



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:05 PM EDT

PDB ID : 1A6E / pdb_00001a6e
Title : THERMOSOME-MG-ADP-ALF3 COMPLEX
Authors : Ditzel, L.; Loewe, J.; Stock, D.; Stetter, K.-O.; Huber, H.; Huber, R.; Steinbacher, S.
Deposited on : 1998-02-24
Resolution : 3.20 Å(reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

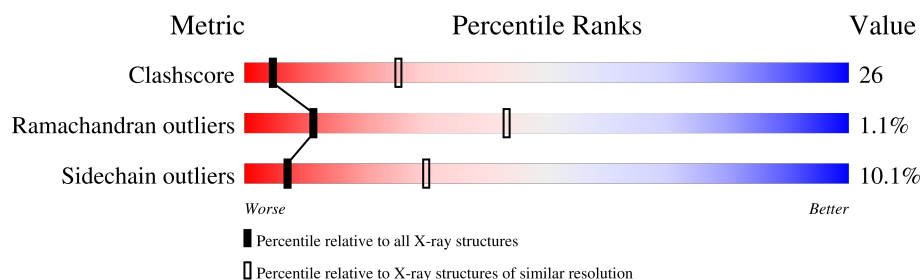
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	545	
2	B	543	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9390 atoms, of which 1742 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 THERMOSOME (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	H	N	O	S	884	0	0
			4668	2356	884	662	752	14			

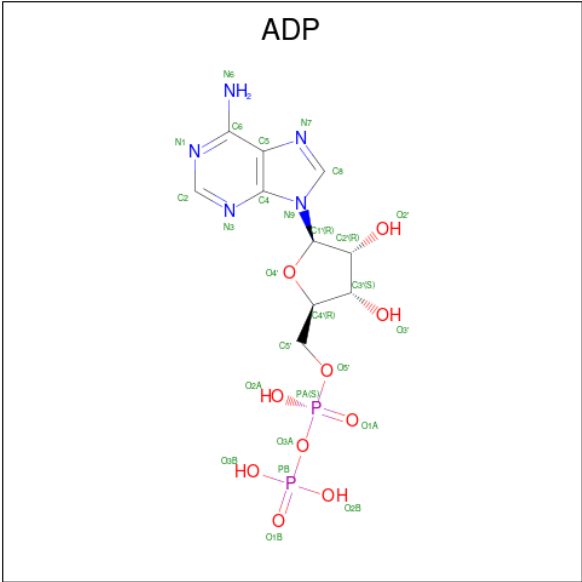
- Molecule 2 is a protein called THERMOSOME (BETA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	502	Total	C	H	N	O	S	858	0	0
			4656	2370	858	651	758	19			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

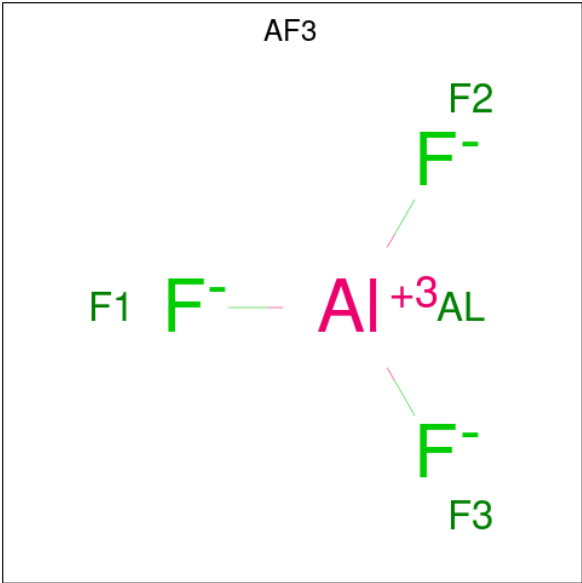
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			4	1	3		
5	B	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is water.

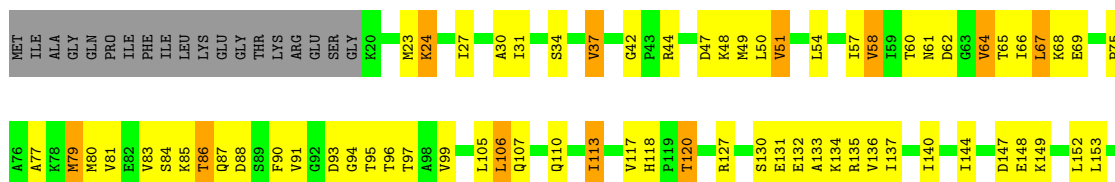
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		

Note EDS was not executed.

- Chain A: 47% 40% 6% 8%

The sequence logo displays the conservation of amino acids at each position. The y-axis lists the amino acids, and the x-axis shows the position number. The color scale at the top indicates the conservation level: 47% (green), 40% (yellow), 6% (orange), and 8% (red). The logo shows that positions 1-100 are highly conserved (green/yellow), while positions 101-250 are less conserved (orange/red).

- Chain B: 45% 39% 7% 8%



T158	A242	A243	G327	D402	A405	A406	G408	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484
T158	P243	L244	S329	Y405	A406	A407	G408	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484
T158	E245	I246	S330	Y406	A407	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484		
T158	K247	K248	S332	G408	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484			
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T158	L255	R256	I337	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
T158	E178	E185	S338	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
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T158	T281	V284	S351	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
T158	N287	I290	S352	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
T158	T291	Q292	S353	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
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T158	D297	M298	S361	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
T158	T211	Q212	S362	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
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T158	I218	V219	S370	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
T158	S304	R305	S371	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
T158	D220	K221	I372	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
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T158	R312	R313	S376	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
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T158	K315	K316	T390	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484				
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T158	E222	K223	G376	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y							

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.80Å 167.80Å 202.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.5 (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.181 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9390	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: AF3, MG, ADP

