58	0.85
1:A:367:VAL:O	1:A:368:LEU:HB2	1.74	0.85
1:A:177:PHE:N	1:A:177:PHE:HD1	1.74	0.84
1:A:392:ILE:N	1:A:392:ILE:HD12	1.93	0.84
1:A:72:VAL:HA	1:A:531:LEU:HD22	1.58	0.84
1:A:196:ALA:HA	1:A:199:ASP:HB2	1.59	0.83
1:A:403:VAL:HG21	1:A:488:THR:HB	1.59	0.82
1:A:177:PHE:N	1:A:177:PHE:CD1	2.47	0.81
1:A:89:SER:HB3	1:A:523:THR:HG22	1.62	0.81
1:A:177:PHE:HD1	1:A:177:PHE:H	1.28	0.81
1:A:381:LEU:HD12	1:A:381:LEU:N	1.94	0.81
1:A:416:ASP:C	1:A:512:GLN:HE22	1.89	0.81
1:A:178:ILE:H	1:A:178:ILE:CD1	1.94	0.81
1:A:435:VAL:CG2	1:A:521:ARG:HH22	1.93	0.81
1:A:304:SER:HB2	1:A:351:LEU:HB3	1.60	0.81
1:A:274:HIS:O	1:A:276:PHE:N	2.15	0.79
1:A:409:GLN:HA	1:A:440:LEU:HA	1.64	0.79
1:A:206:ARG:HB2	1:A:207:GLN:NE2	1.98	0.78
1:A:270:ILE:HD11	1:A:379:TRP:CD1	2.18	0.78
1:A:417:MET:HE3	1:A:534:VAL:HG11	1.65	0.78
1:A:194:ASN:ND2	1:A:219:PHE:O	2.18	0.77
1:A:395:TRP:HD1	1:A:396:THR:HG22	1.50	0.77
1:A:131:MET:HE1	1:A:138:MET:HG2	1.65	0.76
1:A:232:THR:HG21	1:A:236:MET:SD	2.25	0.76
1:A:410:VAL:HG23	1:A:517:THR:O	1.87	0.75
1:A:63:LEU:HD13	1:A:64:TYR:O	1.87	0.75
1:A:119:TRP:HB2	1:A:537:ARG:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:SER:O	1:A:63:LEU:N	2.19	0.75
1:A:235:ILE:HD11	1:A:295:LEU:H	1.50	0.75
1:A:383:TYR:HA	1:A:392:ILE:HD13	1.66	0.75
1:A:431:ASN:O	1:A:521:ARG:CD	2.33	0.75
1:A:422:VAL:HG22	1:A:423:THR:HG23	1.69	0.75
1:A:233:LYS:HB2	1:A:372:ILE:HG21	1.67	0.74
1:A:355:PRO:HG3	1:A:371:LYS:HB3	1.68	0.74
1:A:263:ARG:NH1	1:A:405:CYS:O	2.19	0.74
1:A:301:TYR:CD2	1:A:352:LYS:HD2	2.18	0.74
1:A:304:SER:HB2	1:A:351:LEU:CB	2.16	0.74
1:A:142:LYS:O	1:A:143:PHE:HB3	1.86	0.74
1:A:248:ASP:OD2	1:A:380:TYR:HB2	1.87	0.74
1:A:133:ASN:HB2	1:A:490:SER:CB	2.18	0.74
1:A:235:ILE:HD13	1:A:235:ILE:N	2.03	0.74
1:A:278:GLU:OE1	1:A:280:PHE:HB3	1.88	0.74
1:A:235:ILE:CD1	1:A:293:PRO:HB2	2.17	0.73
1:A:56:ARG:O	1:A:57:TYR:HB3	1.88	0.73
1:A:518:ASP:O	1:A:521:ARG:N	2.22	0.73
1:A:414:LEU:CD1	1:A:417:MET:HB3	2.17	0.73
1:A:72:VAL:HA	1:A:531:LEU:CD2	2.18	0.73
1:A:376:TYR:CE2	1:A:477:ILE:HG21	2.23	0.73
1:A:102:THR:HG23	1:A:105:GLU:CD	2.14	0.72
1:A:143:PHE:HE2	1:A:219:PHE:CZ	2.05	0.72
1:A:147:VAL:HG11	1:A:200:ASN:HD21	1.54	0.72
1:A:147:VAL:HG22	1:A:148:MET:N	2.03	0.72
1:A:93:THR:HG22	1:A:94:THR:O	1.90	0.72
1:A:199:ASP:HA	1:A:202:LEU:HD21	1.70	0.72
1:A:71:LEU:HB3	1:A:532:GLY:O	1.89	0.72
1:A:413:SER:HA	1:A:436:VAL:HG23	1.72	0.72
1:A:424:PHE:CD2	1:A:434:PRO:HA	2.25	0.72
1:A:147:VAL:HG22	1:A:148:MET:H	1.53	0.71
1:A:279:GLY:O	1:A:395:TRP:HZ2	1.73	0.71
1:A:226:LEU:CD2	1:A:241:THR:HG23	2.20	0.71
1:A:418:MET:HE3	1:A:502:LEU:HB2	1.71	0.71
1:A:517:THR:CG2	1:A:521:ARG:HG3	2.19	0.71
1:A:139:PHE:HD1	1:A:139:PHE:N	1.88	0.71
1:A:370:ASP:HB2	1:A:372:ILE:HD11	1.71	0.71
1:A:58:SER:O	1:A:59:GLU:C	2.33	0.71
1:A:133:ASN:HB2	1:A:490:SER:HB3	1.72	0.71
1:A:63:LEU:HD22	1:A:64:TYR:H	1.56	0.71
1:A:159:VAL:CA	1:A:162:THR:HB	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:THR:O	1:A:190:ILE:N	2.24	0.71
1:A:508:ILE:HG23	1:A:512:GLN:HE21	1.56	0.71
1:A:131:MET:HE1	1:A:138:MET:HG3	1.72	0.70
1:A:123:LEU:HD12	1:A:123:LEU:C	2.17	0.70
1:A:475:ASN:HB3	1:A:478:LEU:HD23	1.73	0.69
1:A:161:ASP:OD2	1:A:164:ASP:HB3	1.91	0.69
1:A:91:PHE:CE1	1:A:514:VAL:HG13	2.27	0.69
1:A:134:VAL:HG22	1:A:182:GLY:O	1.92	0.69