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	0.65	0/3812	1.10	24/5139 (0.5%)
2	B	0.69	1/3834 (0.0%)	1.09	19/5166 (0.4%)
All	All	0.67	1/7646 (0.0%)	1.10	43/10305 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	ILE	CA-CB	6.05	1.62	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	ARG	N-CA-C	-7.43	102.87	112.23
2	B	42	GLY	CA-C-N	7.24	126.87	119.56
2	B	42	GLY	C-N-CA	7.24	126.87	119.56
2	B	64	VAL	CB-CA-C	-7.24	102.37	112.14
1	A	43	GLY	CA-C-N	7.22	128.86	119.84
1	A	43	GLY	C-N-CA	7.22	128.86	119.84
1	A	365	ASN	CA-C-N	7.10	126.71	119.19
1	A	365	ASN	C-N-CA	7.10	126.71	119.19
1	A	236	ILE	N-CA-C	6.89	118.78	108.23
1	A	57	ASP	N-CA-C	6.67	125.00	110.80
1	A	160	SER	N-CA-C	6.62	124.91	110.80
1	A	298	ALA	N-CA-C	-6.43	104.19	111.07
2	B	469	ALA	N-CA-C	-6.36	104.27	111.07
1	A	208	ASN	N-CA-C	-6.16	105.59	113.23
2	B	356	ASP	N-CA-C	6.15	118.46	110.53
2	B	487	MET	N-CA-C	6.10	117.93	111.28
2	B	189	GLY	N-CA-C	-5.96	106.72	115.30
1	A	234	ALA	N-CA-C	5.94	119.59	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	GLU	N-CA-C	-5.94	104.88	111.36
1	A	239	ILE	N-CA-C	5.84	116.27	107.75
2	B	499	GLY	N-CA-C	5.82	119.72	112.73
2	B	299	ALA	N-CA-C	-5.79	104.97	111.28
2	B	491	GLY	N-CA-C	5.74	123.00	115.36
2	B	241	ASP	N-CA-C	-5.73	103.66	111.56
1	A	373	ILE	N-CA-C	5.72	116.44	108.89
2	B	90	PHE	N-CA-C	5.70	117.29	111.14
1	A	42	LEU	N-CA-C	5.68	118.49	109.96
2	B	117	VAL	N-CA-C	-5.61	100.50	108.58
1	A	492	VAL	N-CA-C	5.53	116.09	108.12
1	A	119	HIS	CA-C-N	5.46	126.67	119.84
1	A	119	HIS	C-N-CA	5.46	126.67	119.84
1	A	123	ILE	N-CA-C	-5.42	105.44	110.53
2	B	44	ARG	N-CA-C	-5.41	105.12	112.26
1	A	457	ILE	N-CA-C	5.39	116.02	110.36
2	B	60	THR	N-CA-C	5.39	116.17	108.74
1	A	222	LYS	N-CA-C	-5.32	103.00	110.50
1	A	340	VAL	N-CA-C	5.32	116.64	111.91
1	A	302	LEU	N-CA-C	-5.29	105.52	111.28
2	B	120	THR	N-CA-C	-5.22	105.03	111.40
1	A	203	ASN	N-CA-C	5.21	121.89	110.80
1	A	151	LEU	N-CA-C	-5.11	105.72	111.28
2	B	342	LEU	N-CA-C	5.09	117.85	109.76
2	B	277	MET	N-CA-C	-5.03	105.69	111.07

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	3784	884	3935	200	0
2	B	3798	858	3892	211	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	12	1	0
4	B	27	0	12	3	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	7648	1742	7851	399	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 26.

All (399) 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:218:ILE:HD11	1:A:321:LEU:HD11	1.22	1.11
2:B:172:LEU:HD22	2:B:389:ILE:HD11	1.46	0.96
1:A:281:LYS:HD2	1:A:305:GLU:HG3	1.48	0.95
2:B:50:LEU:HB2	2:B:58:VAL:HG13	1.48	0.93
2:B:64:VAL:HG22	2:B:95:THR:HG21	1.49	0.93
2:B:243:PRO:HD3	2:B:293:LYS:HD2	1.52	0.88
2:B:503:ILE:O	2:B:507:THR:HG23	1.75	0.87
1:A:69:LYS:HE2	1:A:86:LYS:HG2	1.56	0.86
2:B:152:LEU:HD11	2:B:400:LEU:HD13	1.60	0.83
2:B:421:ARG:HG3	2:B:421:ARG:HH11	1.45	0.82
2:B:489:LYS:HD3	2:B:490:ASN:HD22	1.45	0.81
2:B:30:ALA:HB1	2:B:80:MET:HE2	1.62	0.79
1:A:163:ASN:HD21	2:B:127:ARG:HH22	1.32	0.78
1:A:213:ILE:HG23	1:A:361:MET:HE3	1.65	0.77
2:B:425:GLN:OE1	2:B:426:LYS:HG3	1.84	0.77
2:B:48:LYS:HG3	2:B:66:ILE:HD13	1.66	0.76
1:A:51:LEU:HA	2:B:520:ILE:O	1.86	0.76
2:B:510:ALA:O	2:B:514:LEU:HB2	1.86	0.76
1:A:328:LYS:HB2	1:A:340:VAL:HB	1.68	0.75
1:A:512:ILE:HA	1:A:515:ILE:HD12	1.69	0.75
2:B:118:HIS:HD2	2:B:120:THR:H	1.35	0.75
2:B:409:GLY:O	2:B:477:ILE:HD12	1.87	0.75
1:A:17:ARG:HG3	1:A:519:ILE:HG12	1.69	0.74
2:B:185:GLU:HB2	2:B:192:TYR:CD1	2.22	0.73
1:A:478:LEU:HD23	1:A:478:LEU:H	1.53	0.73
1:A:51:LEU:HD11	1:A:67:ILE:HA	1.71	0.72
1:A:405:LEU:HD13	1:A:411:VAL:HG11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:O	1:A:136:LYS:HD3	1.89	0.71
1:A:156:LEU:HD13	1:A:172:ALA:HB2	1.71	0.71
1:A:51:LEU:HD23	2:B:520:ILE:HG13	1.71	0.71
2:B:201:VAL:HG11	2:B:358:MET:HE1	1.73	0.71
2:B:87:GLN:HG2	2:B:95:THR:HA	1.74	0.70
2:B:246:ILE:HD12	2:B:246:ILE:O	1.91	0.70
1:A:405:LEU:HD12	1:A:498:LYS:HG3	1.74	0.69
1:A:154:ILE:HD13	1:A:492:VAL:HG23	1.73	0.69
2:B:37:VAL:HG13	2:B:96:THR:HG23	1.75	0.69
2:B:458:ILE:O	2:B:462:LEU:HD22	1.94	0.68
1:A:406:TRP:O	1:A:411:VAL:HG23	1.94	0.68
1:A:75:HIS:ND1	1:A:76:PRO:HD2	2.09	0.68
1:A:486:MET:SD	1:A:491:VAL:HG21	2.34	0.67
1:A:261:LYS:HE2	1:A:261:LYS:HA	1.76	0.67
1:A:132:ASN:ND2	1:A:135:ARG:HH12	1.93	0.66
2:B:80:MET:O	2:B:83:VAL:HB	1.95	0.66
1:A:223:VAL:CG1	1:A:311:ARG:HG2	2.25	0.66
2:B:241:ASP:HB2	2:B:330:ILE:CG2	2.25	0.66
1:A:218:ILE:HD11	1:A:321:LEU:CD1	2.14	0.65
1:A:222:LYS:HD2	1:A:227:MET:HB2	1.78	0.65
2:B:83:VAL:O	2:B:86:THR:HG22	1.96	0.65
1:A:159:LEU:HD21	1:A:391:ALA:HB2	1.76	0.65
2:B:185:GLU:HB2	2:B:192:TYR:CE1	2.31	0.65
1:A:163:ASN:ND2	2:B:127:ARG:HH22	1.94	0.65
1:A:275:GLN:O	1:A:279:LYS:HG2	1.97	0.65
1:A:201:LYS:HB2	1:A:381:VAL:CG1	2.27	0.65
1:A:406:TRP:CH2	1:A:487:LYS:HD2	2.32	0.64
2:B:237:ILE:HD13	2:B:326:THR:HG21	1.79	0.64
1:A:245:ILE:HG12	1:A:273:PHE:CZ	2.31	0.64
2:B:65:THR:O	2:B:69:GLU:HB2	1.97	0.64
1:A:138:ILE:HD11	1:A:499:THR:CG2	2.27	0.64
1:A:204:GLY:HA3	1:A:374:ARG:NH1	2.12	0.64
1:A:218:ILE:CD1	1:A:321:LEU:HD11	2.14	0.63
1:A:51:LEU:CD2	2:B:520:ILE:HG13	2.28	0.63
1:A:213:ILE:HG12	1:A:359:PHE:HE2	1.63	0.63
1:A:352:ILE:HG21	1:A:372:LEU:HD21	1.81	0.62
1:A:231:VAL:HG12	1:A:234:ALA:HB2	1.81	0.62
2:B:64:VAL:HG22	2:B:95:THR:CG2	2.28	0.62
2:B:219:VAL:HB	2:B:359:THR:HG23	1.81	0.62
1:A:67:ILE:O	1:A:71:MET:HB2	1.99	0.62
2:B:460:ILE:HG23	2:B:484:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ILE:O	2:B:361:VAL:HG12	1.98	0.61
1:A:93:GLY:HA3	1:A:393:ARG:HD2	1.82	0.61
2:B:402:ASP:OD2	2:B:497:ARG:HB2	2.00	0.61
1:A:131:VAL:HB	1:A:506:VAL:HG21	1.83	0.61
1:A:417:MET:SD	1:A:468:GLU:HA	2.41	0.60
2:B:409:GLY:HA3	2:B:487:MET:HE3	1.82	0.60
2:B:445:ILE:HB	2:B:446:PRO:HD3	1.82	0.60
1:A:278:GLU:O	1:A:282:LYS:HG3	2.02	0.60
2:B:130:SER:HB2	2:B:507:THR:HG21	1.84	0.59
1:A:112:THR:HG22	1:A:116:GLN:HE21	1.66	0.59
2:B:512:MET:O	2:B:516:ILE:HG13	2.02	0.59
2:B:214:ILE:HG13	2:B:218:ILE:HD11	1.84	0.59
2:B:352:LYS:HG3	2:B:356:ASP:O	2.03	0.59
1:A:17:ARG:HB2	1:A:519:ILE:HG23	1.85	0.59
1:A:50:MET:HE2	1:A:58:ILE:HG21	1.83	0.59
1:A:291:GLN:OE1	1:A:315:LYS:HD3	2.03	0.59
1:A:286:ASN:C	1:A:307:ILE:HG23	2.28	0.58
2:B:137:ILE:HG22	2:B:496:ILE:HG13	1.84	0.58
2:B:144:ILE:HG12	2:B:405:TYR:HD2	1.67	0.58
1:A:205:GLY:O	1:A:206:SER:HB2	2.02	0.58
1:A:406:TRP:CZ3	1:A:487:LYS:HA	2.38	0.58
1:A:137:ILE:O	1:A:141:ILE:HG12	2.03	0.58
1:A:152:ARG:O	1:A:156:LEU:HD22	2.03	0.58
2:B:424:ALA:HB1	2:B:432:GLN:HG3	1.86	0.58
2:B:499:GLY:O	2:B:503:ILE:HG23	2.04	0.57
1:A:218:ILE:HG22	1:A:220:LYS:HB2	1.86	0.57
1:A:445:PRO:HB2	1:A:460:LEU:HD21	1.86	0.57
2:B:67:LEU:HD21	2:B:99:VAL:HG21	1.85	0.57
2:B:68:LYS:HG2	2:B:85:LYS:HE2	1.86	0.57
2:B:212:GLN:HG3	2:B:214:ILE:HD11	1.85	0.57
2:B:133:ALA:HB3	2:B:503:ILE:HD13	1.86	0.57
2:B:107:GLN:O	2:B:110:GLN:HB3	2.05	0.57
2:B:199:GLN:HB3	2:B:371:SER:OG	2.03	0.57