1:A:171:LYS:NZ	1:A:171:LYS:HA	2.08	0.69
1:A:293:PRO:O	1:A:294:ALA:HB2	1.92	0.69
1:A:232:THR:OG1	1:A:234:LEU:HB2	1.92	0.68
1:A:139:PHE:N	1:A:139:PHE:CD1	2.61	0.68
1:A:223:ASN:O	1:A:226:LEU:HD22	1.94	0.68
1:A:98:ASN:ND2	1:A:100:ASP:H	1.92	0.68
1:A:225:ARG:O	1:A:228:TRP:HB2	1.94	0.68
1:A:220:ASP:O	1:A:248:ASP:HB3	1.93	0.68
1:A:198:ILE:O	1:A:202:LEU:HG	1.94	0.68
1:A:132:PRO:CD	1:A:526:TYR:CE2	2.76	0.67
1:A:119:TRP:HA	1:A:539:LEU:HD12	1.77	0.67
1:A:159:VAL:H	1:A:162:THR:HB	1.59	0.67
1:A:206:ARG:HB2	1:A:207:GLN:HE21	1.58	0.67
1:A:119:TRP:N	1:A:119:TRP:CD1	2.63	0.67
1:A:171:LYS:HA	1:A:171:LYS:HZ3	1.58	0.67
1:A:115:GLU:C	1:A:117:SER:N	2.49	0.66
1:A:380:TYR:HB3	1:A:381:LEU:HD12	1.77	0.66
1:A:75:LYS:O	1:A:79:ILE:HD12	1.93	0.66
1:A:202:LEU:HD12	1:A:203:GLU:N	2.10	0.66
1:A:177:PHE:HE2	1:A:197:ILE:HA	1.60	0.66
1:A:215:ILE:HG22	1:A:216:GLY:N	2.10	0.66
1:A:83:ASN:HD21	1:A:92:LEU:HD12	1.60	0.66
1:A:288:GLU:O	1:A:290:GLY:N	2.26	0.66
1:A:517:THR:HG23	1:A:521:ARG:HA	1.78	0.66
1:A:131:MET:HA	1:A:526:TYR:HD2	1.61	0.66
1:A:294:ALA:HA	1:A:374:THR:HG22	1.76	0.66
1:A:117:SER:HA	1:A:541:SER:HA	1.79	0.65
1:A:259:PHE:O	1:A:262:SER:N	2.29	0.65
1:A:369:GLU:O	1:A:371:LYS:N	2.23	0.65
1:A:187:THR:HA	1:A:190:ILE:HD13	1.78	0.65
1:A:159:VAL:N	1:A:162:THR:HB	2.11	0.65
1:A:352:LYS:C	1:A:354:GLN:N	2.52	0.65
1:A:82:LEU:HB2	1:A:92:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:O	1:A:165:HIS:N	2.29	0.65
1:A:244:ALA:CB	1:A:484:PRO:HA	2.27	0.65
1:A:138:MET:HE3	1:A:263:ARG:NH2	2.12	0.64
1:A:360:SER:C	1:A:362:SER:H	2.05	0.64
1:A:470:ASN:HB2	1:A:480:ARG:HB2	1.79	0.64
1:A:158:THR:OG1	1:A:159:VAL:N	2.29	0.64
1:A:263:ARG:O	1:A:265:SER:N	2.31	0.64
1:A:234:LEU:HD21	1:A:294:ALA:HB3	1.78	0.64
1:A:131:MET:N	1:A:492:ASN:ND2	2.30	0.64
1:A:224:PHE:O	1:A:225:ARG:CB	2.45	0.64
1:A:292:ILE:HB	1:A:374:THR:HG23	1.78	0.64
1:A:479:ILE:O	1:A:480:ARG:C	2.40	0.64
1:A:188:MET:O	1:A:192:LEU:HD23	1.97	0.64
1:A:226:LEU:HD21	1:A:241:THR:HG23	1.78	0.64
1:A:235:ILE:HD11	1:A:295:LEU:N	2.13	0.64
1:A:351:LEU:O	1:A:352:LYS:CB	2.39	0.64
1:A:397:LEU:HD22	1:A:398:LEU:H	1.62	0.63
1:A:98:ASN:HD22	1:A:99:ASN:N	1.97	0.63
1:A:179:LEU:HD22	1:A:192:LEU:HB3	1.80	0.63
1:A:416:ASP:HB2	1:A:512:GLN:OE1	1.98	0.63
1:A:125:THR:CG2	1:A:499:HIS:CE1	2.81	0.63
1:A:193:MET:C	1:A:195:ASN:H	2.05	0.63
1:A:397:LEU:HD22	1:A:398:LEU:N	2.12	0.63
1:A:383:TYR:CD1	1:A:383:TYR:C	2.76	0.63
1:A:90:ASN:HB2	1:A:515:THR:OG1	1.99	0.62
1:A:115:GLU:O	1:A:116:ARG:HG2	1.99	0.62
1:A:147:VAL:HG11	1:A:200:ASN:ND2	2.13	0.62
1:A:187:THR:O	1:A:188:MET:C	2.42	0.62
1:A:125:THR:HG21	1:A:499:HIS:CE1	2.35	0.62
1:A:379:TRP:CZ2	1:A:383:TYR:HD2	2.18	0.62
1:A:418:MET:HG3	1:A:436:VAL:HG13	1.82	0.62
1:A:440:LEU:HD12	1:A:440:LEU:H	1.63	0.62
1:A:83:ASN:ND2	1:A:92:LEU:CD1	2.63	0.61
1:A:83:ASN:ND2	1:A:92:LEU:HD12	2.15	0.61
1:A:517:THR:HG21	1:A:521:ARG:CG	2.27	0.61
1:A:288:GLU:C	1:A:387:ASN:HD21	2.08	0.61
1:A:82:LEU:CD1	1:A:92:LEU:HD13	2.30	0.61
1:A:187:THR:CG2	1:A:484:PRO:HD3	2.31	0.61
1:A:239:VAL:HG13	1:A:476:GLN:HE22	1.65	0.61
1:A:79:ILE:O	1:A:80:ALA:C	2.40	0.61
1:A:129:THR:HG22	1:A:527:VAL:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PRO:CD	1:A:526:TYR:HE2	2.08	0.61
1:A:379:TRP:HH2	1:A:396:THR:HG1	1.45	0.61
1:A:232:THR:HG23	1:A:234:LEU:H	1.66	0.61
1:A:466:THR:HG22	1:A:467:HIS:N	2.16	0.61
1:A:246:HIS:CE1	1:A:398:LEU:HD11	2.36	0.61
1:A:128:HIS:HB3	1:A:528:TYR:HD2	1.66	0.61
1:A:267:LEU:C	1:A:267:LEU:HD12	2.26	0.61
1:A:369:GLU:C	1:A:371:LYS:H	2.09	0.61
1:A:111:ILE:HG22	1:A:508:ILE:HB	1.83	0.60
1:A:82:LEU:CB	1:A:92:LEU:HD13	2.31	0.60
1:A:187:THR:HG23	1:A:484:PRO:HD3	1.83	0.60
1:A:287:LEU:H	1:A:287:LEU:HD22	1.67	0.60
1:A:287:LEU:HD12	1:A:379:TRP:HA	1.83	0.60
1:A:288:GLU:C	1:A:290:GLY:H	2.08	0.60
1:A:224:PHE:O	1:A:225:ARG:HB3	2.00	0.60
1:A:226:LEU:HG	1:A:241:THR:HG23	1.84	0.60
1:A:111:ILE:CG2	1:A:508:ILE:HB	2.32	0.60
1:A:177:PHE:CE2	1:A:197:ILE:HA	2.37	0.60
1:A:65:ASP:O	1:A:66:THR:HB	2.02	0.59
1:A:246:HIS:NE2	1:A:398:LEU:HD11	2.17	0.59
1:A:83:ASN:HD21	1:A:92:LEU:CD1	2.15	0.59
1:A:92:LEU:HD12	1:A:92:LEU:N	2.17	0.59
1:A:418:MET:C	1:A:420:ASP:H	2.10	0.59
1:A:421:PRO:HG2	1:A:424:PHE:CD1	2.38	0.59
1:A:65:ASP:O	1:A:66:THR:CB	2.50	0.59
1:A:388:PRO:HB2	1:A:389:GLU:HG3	1.85	0.59
1:A:508:ILE:HG23	1:A:512:GLN:NE2	2.18	0.59
1:A:157:VAL:HB	1:A:158:THR:HG22	1.85	0.59
1:A:223:ASN:HB3	1:A:226:LEU:HD13	1.84	0.59
1:A:125:THR:CG2	1:A:499:HIS:HE1	2.15	0.59
1:A:277:GLN:O	1:A:278:GLU:HG2	2.02	0.59
1:A:399:THR:OG1	1:A:400:THR:N	2.34	0.59
1:A:107:SER:HB2	1:A:511:VAL:CG2	2.33	0.58
1:A:119:TRP:HB3	1:A:538:VAL:HA	1.85	0.58
1:A:90:ASN:HB2	1:A:515:THR:HG1	1.67	0.58
1:A:98:ASN:HD22	1:A:98:ASN:C	2.11	0.58
1:A:418:MET:CE	1:A:502:LEU:HB2	2.34	0.58
1:A:469:PHE:O	1:A:470:ASN:CB	2.51	0.58
1:A:392:ILE:HD12	1:A:392:ILE:H	1.67	0.58
1:A:417:MET:CE	1:A:534:VAL:HG11	2.33	0.58
1:A:122:GLN:HB2	1:A:501:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:HIS:N	1:A:275:PRO:CD	2.67	0.58
1:A:267:LEU:HD12	1:A:267:LEU:O	2.03	0.58
1:A:383:TYR:C	1:A:383:TYR:HD1	2.11	0.57
1:A:387:ASN:O	1:A:388:PRO:C	2.46	0.57
1:A:478:LEU:N	1:A:478:LEU:HD22	2.19	0.57
1:A:395:TRP:CD1	1:A:396:THR:HG22	2.35	0.57
1:A:145:ALA:HA	1:A:257:VAL:HA	1.87	0.57
1:A:108:THR:HG23	1:A:109:GLN:N	2.20	0.57
1:A:150:SER:HB3	1:A:171:LYS:CB	2.35	0.57
1:A:187:THR:O	1:A:189:THR:N	2.38	0.57
1:A:223:ASN:O	1:A:224:PHE:C	2.47	0.57
1:A:198:ILE:C	1:A:200:ASN:H	2.12	0.56
1:A:89:SER:CB	1:A:523:THR:HG22	2.35	0.56
1:A:184:PHE:HB3	1:A:188:MET:HB3	1.86	0.56
1:A:248:ASP:OD1	1:A:249:ILE:N	2.39	0.56
1:A:133:ASN:HB3	1:A:183:ASN:HB2	1.87	0.56
1:A:293:PRO:O	1:A:294:ALA:CB	2.52	0.56
1:A:417:MET:HB2	1:A:512:GLN:NE2	2.19	0.56
1:A:136:GLU:HA	1:A:141:ASN:HB3	1.87	0.56
1:A:61:SER:O	1:A:62:PRO:C	2.49	0.55
1:A:150:SER:HB3	1:A:171:LYS:HB3	1.87	0.55
1:A:223:ASN:C	1:A:223:ASN:HD22	2.12	0.55
1:A:226:LEU:HD23	1:A:227:GLY:N	2.18	0.55
1:A:433:TYR:O	1:A:434:PRO:C	2.49	0.55
1:A:226:LEU:HG	1:A:241:THR:CG2	2.37	0.55
1:A:234:LEU:CD2	1:A:294:ALA:HB3	2.36	0.55
1:A:263:ARG:C	1:A:265:SER:N	2.64	0.55
1:A:92:LEU:HD12	1:A:92:LEU:H	1.71	0.55
1:A:111:ILE:CG2	1:A:111:ILE:O	2.55	0.55
1:A:427:THR:HG21	1:A:432:ASN:HB3	1.88	0.55
1:A:202:LEU:HB2	1:A:206:ARG:HH21	1.72	0.55
1:A:203:GLU:C	1:A:204:ILE:HD12	2.32	0.55
1:A:133:ASN:H	1:A:183:ASN:HB3	1.72	0.55
1:A:185:SER:O	1:A:186:ALA:C	2.50	0.54
1:A:233:LYS:O	1:A:372:ILE:HG22	2.05	0.54
1:A:272:LYS:HD2	1:A:280:PHE:HB2	1.89	0.54
1:A:379:TRP:HH2	1:A:396:THR:OG1	1.90	0.54