1:A:201:LYS:HB2	1:A:381:VAL:HG11	1.86	0.57
1:A:48:ASP:OD1	1:A:62:ASN:HB2	2.03	0.57
1:A:412:GLU:OE2	1:A:498:LYS:HE3	2.05	0.57
2:B:239:LEU:HD22	2:B:328:ALA:HB3	1.86	0.57
2:B:301:HIS:CE1	2:B:305:ARG:HD2	2.39	0.57
1:A:65:ALA:HB1	1:A:69:LYS:HE3	1.87	0.56
2:B:132:GLU:OE2	2:B:135:ARG:HD3	2.05	0.56
2:B:152:LEU:CD1	2:B:400:LEU:HD13	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:SER:HB2	1:A:386:ARG:NH1	2.20	0.56
1:A:289:LEU:HD23	1:A:321:LEU:HD13	1.88	0.56
2:B:347:ARG:CB	2:B:347:ARG:HH11	2.18	0.56
2:B:421:ARG:HG3	2:B:421:ARG:NH1	2.18	0.56
1:A:405:LEU:CD1	1:A:498:LYS:HG3	2.35	0.56
2:B:472:ASN:HB3	2:B:475:TYR:CD1	2.40	0.56
1:A:204:GLY:HA3	1:A:374:ARG:CZ	2.36	0.55
1:A:450:GLU:HG2	1:A:456:PRO:HG3	1.88	0.55
1:A:206:SER:HB3	1:A:209:ASP:HB2	1.88	0.55
2:B:222:GLU:HB2	2:B:350:GLN:OE1	2.06	0.55
2:B:399:ALA:HB2	2:B:495:PRO:HG3	1.88	0.55
2:B:27:ILE:O	2:B:31:ILE:HG13	2.06	0.55
1:A:58:ILE:HD13	2:B:79:MET:SD	2.47	0.55
2:B:140:ILE:HG21	2:B:415:GLU:HG2	1.88	0.55
1:A:235:LYS:HE2	1:A:341:LEU:HD12	1.89	0.55
2:B:87:GLN:HE22	2:B:502:ALA:N	2.05	0.55
1:A:486:MET:HB3	1:A:491:VAL:HG22	1.89	0.54
1:A:510:THR:O	1:A:514:ARG:HG3	2.08	0.54
2:B:64:VAL:HA	2:B:84:SER:OG	2.06	0.54
2:B:118:HIS:CD2	2:B:120:THR:H	2.20	0.54
1:A:196:ASN:HD21	1:A:323:LYS:HE2	1.72	0.54
1:A:206:SER:C	1:A:208:ASN:H	2.16	0.54
1:A:192:VAL:HG21	1:A:396:ALA:HB1	1.89	0.54
2:B:292:GLN:HE22	2:B:316:LYS:HD3	1.73	0.54
2:B:236:LYS:H	2:B:287:ASN:HB2	1.72	0.54
2:B:292:GLN:O	2:B:313:ARG:HA	2.08	0.54
2:B:241:ASP:HB2	2:B:330:ILE:HG22	1.89	0.54
2:B:511:ILE:O	2:B:515:ARG:HG3	2.07	0.53
2:B:195:PHE:C	2:B:197:ASN:H	2.16	0.53
1:A:201:LYS:HD2	1:A:381:VAL:HG12	1.89	0.53
2:B:292:GLN:NE2	2:B:316:LYS:HD3	2.23	0.53
1:A:281:LYS:CD	1:A:305:GLU:HG3	2.31	0.53
2:B:200:VAL:HG13	2:B:372:ILE:HB	1.90	0.53
1:A:17:ARG:HH21	1:A:19:GLN:HG3	1.73	0.53
2:B:232:VAL:HG22	2:B:348:VAL:HB	1.91	0.53
1:A:50:MET:HE2	1:A:58:ILE:CG2	2.39	0.52
1:A:223:VAL:HG12	1:A:311:ARG:HG2	1.90	0.52
1:A:144:LYS:O	1:A:145:SER:HB2	2.08	0.52
1:A:200:ASP:O	1:A:373:ILE:HG13	2.09	0.52
1:A:427:GLY:O	1:A:431:GLN:HB2	2.09	0.52
1:A:486:MET:SD	1:A:491:VAL:CG2	2.96	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ALA:HB1	2:B:172:LEU:CD1	2.40	0.52
1:A:486:MET:HB3	1:A:491:VAL:CG2	2.40	0.52
1:A:233:ASN:N	1:A:345:GLU:O	2.39	0.52
1:A:127:TYR:O	1:A:131:VAL:HG12	2.10	0.52
2:B:366:ASN:ND2	2:B:368:LYS:H	2.07	0.52
1:A:138:ILE:HD11	1:A:499:THR:HG22	1.91	0.52
2:B:347:ARG:HH11	2:B:347:ARG:CG	2.22	0.52
2:B:432:GLN:O	2:B:436:GLU:HG3	2.09	0.52
2:B:446:PRO:HB2	2:B:461:LEU:HD21	1.91	0.52
2:B:241:ASP:HB3	2:B:332:SER:OG	2.10	0.51
1:A:192:VAL:CG2	1:A:396:ALA:HB1	2.41	0.51
1:A:227:MET:HE1	1:A:309:ALA:HB3	1.92	0.51
1:A:426:VAL:HG12	1:A:427:GLY:N	2.26	0.51
2:B:245:GLU:HA	2:B:274:LEU:HD21	1.92	0.51
2:B:334:ILE:HD12	2:B:334:ILE:H	1.75	0.51
1:A:174:LEU:HD22	1:A:212:PHE:HB2	1.92	0.51
1:A:192:VAL:HG23	1:A:192:VAL:O	2.11	0.51
1:A:291:GLN:HB2	1:A:318:MET:HG3	1.92	0.51
2:B:239:LEU:HD22	2:B:328:ALA:CB	2.41	0.51
2:B:338:SER:O	2:B:341:ASP:HB2	2.11	0.51
2:B:346:GLU:HB2	2:B:363:GLY:HA3	1.93	0.51
1:A:31:ALA:O	1:A:34:ILE:HG22	2.12	0.50
1:A:166:LEU:HD22	1:A:166:LEU:N	2.26	0.50
1:A:177:LYS:HD3	1:A:212:PHE:CD2	2.46	0.50
2:B:237:ILE:HG22	2:B:239:LEU:HD13	1.91	0.50
1:A:44:PRO:O	1:A:161:GLY:HA2	2.10	0.50
1:A:213:ILE:HG12	1:A:359:PHE:CE2	2.46	0.50
1:A:255:GLN:NE2	2:B:256:ARG:HB2	2.26	0.50
1:A:406:TRP:O	1:A:410:ALA:HB3	2.10	0.50
2:B:47:ASP:OD1	2:B:61:ASN:HB2	2.12	0.50
2:B:490:ASN:HD22	2:B:490:ASN:N	2.08	0.50
1:A:138:ILE:CG2	1:A:415:LEU:HD11	2.42	0.50
2:B:62:ASP:O	2:B:66:ILE:HG13	2.11	0.50
1:A:377:THR:O	1:A:378:ASP:HB2	2.12	0.50
1:A:25:ARG:O	1:A:29:GLU:HG2	2.12	0.50
1:A:224:HIS:CE1	1:A:226:LYS:HB2	2.47	0.50
2:B:290:ILE:O	2:B:319:MET:HE1	2.11	0.50
2:B:328:ALA:HB2	2:B:343:GLY:HA3	1.93	0.50
1:A:422:TYR:O	1:A:426:VAL:HG23	2.11	0.50
2:B:50:LEU:HB2	2:B:58:VAL:CG1	2.32	0.50
2:B:331:VAL:HG21	2:B:337:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ILE:HB	1:A:445:PRO:HD3	1.94	0.49
2:B:134:LYS:HG3	2:B:503:ILE:HD11	1.94	0.49
2:B:456:ASP:O	2:B:460:ILE:HG12	2.12	0.49
2:B:423:TYR:HA	2:B:426:LYS:HD2	1.95	0.49
1:A:146:THR:HG22	1:A:402:GLY:HA2	1.94	0.49
1:A:253:LYS:HB2	1:A:253:LYS:NZ	2.27	0.49
1:A:198:LYS:O	1:A:370:SER:HA	2.11	0.49
1:A:371:ILE:HD12	1:A:392:ILE:HD11	1.93	0.49
1:A:397:ILE:HG12	1:A:496:ARG:NH2	2.28	0.49
2:B:58:VAL:HG11	2:B:69:GLU:HG2	1.93	0.49
1:A:305:GLU:OE1	1:A:305:GLU:HA	2.12	0.49
1:A:73:VAL:HG21	1:A:82:VAL:HG21	1.95	0.48