1:A:226:LEU:CD2	1:A:226:LEU:H	2.21	0.54
1:A:197:ILE:HD12	1:A:217:VAL:O	2.08	0.54
1:A:258:ASP:OD1	1:A:258:ASP:C	2.49	0.54
1:A:352:LYS:C	1:A:354:GLN:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TYR:CA	1:A:392:ILE:HD13	2.37	0.54
1:A:143:PHE:O	1:A:143:PHE:CD1	2.60	0.54
1:A:58:SER:O	1:A:60:LEU:N	2.40	0.54
1:A:82:LEU:HB2	1:A:92:LEU:CD1	2.38	0.54
1:A:147:VAL:CG2	1:A:148:MET:H	2.19	0.54
1:A:352:LYS:O	1:A:353:ILE:C	2.51	0.54
1:A:215:ILE:CG2	1:A:216:GLY:N	2.72	0.53
1:A:147:VAL:CG2	1:A:148:MET:N	2.70	0.53
1:A:376:TYR:CD2	1:A:477:ILE:HG13	2.43	0.53
1:A:177:PHE:HD2	1:A:196:ALA:O	1.92	0.53
1:A:178:ILE:CD1	1:A:178:ILE:N	2.65	0.53
1:A:230:PRO:O	1:A:233:LYS:HG2	2.08	0.53
1:A:263:ARG:HD2	1:A:406:GLY:CA	2.34	0.53
1:A:359:ASP:CG	1:A:360:SER:N	2.67	0.53
1:A:441:MET:C	1:A:443:VAL:H	2.14	0.53
1:A:467:HIS:HE1	2:P:20:GLU:HB3	1.73	0.53
1:A:414:LEU:HD13	1:A:417:MET:HB3	1.90	0.53
1:A:304:SER:O	1:A:351:LEU:HD13	2.09	0.53
1:A:218:LYS:O	1:A:250:VAL:HG23	2.08	0.53
1:A:60:LEU:O	1:A:61:SER:C	2.52	0.52
1:A:132:PRO:HD2	1:A:526:TYR:CD2	2.44	0.52
1:A:226:LEU:CG	1:A:241:THR:HG23	2.38	0.52
1:A:417:MET:HG2	1:A:418:MET:SD	2.50	0.52
1:A:67:THR:O	1:A:536:PRO:HD2	2.10	0.52
1:A:136:GLU:HA	1:A:141:ASN:CB	2.40	0.52
1:A:367:VAL:O	1:A:368:LEU:CB	2.52	0.52
1:A:418:MET:HG3	1:A:436:VAL:CG1	2.39	0.52
1:A:107:SER:HB2	1:A:511:VAL:HG22	1.91	0.52
1:A:171:LYS:HZ2	1:A:172:TYR:H	1.58	0.52
1:A:293:PRO:O	1:A:373:ASN:CA	2.50	0.52
1:A:119:TRP:CB	1:A:537:ARG:O	2.57	0.52
1:A:246:HIS:ND1	1:A:247:PRO:O	2.43	0.52
1:A:292:ILE:HG12	1:A:376:TYR:O	2.10	0.52
1:A:113:PHE:CE1	1:A:536:PRO:CB	2.93	0.52
1:A:144:LYS:HB2	1:A:258:ASP:HB3	1.91	0.52
1:A:352:LYS:O	1:A:354:GLN:N	2.43	0.52
1:A:486:ILE:HG22	1:A:486:ILE:O	2.09	0.52
1:A:75:LYS:O	1:A:79:ILE:CD1	2.58	0.51
1:A:356:LEU:HD11	1:A:358:LYS:O	2.10	0.51
1:A:259:PHE:O	1:A:261:GLU:N	2.43	0.51
1:A:78:ASP:OD1	1:A:94:THR:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:HB2	1:A:490:SER:OG	2.11	0.51
1:A:216:GLY:HA2	1:A:252:LEU:HB2	1.90	0.51
1:A:91:PHE:C	1:A:92:LEU:HG	2.35	0.51
1:A:267:LEU:C	1:A:269:GLY:H	2.19	0.51
1:A:90:ASN:CB	1:A:515:THR:OG1	2.58	0.51
1:A:51:GLY:HA3	1:A:53:ASN:ND2	2.25	0.51
1:A:353:ILE:O	1:A:355:PRO:HD3	2.11	0.51
1:A:475:ASN:O	1:A:477:ILE:N	2.44	0.51
1:A:250:VAL:HG13	1:A:378:SER:HB2	1.93	0.50
1:A:288:GLU:O	1:A:387:ASN:ND2	2.44	0.50
1:A:135:ASN:OD1	1:A:137:TYR:N	2.43	0.50
1:A:280:PHE:O	1:A:280:PHE:CD1	2.65	0.50
1:A:57:TYR:O	1:A:58:SER:C	2.54	0.50
1:A:78:ASP:O	1:A:79:ILE:O	2.29	0.50
1:A:143:PHE:HE2	1:A:219:PHE:HZ	1.52	0.50
1:A:224:PHE:CG	1:A:292:ILE:HD12	2.47	0.50
1:A:126:ILE:HD11	1:A:496:LEU:HD13	1.93	0.50
1:A:143:PHE:CE2	1:A:219:PHE:HZ	2.29	0.50
1:A:189:THR:O	1:A:192:LEU:HB2	2.12	0.50
1:A:114:ASP:H	1:A:119:TRP:HZ2	1.59	0.50
1:A:294:ALA:O	1:A:295:LEU:CB	2.60	0.50
1:A:383:TYR:CE1	1:A:393:ARG:HG3	2.47	0.50
1:A:259:PHE:O	1:A:260:THR:C	2.54	0.50
1:A:383:TYR:HA	1:A:392:ILE:CD1	2.40	0.50
1:A:83:ASN:OD1	1:A:85:GLN:OE1	2.30	0.49
1:A:272:LYS:HZ1	1:A:279:GLY:H	1.59	0.49
1:A:143:PHE:CE2	1:A:219:PHE:CZ	2.95	0.49
1:A:414:LEU:HG	1:A:436:VAL:HG21	1.93	0.49
1:A:304:SER:HB2	1:A:351:LEU:HB2	1.94	0.49
1:A:235:ILE:HD12	1:A:293:PRO:HB2	1.91	0.49
1:A:269:GLY:C	1:A:399:THR:HG23	2.37	0.49
1:A:464:SER:C	1:A:466:THR:H	2.19	0.49