2:B:237:ILE:CG2	2:B:239:LEU:HD13	2.43	0.48
1:A:41:THR:HB	1:A:62:ASN:ND2	2.28	0.48
2:B:64:VAL:CG2	2:B:95:THR:HG21	2.32	0.48
2:B:274:LEU:HD22	2:B:299:ALA:HB2	1.95	0.48
2:B:423:TYR:CZ	2:B:427:ILE:HG13	2.48	0.48
2:B:441:ALA:O	2:B:444:GLU:HG2	2.13	0.48
1:A:51:LEU:HD13	1:A:70:GLU:HB2	1.95	0.48
1:A:261:LYS:HE2	1:A:261:LYS:CA	2.41	0.48
2:B:67:LEU:HB3	2:B:81:VAL:HG13	1.96	0.48
1:A:128:ARG:HG3	1:A:132:ASN:OD1	2.14	0.48
1:A:51:LEU:CD1	1:A:70:GLU:HB2	2.44	0.48
2:B:165:ALA:HB1	2:B:172:LEU:HD12	1.96	0.48
2:B:296:ASP:O	2:B:300:GLN:HG3	2.14	0.48
2:B:325:ALA:O	2:B:366:ASN:HB3	2.14	0.48
1:A:138:ILE:HD11	1:A:499:THR:HG23	1.95	0.47
1:A:210:THR:HG23	1:A:373:ILE:HA	1.96	0.47
1:A:443:ILE:HD13	1:A:443:ILE:O	2.15	0.47
2:B:34:SER:HA	2:B:99:VAL:HG12	1.97	0.47
1:A:405:LEU:HB3	1:A:411:VAL:CG2	2.44	0.47
2:B:64:VAL:HG21	2:B:88:ASP:OD1	2.13	0.47
1:A:278:GLU:HG2	1:A:282:LYS:HD2	1.97	0.47
1:A:463:LEU:HD11	1:A:474:VAL:O	2.15	0.47
1:A:475:GLY:C	1:A:486:MET:HE3	2.40	0.47
1:A:477:ASP:HB3	1:A:480:ASN:HB2	1.96	0.47
2:B:137:ILE:HG12	2:B:416:ILE:HD11	1.95	0.47
2:B:337:ILE:HG23	2:B:337:ILE:O	2.14	0.47
1:A:405:LEU:HD13	1:A:411:VAL:CG1	2.44	0.47
1:A:477:ASP:HB2	1:A:484:GLY:HA3	1.97	0.47
2:B:513:ILE:HA	2:B:516:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:CB	1:A:506:VAL:HG21	2.45	0.47
1:A:351:LYS:HE3	1:A:353:GLY:O	2.15	0.47
2:B:152:LEU:HD11	2:B:400:LEU:CD1	2.38	0.47
2:B:158:THR:HG23	4:B:998:ADP:C8	2.50	0.47
2:B:407:ALA:O	2:B:412:THR:HG22	2.14	0.47
2:B:136:VAL:O	2:B:140:ILE:HG12	2.14	0.47
1:A:217:VAL:HG22	1:A:357:MET:HE2	1.96	0.46
1:A:471:ARG:HB3	1:A:474:VAL:HG23	1.97	0.46
2:B:185:GLU:HB2	2:B:192:TYR:HD1	1.75	0.46
1:A:78:ALA:O	1:A:82:VAL:HG23	2.15	0.46
1:A:130:ALA:HB2	1:A:434:ILE:HG23	1.96	0.46
2:B:221:LYS:HG3	2:B:314:VAL:HG22	1.97	0.46
2:B:492:VAL:HG23	2:B:492:VAL:O	2.14	0.46
1:A:405:LEU:HB3	1:A:411:VAL:HG22	1.97	0.46
2:B:487:MET:HE3	2:B:492:VAL:HG21	1.98	0.46
1:A:256:ILE:HG23	1:A:261:LYS:HB2	1.97	0.46
2:B:51:VAL:HG13	2:B:57:ILE:HG12	1.95	0.46
2:B:199:GLN:O	2:B:371:SER:HA	2.14	0.46
1:A:69:LYS:HG2	1:A:86:LYS:HD3	1.97	0.46
1:A:154:ILE:HD13	1:A:492:VAL:CG2	2.44	0.46
2:B:132:GLU:O	2:B:136:VAL:HG23	2.16	0.46
2:B:315:LYS:HD2	2:B:317:SER:OG	2.15	0.46
1:A:291:GLN:HB2	1:A:318:MET:HE2	1.98	0.46
2:B:149:LYS:HD2	2:B:177:TYR:CE2	2.50	0.46
2:B:366:ASN:HD22	2:B:366:ASN:C	2.23	0.46
1:A:94:ASP:OD1	4:A:898:ADP:O2B	2.34	0.46
1:A:308:TYR:OH	1:A:349:GLU:HB2	2.16	0.46
1:A:235:LYS:HB3	1:A:341:LEU:HD13	1.98	0.46
1:A:145:SER:HB3	1:A:404:PHE:HE2	1.81	0.45
1:A:224:HIS:HE1	1:A:226:LYS:HB2	1.80	0.45
2:B:67:LEU:HD23	2:B:84:SER:OG	2.16	0.45
2:B:207:ALA:O	2:B:210:ASP:HB2	2.16	0.45
2:B:278:VAL:HG21	2:B:302:TYR:HB2	1.99	0.45
1:A:222:LYS:HE2	1:A:227:MET:O	2.17	0.45
1:A:294:ILE:HG13	1:A:311:ARG:HB3	1.99	0.45
1:A:491:VAL:HG23	1:A:491:VAL:O	2.16	0.45
1:A:50:MET:O	2:B:519:VAL:HA	2.16	0.45
1:A:409:GLY:CA	1:A:445:PRO:HG3	2.46	0.45
2:B:370:VAL:HG22	2:B:371:SER:N	2.32	0.45
1:A:222:LYS:CD	1:A:227:MET:HB2	2.46	0.45
2:B:79:MET:HE3	2:B:79:MET:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:HIS:CD2	2:B:120:THR:OG1	2.70	0.45
2:B:217:ILE:O	2:B:361:VAL:CG1	2.65	0.45
1:A:20:GLY:N	1:A:516:ASP:O	2.50	0.45
1:A:84:VAL:HG12	1:A:508:VAL:HG21	1.99	0.45
2:B:408:GLY:O	2:B:487:MET:HG3	2.17	0.44
1:A:269:GLU:O	1:A:272:THR:HB	2.17	0.44
2:B:147:ASP:O	2:B:148:GLU:C	2.59	0.44
1:A:186:ARG:O	1:A:188:GLY:N	2.51	0.44
1:A:446:ARG:HB2	1:A:460:LEU:HD11	1.99	0.44
2:B:219:VAL:HB	2:B:359:THR:CG2	2.46	0.44
1:A:18:GLU:O	1:A:517:ASP:HA	2.17	0.44
1:A:266:LEU:HD12	2:B:249:PRO:HG3	1.99	0.44
2:B:290:ILE:HG12	2:B:311:VAL:HG22	1.99	0.44
2:B:218:ILE:HG22	2:B:358:MET:HE2	2.00	0.44
1:A:382:SER:O	1:A:385:GLU:HB3	2.17	0.44
2:B:489:LYS:HD3	2:B:490:ASN:ND2	2.22	0.44
2:B:68:LYS:HE3	2:B:85:LYS:HG2	2.00	0.44
2:B:93:ASP:O	2:B:498:VAL:HG13	2.17	0.44
2:B:472:ASN:O	2:B:474:THR:N	2.51	0.44
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.82	0.43
2:B:23:MET:SD	2:B:113:ILE:HD13	2.58	0.43
2:B:395:VAL:O	2:B:396:VAL:C	2.58	0.43
1:A:253:LYS:HB2	1:A:253:LYS:HZ3	1.82	0.43
2:B:224:VAL:HG12	2:B:228:MET:SD	2.58	0.43
2:B:211:THR:HG23	2:B:374:VAL:HA	2.00	0.43
1:A:201:LYS:HA	1:A:373:ILE:O	2.18	0.43
1:A:406:TRP:CZ2	1:A:487:LYS:HD2	2.53	0.43
1:A:167:SER:O	1:A:170:PHE:N	2.51	0.43
2:B:477:ILE:O	4:B:998:ADP:H2	2.01	0.43
1:A:56:GLY:O	1:A:57:ASP:HB2	2.17	0.43
2:B:152:LEU:HD23	2:B:152:LEU:HA	1.82	0.43
2:B:352:LYS:HD3	2:B:357:TYR:CZ	2.54	0.43
1:A:57:ASP:HB3	1:A:58:ILE:H	1.59	0.43
2:B:77:ALA:O	2:B:81:VAL:HG23	2.19	0.43
2:B:137:ILE:HG22	2:B:496:ILE:CG1	2.49	0.43
2:B:366:ASN:ND2	2:B:366:ASN:C	2.77	0.43
1:A:58:ILE:HD11	2:B:75:PRO:HA	2.00	0.43
1:A:98:THR:O	1:A:102:LEU:HB2	2.19	0.43
1:A:186:ARG:HG3	1:A:191:ILE:HD11	2.00	0.43
2:B:212:GLN:HG3	2:B:214:ILE:CD1	2.49	0.43
2:B:240:LEU:O	2:B:319:MET:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:VAL:HG22	2:B:339:SER:CA	2.49	0.43
2:B:30:ALA:HB1	2:B:80:MET:CE	2.43	0.43
2:B:240:LEU:HA	2:B:331:VAL:O	2.19	0.43
1:A:266:LEU:CD1	2:B:249:PRO:HG3	2.49	0.42
1:A:474:VAL:HA	1:A:484:GLY:O	2.19	0.42
2:B:244:LEU:O	2:B:245:GLU:HG3	2.19	0.42
1:A:183:ALA:HB2	1:A:192:VAL:HG12	1.99	0.42
1:A:288:VAL:HG23	1:A:307:ILE:HG21	2.01	0.42
1:A:455:ASP:HA	1:A:456:PRO:HD3	1.80	0.42
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.84	0.42
1:A:17:ARG:CG	1:A:519:ILE:HG12	2.45	0.42
1:A:477:ASP:N	1:A:482:GLY:O	2.52	0.42
1:A:186:ARG:HG3	1:A:191:ILE:CD1	2.49	0.42
2:B:130:SER:CB	2:B:507:THR:HG21	2.48	0.42
2:B:469:ALA:C	2:B:471:GLY:H	2.27	0.42
2:B:232:VAL:HG23	2:B:235:ALA:HB2	2.02	0.42
2:B:430:ARG:HA	2:B:433:LEU:HD13	2.01	0.42
1:A:138:ILE:HA	1:A:141:ILE:HG12	2.02	0.42
1:A:277:VAL:HG21	1:A:301:TYR:HB2	2.00	0.42
2:B:106:LEU:HD12	2:B:106:LEU:HA	1.86	0.42
2:B:133:ALA:O	2:B:137:ILE:HG13	2.20	0.42
2:B:228:MET:HE1	2:B:310:ALA:HB3	2.02	0.42
2:B:297:ASP:O	2:B:300:GLN:HB2	2.19	0.42
1:A:376:GLY:O	1:A:377:THR:C	2.63	0.42
2:B:457:PRO:O	2:B:461:LEU:HB2	2.20	0.42
1:A:19:GLN:HG2	1:A:517:ASP:CG	2.45	0.42
1:A:58:ILE:HG21	2:B:79:MET:SD	2.59	0.42
1:A:128:ARG:HH22	1:A:503:GLU:CD	2.28	0.42
2:B:50:LEU:HD13	2:B:69:GLU:HG2	2.02	0.42
2:B:484:ILE:HD12	2:B:484:ILE:N	2.35	0.42
2:B:487:MET:SD	2:B:492:VAL:HG22	2.60	0.42
1:A:197:ILE:HG21	1:A:392:ILE:HD13	2.02	0.41
1:A:327:ALA:HB2	1:A:342:GLY:N	2.35	0.41
1:A:376:GLY:O	1:A:378:ASP:N	2.53	0.41
2:B:91:VAL:HG21	2:B:498:VAL:HA	2.01	0.41
1:A:203:ASN:O	1:A:204:GLY:C	2.63	0.41
2:B:221:LYS:O	2:B:359:THR:HG22	2.19	0.41
1:A:69:LYS:CE	1:A:86:LYS:HG2	2.40	0.41
1:A:243:LEU:HD11	1:A:280:ILE:HD11	2.02	0.41
1:A:397:ILE:HD13	1:A:397:ILE:HG21	1.80	0.41
1:A:167:SER:O	1:A:170:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HG23	1:A:348:GLU:HB3	2.02	0.41
1:A:242:ALA:HB2	1:A:292:LYS:HB3	2.02	0.41
1:A:324:ALA:O	1:A:363:CYS:HB3	2.20	0.41
2:B:48:LYS:CG	2:B:66:ILE:HD13	2.46	0.41
2:B:215:ASN:O	2:B:362:THR:HG23	2.20	0.41
2:B:88:ASP:HB2	2:B:95:THR:HG21	2.02	0.41
2:B:97:THR:HG22	2:B:502:ALA:HB1	2.02	0.41
2:B:195:PHE:C	2:B:197:ASN:N	2.78	0.41
2:B:442:ILE:C	2:B:444:GLU:H	2.27	0.41
2:B:443:GLU:C	2:B:446:PRO:HD2	2.46	0.41
2:B:144:ILE:HG12	2:B:405:TYR:CD2	2.51	0.41
2:B:298:MET:HG3	2:B:302:TYR:CE2	2.56	0.41
2:B:352:LYS:HD2	2:B:355:GLU:O	2.19	0.41
2:B:391:ASP:O	2:B:395:VAL:HG23	2.19	0.41
2:B:440:ASP:O	2:B:443:GLU:HB2	2.21	0.41
2:B:450:ALA:HA	2:B:455:LEU:HD12	2.03	0.41
2:B:236:LYS:H	2:B:287:ASN:CB	2.33	0.41
1:A:44:PRO:C	1:A:46:GLY:H	2.28	0.41
2:B:94:GLY:HA2	4:B:998:ADP:O3B	2.20	0.41
1:A:177:LYS:HD3	1:A:212:PHE:CE2	2.55	0.41
2:B:64:VAL:HG21	2:B:88:ASP:CG	2.46	0.41
2:B:118:HIS:HD2	2:B:120:THR:N	2.11	0.41
2:B:204:GLN:HA	2:B:376:GLY:O	2.21	0.41
2:B:284:VAL:CG2	2:B:339:SER:N	2.83	0.41
2:B:290:ILE:HD13	2:B:322:LEU:CD1	2.50	0.41
2:B:303:LEU:HD13	2:B:310:ALA:CB	2.51	0.41
2:B:334:ILE:HD12	2:B:334:ILE:N	2.34	0.41
2:B:272:ASN:O	2:B:276:GLU:HG3	2.20	0.41
1:A:119:HIS:HA	1:A:120:PRO:HD3	2.00	0.40
1:A:133:GLU:OE1	1:A:133:GLU:HA	2.20	0.40
1:A:478:LEU:H	1:A:478:LEU:CD2	2.28	0.40
2:B:24:LYS:NZ	2:B:24:LYS:HB3	2.36	0.40
2:B:390:THR:HG22	2:B:394:HIS:HD2	1.86	0.40
2:B:489:LYS:C	2:B:491:GLY:H	2.30	0.40
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.85	0.40
1:A:189:LYS:HD2	1:A:189:LYS:O	2.21	0.40
2:B:195:PHE:HA	2:B:198:ILE:HD12	2.04	0.40
2:B:203:LYS:HG2	2:B:353:VAL:HG12	2.04	0.40
2:B:281:ILE:O	2:B:284:VAL:HG12	2.22	0.40
1:A:42:LEU:HD23	1:A:447:THR:CG2	2.52	0.40
1:A:53:ASP:OD1	1:A:57:ASP:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:ASN:HA	2:B:370:VAL:HG23	2.04	0.40
2:B:236:LYS:HB3	2:B:342:LEU:HD23	2.03	0.40
2:B:420:LEU:HA	2:B:420:LEU:HD23	1.86	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	501/545 (92%)	450 (90%)	41 (8%)	10 (2%)	6	31
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	43	73
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	11	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	145	SER
1	A	377	THR
1	A	378	ASP
1	A	160	SER
1	A	206	SER
1	A	207	VAL
2	B	473	LYS
1	A	203	ASN
1	A	427	GLY
1	A	375	GLY