1:A:132:PRO:CD	1:A:526:TYR:CD2	2.96	0.49
1:A:263:ARG:O	1:A:264:LEU:C	2.55	0.49
1:A:363:ARG:HD3	1:A:475:ASN:CG	2.38	0.49
1:A:134:VAL:HG23	1:A:134:VAL:O	2.13	0.49
1:A:219:PHE:CD2	1:A:249:ILE:HG22	2.48	0.49
1:A:294:ALA:HA	1:A:374:THR:CG2	2.43	0.49
1:A:82:LEU:HD13	1:A:92:LEU:HD13	1.95	0.49
1:A:193:MET:C	1:A:195:ASN:N	2.68	0.49
1:A:235:ILE:HD13	1:A:235:ILE:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG13	1:A:476:GLN:NE2	2.27	0.49
1:A:295:LEU:HD23	1:A:296:LEU:O	2.13	0.49
1:A:517:THR:CG2	1:A:521:ARG:CG	2.88	0.49
1:A:234:LEU:HD11	1:A:355:PRO:HB3	1.94	0.48
1:A:244:ALA:HB1	1:A:484:PRO:HA	1.95	0.48
1:A:276:PHE:C	1:A:277:GLN:HG3	2.38	0.48
1:A:292:ILE:HB	1:A:374:THR:CG2	2.43	0.48
1:A:534:VAL:O	1:A:534:VAL:HG13	2.13	0.48
1:A:101:PHE:HA	1:A:105:GLU:OE2	2.13	0.48
1:A:135:ASN:ND2	1:A:138:MET:H	2.10	0.48
1:A:474:GLU:CD	1:A:474:GLU:N	2.72	0.48
1:A:201:TYR:CD2	1:A:202:LEU:N	2.82	0.48
1:A:106:ALA:O	1:A:109:GLN:HG2	2.13	0.48
1:A:226:LEU:CD2	1:A:226:LEU:N	2.77	0.48
1:A:226:LEU:HD22	1:A:226:LEU:H	1.78	0.48
1:A:270:ILE:HD11	1:A:379:TRP:CG	2.47	0.48
1:A:472:PHE:CD1	1:A:478:LEU:HB3	2.47	0.48
1:A:53:ASN:ND2	1:A:53:ASN:H	2.12	0.48
1:A:363:ARG:HB2	1:A:475:ASN:HD21	1.77	0.48
1:A:414:LEU:HD12	1:A:414:LEU:C	2.39	0.48
1:A:540:SER:O	1:A:541:SER:CB	2.62	0.48
1:A:160:ASN:ND2	1:A:160:ASN:H	2.12	0.48
1:A:227:GLY:C	1:A:235:ILE:HG22	2.38	0.48
1:A:396:THR:OG1	1:A:397:LEU:N	2.45	0.48
1:A:253:PRO:HA	1:A:284:TYR:CG	2.49	0.48
1:A:135:ASN:ND2	1:A:138:MET:N	2.62	0.47
1:A:152:LYS:C	1:A:169:ILE:HG22	2.39	0.47
1:A:198:ILE:C	1:A:200:ASN:N	2.72	0.47
1:A:236:MET:HA	1:A:296:LEU:CD2	2.44	0.47
1:A:367:VAL:O	1:A:373:ASN:O	2.32	0.47
1:A:467:HIS:CE1	2:P:20:GLU:HB3	2.49	0.47
1:A:88:HIS:CD2	1:A:528:TYR:O	2.67	0.47
1:A:108:THR:HG23	1:A:109:GLN:H	1.79	0.47
1:A:475:ASN:O	1:A:476:GLN:C	2.56	0.47
1:A:143:PHE:CD1	1:A:143:PHE:C	2.89	0.47
1:A:469:PHE:O	1:A:470:ASN:HB3	2.14	0.47
1:A:119:TRP:HA	1:A:539:LEU:CD1	2.44	0.47
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.55	0.47
1:A:96:VAL:HG21	1:A:106:ALA:HB1	1.97	0.47
1:A:457:GLN:NE2	1:A:480:ARG:HG2	2.30	0.47
1:A:56:ARG:O	1:A:57:TYR:CB	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:HA	1:A:79:ILE:CD1	2.45	0.47
1:A:301:TYR:HA	1:A:351:LEU:O	2.15	0.47
1:A:392:ILE:N	1:A:392:ILE:CD1	2.64	0.47
1:A:477:ILE:HG22	1:A:478:LEU:HD22	1.97	0.47
1:A:67:THR:OG1	1:A:68:LYS:N	2.47	0.47
1:A:435:VAL:HG12	1:A:437:GLY:N	2.29	0.47
1:A:122:GLN:CB	1:A:501:THR:HG22	2.45	0.47
1:A:511:VAL:HG23	1:A:511:VAL:O	2.15	0.47
1:A:69:LEU:HD22	1:A:95:VAL:HG22	1.96	0.46
1:A:116:ARG:O	1:A:117:SER:HB3	2.15	0.46
1:A:120:GLY:HA2	1:A:504:LEU:HG	1.96	0.46
1:A:252:LEU:HD22	1:A:253:PRO:HD3	1.97	0.46
1:A:355:PRO:O	1:A:356:LEU:C	2.56	0.46
1:A:418:MET:C	1:A:420:ASP:N	2.73	0.46
1:A:89:SER:HA	1:A:516:VAL:HG12	1.97	0.46
1:A:234:LEU:CD1	1:A:355:PRO:HB3	2.45	0.46
1:A:258:ASP:OD1	1:A:259:PHE:N	2.48	0.46
1:A:264:LEU:O	1:A:267:LEU:HB3	2.15	0.46
1:A:417:MET:CA	1:A:512:GLN:HE22	2.28	0.46
1:A:498:ASP:C	1:A:498:ASP:OD1	2.56	0.46
1:A:252:LEU:HG	1:A:376:TYR:HE1	1.81	0.46
1:A:371:LYS:C	1:A:372:ILE:HG13	2.39	0.46
1:A:440:LEU:HD12	1:A:440:LEU:N	2.29	0.46
1:A:508:ILE:CG2	1:A:512:GLN:HE21	2.26	0.46
1:A:114:ASP:OD1	1:A:115:GLU:N	2.49	0.46
1:A:135:ASN:HD21	1:A:138:MET:N	2.14	0.46
1:A:151:ARG:C	1:A:152:LYS:HG3	2.40	0.46
1:A:349:LYS:C	1:A:351:LEU:HG	2.41	0.46
1:A:350:GLU:H	1:A:350:GLU:CD	2.23	0.46
1:A:138:MET:HB3	1:A:263:ARG:HH22	1.80	0.46
1:A:273:ARG:C	1:A:275:PRO:CD	2.89	0.46
1:A:127:MET:HB2	1:A:127:MET:HE3	1.82	0.46
1:A:119:TRP:N	1:A:119:TRP:HD1	2.12	0.46
1:A:417:MET:N	1:A:512:GLN:HE22	2.14	0.46
1:A:466:THR:HG22	1:A:468:VAL:N	2.31	0.46
1:A:195:ASN:O	1:A:198:ILE:N	2.49	0.45
1:A:414:LEU:HD11	1:A:418:MET:HG2	1.98	0.45
1:A:478:LEU:HD22	1:A:478:LEU:H	1.80	0.45
1:A:519:ALA:C	1:A:521:ARG:H	2.23	0.45
1:A:161:ASP:O	1:A:165:HIS:HB2	2.16	0.45
1:A:196:ALA:HA	1:A:199:ASP:CB	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HG22	1:A:216:GLY:H	1.80	0.45
1:A:233:LYS:HB2	1:A:372:ILE:CG2	2.40	0.45
1:A:235:ILE:N	1:A:235:ILE:CD1	2.68	0.45
1:A:273:ARG:NH2	1:A:397:LEU:HD23	2.31	0.45
1:A:283:MET:O	1:A:284:TYR:C	2.58	0.45
1:A:202:LEU:HD12	1:A:203:GLU:H	1.77	0.45
1:A:134:VAL:HG21	1:A:184:PHE:CE2	2.52	0.45
1:A:387:ASN:HA	1:A:388:PRO:HD2	1.61	0.45
1:A:263:ARG:C	1:A:265:SER:H	2.24	0.45
1:A:98:ASN:HD22	1:A:100:ASP:H	1.64	0.45
1:A:137:TYR:HE1	1:A:522:ARG:CZ	2.30	0.45
1:A:63:LEU:HD13	1:A:64:TYR:N	2.32	0.45
1:A:131:MET:HA	1:A:526:TYR:CD2	2.47	0.45
1:A:405:CYS:O	1:A:405:CYS:SG	2.75	0.45
1:A:83:ASN:ND2	1:A:92:LEU:HD11	2.32	0.45
1:A:135:ASN:OD1	1:A:136:GLU:N	2.50	0.45
1:A:138:MET:HE3	1:A:263:ARG:HH22	1.79	0.45
1:A:252:LEU:CG	1:A:376:TYR:HE1	2.30	0.45
1:A:392:ILE:HA	1:A:395:TRP:HB3	1.98	0.45
1:A:413:SER:HB2	1:A:433:TYR:O	2.16	0.45
1:A:102:THR:O	1:A:103:PRO:C	2.60	0.44
1:A:248:ASP:OD2	1:A:378:SER:OG	2.35	0.44
1:A:370:ASP:HB2	1:A:372:ILE:CD1	2.42	0.44
1:A:466:THR:HB	1:A:468:VAL:HG22	1.99	0.44
1:A:224:PHE:CB	1:A:292:ILE:HD12	2.48	0.44
1:A:236:MET:HA	1:A:296:LEU:HD22	1.99	0.44
1:A:433:TYR:O	1:A:434:PRO:O	2.35	0.44
1:A:248:ASP:OD2	1:A:380:TYR:CB	2.63	0.44
1:A:466:THR:CG2	1:A:467:HIS:N	2.80	0.44
1:A:170:LEU:HD13	1:A:170:LEU:N	2.32	0.44
1:A:277:GLN:O	1:A:278:GLU:CG	2.65	0.44
1:A:252:LEU:HD21	1:A:376:TYR:CE1	2.52	0.44
1:A:418:MET:HE3	1:A:502:LEU:CB	2.43	0.44
1:A:493:VAL:HG22	1:A:494:PRO:N	2.32	0.44
1:A:125:THR:CG2	1:A:412:TRP:CZ3	3.01	0.44
1:A:133:ASN:CB	1:A:490:SER:OG	2.66	0.44
1:A:107:SER:HB2	1:A:511:VAL:HG21	2.00	0.44
1:A:201:TYR:O	1:A:205:GLY:N	2.40	0.44
1:A:496:LEU:HD23	1:A:496:LEU:N	2.32	0.44
1:A:435:VAL:CG2	1:A:521:ARG:NH2	2.73	0.44
1:A:137:TYR:CE1	1:A:522:ARG:CZ	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:C	1:A:371:LYS:N	2.75	0.43
1:A:89:SER:HA	1:A:516:VAL:CG1	2.48	0.43
1:A:90:ASN:ND2	1:A:513:ARG:HH21	2.15	0.43
1:A:85:GLN:O	1:A:86:ASN:CG	2.61	0.43
1:A:111:ILE:HG22	1:A:111:ILE:O	2.18	0.43
1:A:219:PHE:CD2	1:A:249:ILE:CG2	3.02	0.43
1:A:159:VAL:H	1:A:162:THR:CB	2.30	0.43
1:A:239:VAL:HG22	1:A:476:GLN:NE2	2.33	0.43
2:P:17:TYR:O	2:P:18:ASP:HB2	2.18	0.43
1:A:51:GLY:O	1:A:52:ARG:HD3	2.18	0.43
1:A:85:GLN:O	1:A:86:ASN:ND2	2.52	0.43
1:A:520:ARG:HG3	1:A:522:ARG:NE	2.33	0.43
1:A:146:ARG:HB3	1:A:174:TRP:CE3	2.53	0.43
1:A:198:ILE:O	1:A:200:ASN:N	2.51	0.43
1:A:69:LEU:HD22	1:A:95:VAL:CG2	2.49	0.43
1:A:72:VAL:HG12	1:A:73:ASP:H	1.84	0.43
1:A:124:LYS:HB2	1:A:533:ILE:CD1	2.48	0.43
1:A:138:MET:HB3	1:A:263:ARG:NH2	2.34	0.43
1:A:246:HIS:CE1	1:A:398:LEU:CD1	3.02	0.43