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	411/442 (93%)	376 (92%)	35 (8%)	10	37
2	B	410/446 (92%)	362 (88%)	48 (12%)	5	23
All	All	821/888 (92%)	738 (90%)	83 (10%)	7	30

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	40	THR
1	A	52	VAL
1	A	57	ASP
1	A	59	ILE
1	A	84	VAL
1	A	92	VAL
1	A	102	LEU
1	A	120	PRO
1	A	122	VAL
1	A	135	ARG
1	A	143	GLU
1	A	156	LEU
1	A	162	LYS
1	A	166	LEU
1	A	189	LYS
1	A	194	THR
1	A	223	VAL
1	A	230	VAL
1	A	240	ASP
1	A	249	GLU
1	A	251	GLU
1	A	253	LYS
1	A	305	GLU
1	A	311	ARG
1	A	333	LEU
1	A	361	MET

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Mol	Chain	Res	Type
1	A	380	VAL
1	A	388	LEU
1	A	443	ILE
1	A	466	ASP
1	A	467	ASP
1	A	496	ARG
1	A	513	LEU
1	A	516	ASP
2	B	24	LYS
2	B	37	VAL
2	B	49	MET
2	B	51	VAL
2	B	54	LEU
2	B	58	VAL
2	B	67	LEU
2	B	79	MET
2	B	86	THR
2	B	105	LEU
2	B	106	LEU
2	B	113	ILE
2	B	131	GLU
2	B	153	LEU
2	B	161	ASN
2	B	163	LYS
2	B	178	GLU
2	B	192	TYR
2	B	200	VAL
2	B	203	LYS
2	B	209	ASP
2	B	239	LEU
2	B	248	LYS
2	B	250	GLU
2	B	255	LEU
2	B	269	GLN
2	B	305	ARG
2	B	339	SER
2	B	340	SER
2	B	342	LEU
2	B	344	THR
2	B	347	ARG
2	B	352	LYS
2	B	361	VAL