1:A:353:ILE:H	1:A:353:ILE:HG13	1.60	0.43
1:A:298:VAL:HG22	1:A:299:THR:N	2.33	0.43
1:A:133:ASN:HB3	1:A:183:ASN:CB	2.49	0.42
1:A:376:TYR:CD2	1:A:477:ILE:CG1	3.02	0.42
1:A:474:GLU:N	1:A:474:GLU:OE1	2.52	0.42
1:A:78:ASP:O	1:A:79:ILE:C	2.62	0.42
1:A:102:THR:O	1:A:105:GLU:HG2	2.19	0.42
1:A:125:THR:HG21	1:A:412:TRP:CZ3	2.55	0.42
1:A:132:PRO:HA	1:A:183:ASN:HB3	2.00	0.42
1:A:403:VAL:HG22	1:A:488:THR:HB	1.94	0.42
1:A:518:ASP:O	1:A:521:ARG:HA	2.20	0.42
1:A:249:ILE:HD12	1:A:257:VAL:HG11	2.01	0.42
1:A:64:TYR:O	1:A:65:ASP:CB	2.67	0.42
1:A:124:LYS:HB2	1:A:533:ILE:HD13	2.01	0.42
1:A:214:ASP:HA	1:A:252:LEU:CD1	2.49	0.42
1:A:369:GLU:H	1:A:369:GLU:CD	2.27	0.42
1:A:111:ILE:HG22	1:A:508:ILE:CB	2.47	0.42
1:A:203:GLU:HB3	1:A:204:ILE:HD12	2.01	0.42
1:A:113:PHE:HE1	1:A:536:PRO:CB	2.31	0.42
1:A:235:ILE:CD1	1:A:235:ILE:H	2.32	0.42
1:A:263:ARG:O	1:A:266:ASN:N	2.51	0.42
1:A:378:SER:O	1:A:379:TRP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HB3	1:A:116:ARG:H	1.10	0.42
1:A:164:ASP:HA	1:A:167:GLU:HG2	2.00	0.42
1:A:126:ILE:HG13	1:A:496:LEU:HD22	2.02	0.42
1:A:235:ILE:HD11	1:A:293:PRO:HB2	1.98	0.42
1:A:416:ASP:O	1:A:512:GLN:NE2	2.46	0.42
1:A:435:VAL:HG12	1:A:437:GLY:H	1.84	0.42
1:A:218:LYS:HE2	1:A:220:ASP:HB2	2.01	0.41
1:A:388:PRO:HB2	1:A:389:GLU:H	1.68	0.41
1:A:389:GLU:HG3	1:A:389:GLU:H	1.66	0.41
1:A:427:THR:OG1	1:A:428:ARG:N	2.53	0.41
1:A:111:ILE:HA	1:A:111:ILE:HD12	1.85	0.41
1:A:133:ASN:H	1:A:183:ASN:CB	2.31	0.41
1:A:190:ILE:HG22	1:A:191:ASP:N	2.35	0.41
1:A:252:LEU:C	1:A:284:TYR:CD1	2.98	0.41
1:A:273:ARG:HH21	1:A:397:LEU:HD23	1.86	0.41
1:A:134:VAL:HG23	1:A:181:GLU:HA	2.01	0.41
1:A:379:TRP:O	1:A:380:TYR:C	2.63	0.41
1:A:169:ILE:HD12	1:A:169:ILE:HA	1.91	0.41
1:A:475:ASN:O	1:A:478:LEU:N	2.54	0.41
1:A:295:LEU:HD23	1:A:296:LEU:N	2.35	0.41
1:A:115:GLU:C	1:A:117:SER:H	2.21	0.41
1:A:240:TYR:O	1:A:241:THR:C	2.64	0.41
1:A:240:TYR:CE2	1:A:295:LEU:HD12	2.56	0.41
1:A:397:LEU:HD13	1:A:397:LEU:C	2.46	0.41
1:A:479:ILE:O	1:A:481:PRO:N	2.54	0.41
1:A:150:SER:HB3	1:A:171:LYS:HB2	2.01	0.41
1:A:201:TYR:O	1:A:202:LEU:C	2.63	0.41
1:A:220:ASP:N	1:A:248:ASP:O	2.48	0.41
1:A:232:THR:O	1:A:233:LYS:HB2	2.20	0.41
1:A:252:LEU:HG	1:A:376:TYR:CE1	2.55	0.41
1:A:194:ASN:HD21	1:A:219:PHE:N	2.18	0.40
1:A:267:LEU:C	1:A:267:LEU:CD1	2.94	0.40
1:A:365:TYR:O	1:A:366:ASN:C	2.63	0.40
1:A:414:LEU:HD11	1:A:417:MET:HB3	1.97	0.40
1:A:442:PRO:HD2	1:A:443:VAL:HG23	2.04	0.40
1:A:223:ASN:HD21	1:A:385:TYR:HE2	1.68	0.40
1:A:441:MET:C	1:A:443:VAL:N	2.79	0.40
1:A:257:VAL:O	1:A:257:VAL:HG13	2.20	0.40
1:A:380:TYR:CE1	1:A:384:ASN:ND2	2.89	0.40
1:A:57:TYR:CE1	1:A:58:SER:HB3	2.57	0.40
1:A:419:GLN:O	1:A:420:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:HIS:ND1	1:A:246:HIS:C	2.80	0.40
1:A:379:TRP:CZ2	1:A:383:TYR:CD2	3.05	0.40
1:A:392:ILE:C	1:A:394:SER:N	2.78	0.40
1:A:427:THR:HG21	1:A:432:ASN:HD22	1.87	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	451/509 (89%)	320 (71%)	81 (18%)	50 (11%)	0	5
2	P	8/21 (38%)	5 (62%)	2 (25%)	1 (12%)	0	4
All	All	459/530 (87%)	325 (71%)	83 (18%)	51 (11%)	0	5

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	57	TYR
1	A	59	GLU
1	A	66	THR
1	A	79	ILE
1	A	117	SER
1	A	143	PHE
1	A	188	MET
1	A	242	TYR
1	A	260	THR
1	A	275	PRO
1	A	278	GLU
1	A	351	LEU
1	A	352	LYS

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Mol	Chain	Res	Type
1	A	368	LEU
1	A	370	ASP
1	A	388	PRO
1	A	392	ILE
1	A	415	PRO
1	A	434	PRO
1	A	470	ASN
1	A	519	ALA
1	A	541	SER
1	A	58	SER
1	A	222	ARG
1	A	225	ARG
1	A	264	LEU
1	A	289	GLY
1	A	294	ALA
1	A	405	CYS
1	A	430	VAL
1	A	476	GLN
1	A	152	LYS
1	A	199	ASP
1	A	241	THR
1	A	423	THR
1	A	453	ALA
1	A	521	ARG
1	A	62	PRO
1	A	295	LEU
1	A	420	ASP
1	A	87	ASP
1	A	145	ALA
1	A	379	TRP
1	A	419	GLN
1	A	190	ILE
1	A	372	ILE
1	A	481	PRO
1	A	367	VAL
2	P	14	VAL
1	A	159	VAL

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	412/457 (90%)	284 (69%)	128 (31%)	0	1
2	P	10/20 (50%)	10 (100%)	0	100	100
All	All	422/477 (88%)	294 (70%)	128 (30%)	0	2

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	52	ARG
1	A	54	SER
1	A	57	TYR
1	A	59	GLU
1	A	60	LEU
1	A	63	LEU
1	A	71	LEU
1	A	72	VAL
1	A	75	LYS
1	A	76	SER
1	A	82	LEU
1	A	85	GLN
1	A	92	LEU
1	A	96	VAL
1	A	100	ASP
1	A	102	THR
1	A	104	THR
1	A	107	SER
1	A	110	THR
1	A	116	ARG
1	A	119	TRP
1	A	123	LEU
1	A	126	ILE
1	A	130	ASN
1	A	131	MET
1	A	133	ASN
1	A	135	ASN
1	A	139	PHE
1	A	143	PHE
1	A	149	VAL

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Mol	Chain	Res	Type
1	A	157	VAL
1	A	158	THR
1	A	160	ASN
1	A	161	ASP
1	A	163	TYR
1	A	164	ASP
1	A	170	LEU
1	A	171	LYS
1	A	177	PHE
1	A	178	ILE
1	A	189	THR
1	A	191	ASP
1	A	193	MET
1	A	197	ILE
1	A	199	ASP
1	A	200	ASN
1	A	202	LEU
1	A	207	GLN
1	A	211	LEU
1	A	212	GLU
1	A	214	ASP
1	A	215	ILE
1	A	220	ASP
1	A	221	THR
1	A	222	ARG
1	A	226	LEU
1	A	228	TRP
1	A	229	ASP
1	A	231	GLU
1	A	232	THR
1	A	235	ILE
1	A	241	THR
1	A	243	GLU
1	A	246	HIS
1	A	249	ILE
1	A	250	VAL
1	A	255	CYS
1	A	261	GLU
1	A	267	LEU
1	A	270	ILE
1	A	273	ARG
1	A	285	GLU

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	288	GLU
1	A	296	LEU
1	A	298	VAL
1	A	301	TYR
1	A	349	LYS
1	A	351	LEU
1	A	354	GLN
1	A	363	ARG
1	A	366	ASN
1	A	372	ILE
1	A	374	THR
1	A	376	TYR
1	A	381	LEU
1	A	383	TYR
1	A	389	GLU
1	A	392	ILE
1	A	396	THR
1	A	399	THR
1	A	400	THR
1	A	401	SER
1	A	403	VAL
1	A	408	GLU
1	A	410	VAL
1	A	412	TRP
1	A	417	MET
1	A	429	GLN
1	A	430	VAL
1	A	439	GLU
1	A	440	LEU
1	A	451	GLU
1	A	460	ARG
1	A	468	VAL
1	A	469	PHE
1	A	472	PHE
1	A	474	GLU
1	A	477	ILE
1	A	478	LEU
1	A	485	THR
1	A	486	ILE
1	A	487	THR
1	A	488	THR

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Mol	Chain	Res	Type
1	A	492	ASN
1	A	496	LEU
1	A	497	THR
1	A	504	LEU
1	A	514	VAL
1	A	515	THR
1	A	518	ASP
1	A	520	ARG
1	A	522	ARG
1	A	523	THR
1	A	533	ILE
1	A	538	VAL
1	A	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	83	ASN
1	A	86	ASN
1	A	88	HIS
1	A	90	ASN
1	A	98	ASN
1	A	112	ASN
1	A	130	ASN
1	A	141	ASN
1	A	160	ASN
1	A	200	ASN
1	A	207	GLN
1	A	223	ASN
1	A	354	GLN
1	A	366	ASN
1	A	387	ASN
1	A	429	GLN
1	A	432	ASN
1	A	461	GLN
1	A	475	ASN
1	A	476	GLN
1	A	492	ASN
1	A	499	HIS
1	A	512	GLN

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	455/509 (89%)	-0.68	0 100 100	13, 61, 170, 199	0
2	P	10/21 (47%)	-0.21	0 100 100	121, 128, 130, 130	10 (100%)
All	All	465/530 (87%)	-0.67	0 100 100	13, 61, 169, 199	10 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
3	CA	A	999	1/1	0.96	0.07	72,72,72,72	1

6.5 Other polymers [i](#)

There are no such residues in this entry.