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Mol	Chain	Res	Type
2	B	391	ASP
2	B	396	VAL
2	B	412	THR
2	B	425	GLN
2	B	461	LEU
2	B	462	LEU
2	B	489	LYS
2	B	501	GLN
2	B	503	ILE
2	B	507	THR
2	B	513	ILE
2	B	514	LEU
2	B	519	VAL
2	B	520	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	27	ASN
1	A	109	GLN
1	A	116	GLN
1	A	163	ASN
1	A	180	ASN
1	A	196	ASN
1	A	208	ASN
1	A	233	ASN
1	A	255	GLN
1	A	267	ASN
1	A	275	GLN
1	A	299	GLN
1	A	389	ASN
1	A	424	ASN
1	A	431	GLN
1	A	451	ASN
1	A	480	ASN
2	B	26	ASN
2	B	35	ASN
2	B	87	GLN
2	B	108	GLN
2	B	118	HIS
2	B	272	ASN

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Mol	Chain	Res	Type
2	B	300	GLN
2	B	301	HIS
2	B	366	ASN
2	B	394	HIS
2	B	432	GLN
2	B	490	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
4	ADP	A	898	3,5	28,29,29	1.43	4 (14%)	43,45,45	2.07	9 (20%)
5	AF3	B	999	6,4	0,3,3	-	-	-		
5	AF3	A	899	6,4	0,3,3	-	-	-		
4	ADP	B	998	3,5	28,29,29	1.33	4 (14%)	43,45,45	2.05	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	898	3,5	-	6/16/32/32	0/3/3/3
4	ADP	B	998	3,5	-	2/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C5-N7	-4.35	1.31	1.39
4	B	998	ADP	C5-N7	-3.95	1.31	1.39
4	A	898	ADP	C4-N9	-2.89	1.31	1.37
4	B	998	ADP	C4-N9	-2.84	1.31	1.37
4	A	898	ADP	PB-O2B	2.82	1.65	1.54
4	B	998	ADP	PB-O2B	2.69	1.64	1.54
4	B	998	ADP	C8-N9	-2.58	1.33	1.37
4	A	898	ADP	C8-N9	-2.35	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	ADP	N3-C2-N1	-6.06	119.41	128.58
4	A	898	ADP	N3-C2-N1	-5.81	119.79	128.58
4	A	898	ADP	C5-C4-N3	-5.51	119.13	126.72
4	B	998	ADP	C5-C4-N3	-5.49	119.16	126.72
4	B	998	ADP	C2-N3-C4	4.49	122.80	111.83
4	A	898	ADP	C2-N3-C4	4.22	122.14	111.83
4	B	998	ADP	N3-C4-N9	3.93	133.85	127.17
4	A	898	ADP	N3-C4-N9	3.90	133.80	127.17
4	B	998	ADP	N9-C8-N7	-3.71	108.67	113.94
4	A	898	ADP	N9-C8-N7	-3.62	108.80	113.94
4	A	898	ADP	C5-N7-C8	3.51	108.96	103.45
4	A	898	ADP	O4'-C1'-N9	3.45	114.71	108.09
4	A	898	ADP	C4-C5-N7	-3.42	106.67	110.58
4	B	998	ADP	C5-N7-C8	3.38	108.77	103.45
4	B	998	ADP	C4-C5-N7	-3.29	106.82	110.58
4	B	998	ADP	C4-N9-C8	2.87	108.75	105.74
4	A	898	ADP	C4-N9-C8	2.62	108.49	105.74
4	B	998	ADP	O3B-PB-O3A	2.03	111.45	104.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

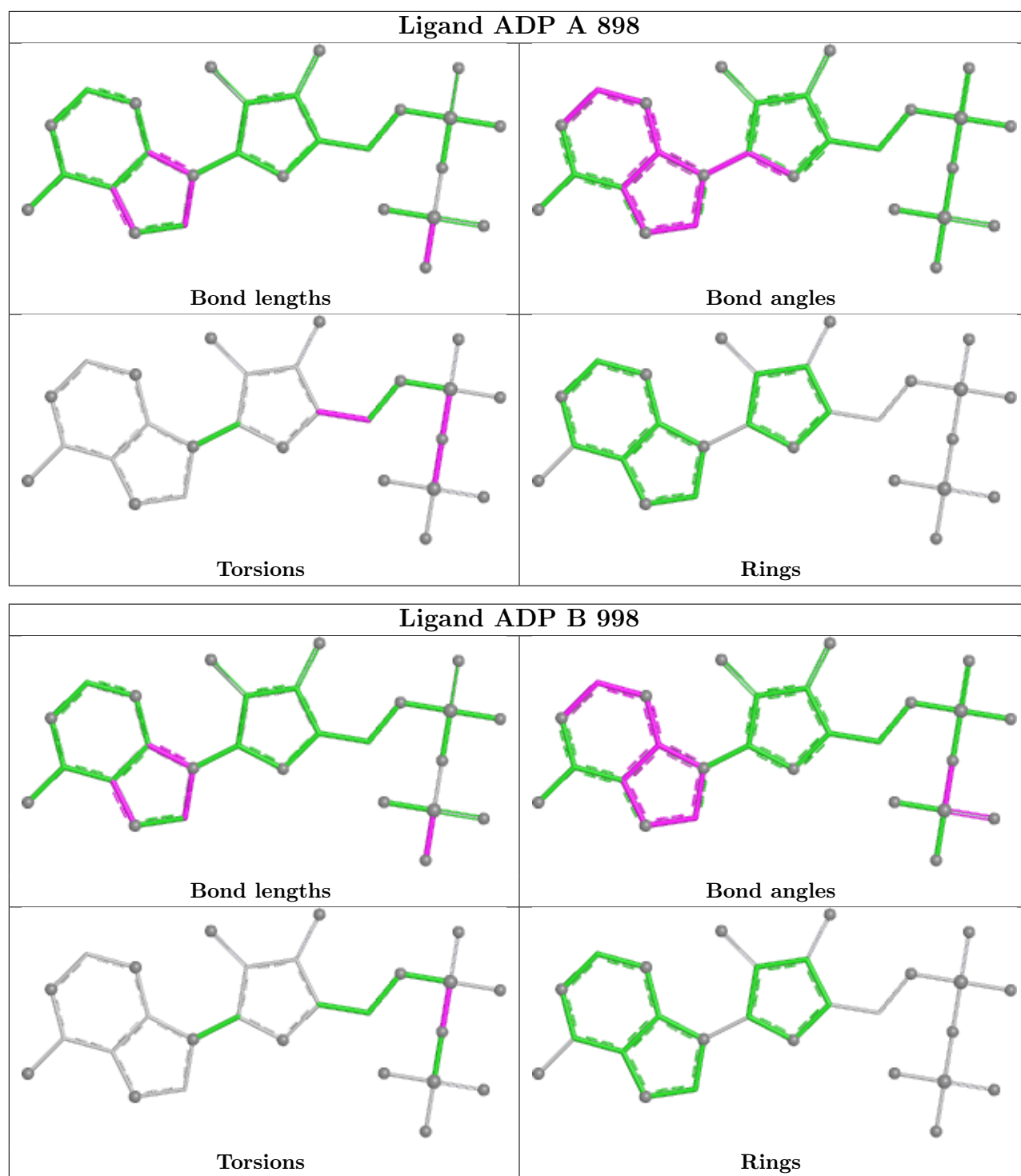
Mol	Chain	Res	Type	Atoms
4	A	898	ADP	PA-O3A-PB-O2B
4	A	898	ADP	C3'-C4'-C5'-O5'
4	A	898	ADP	PA-O3A-PB-O1B
4	A	898	ADP	PA-O3A-PB-O3B
4	B	998	ADP	PB-O3A-PA-O1A
4	A	898	ADP	O4'-C4'-C5'-O5'
4	A	898	ADP	PB-O3A-PA-O2A
4	B	998	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	898	ADP	1	0
4	B	998	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.