



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 06:41 pm GMT

PDB ID : 1A6E  
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)

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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

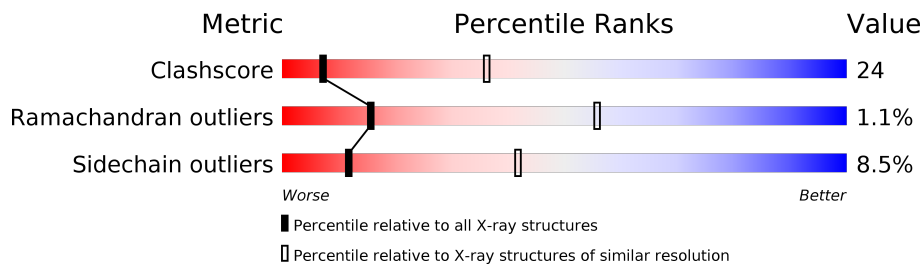
# 1 Overall quality at a glance

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	122078	1092 (3.20-3.20)
Ramachandran outliers	120005	1075 (3.20-3.20)
Sidechain outliers	119972	1074 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

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 (three-letter code: MG) (formula: Mg).

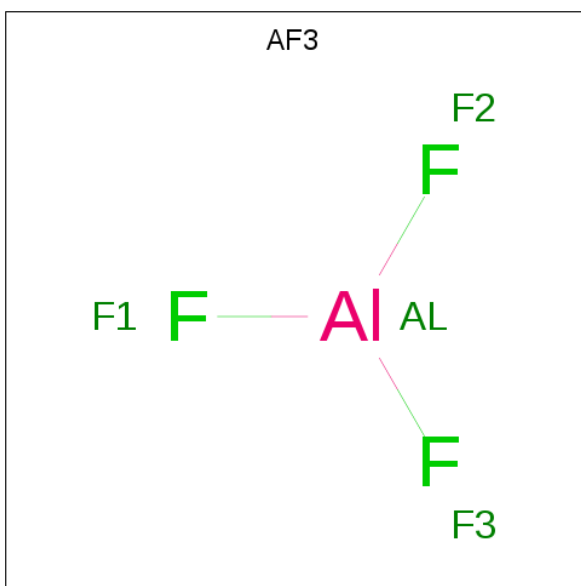
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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 (three-letter code: AF3) (formula:  $\text{AlF}_3$ ).



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

- Molecule 6 is water.

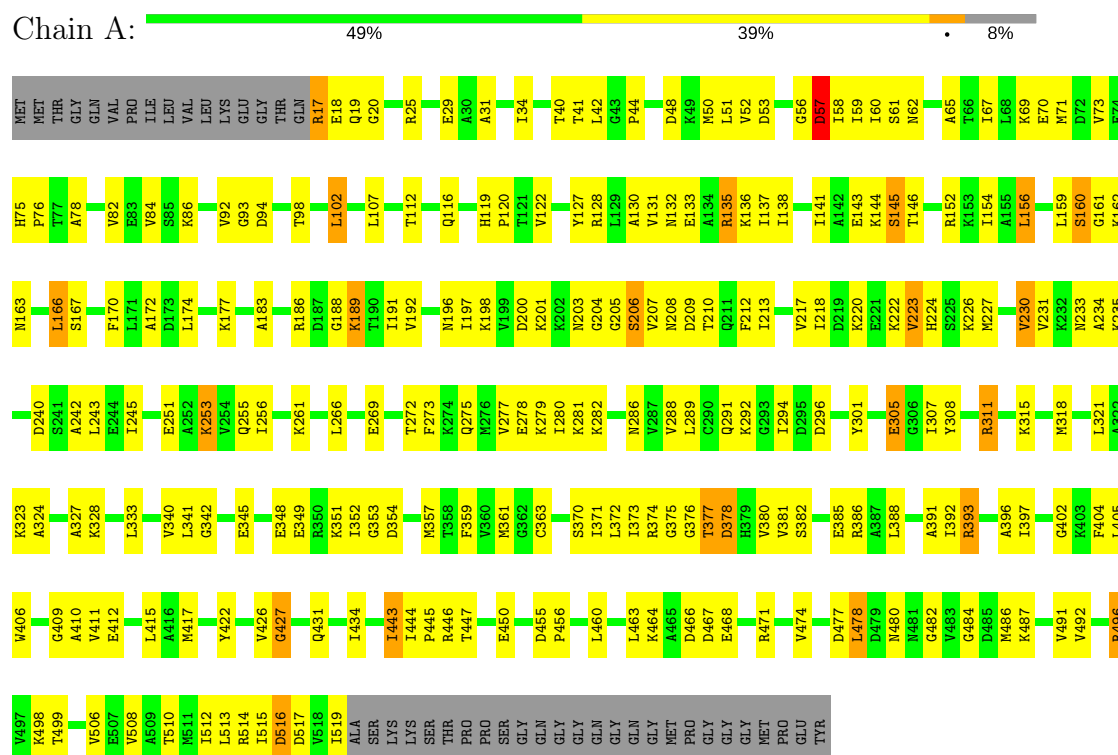
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

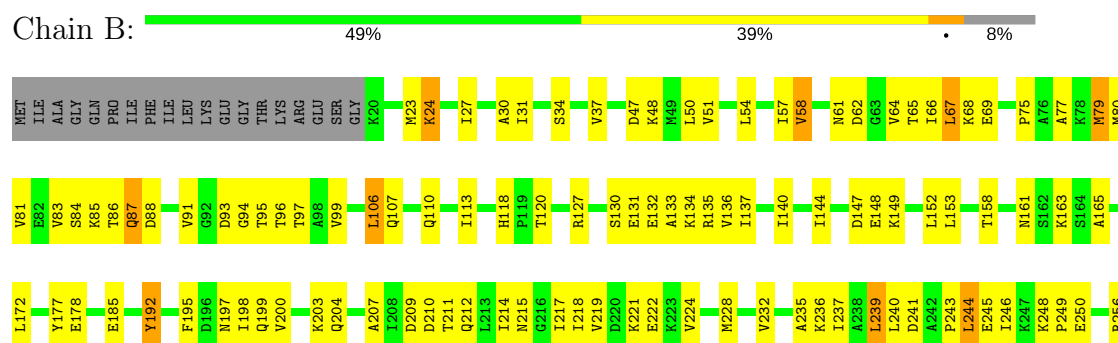
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: THERMOSOME (ALPHA SUBUNIT)



#### • Molecule 2: THERMOSOME (BETA SUBUNIT)



I511	A424	E346	N272
M512	Q425	R347	N273
I513	K426	V348	L274
I514	I427	E349	E275
R515	R430	Q350	E276
I516	Q431	V351	N277
	Q432	K352	V278
V519	L433	G354	
I520	E436	E355	I281
A521		D356	V284
THR	LYS	Y357	
LYS	D440	N358	N287
SER	A441	T359	
SER	I442	F360	I290
SER	E443	V361	T291
SER	E444	T362	Q292
SER	I445	G363	K293
SER	P446		
ASN		N366	D296
PRO	A450	P367	D297
LYS		K368	N298
LYS	L455	A369	A299
SER	D456	V370	Q300
GLY	P457	S371	H301
SER	I458	L372	Y302
SER	D459	L373	L303
SER	T460	V374	S304
GLU	L461	R375	R305
SER	L462	G376	
SER		I389	A310
GLU	N472	T390	V311
ASP	K473	D391	R312
	T474		R313
	Y475	H394	V314
	G476	V395	K315
	I477	V396	K316
			S317
	I484		
		A399	L322
	N487	L400	
	V488	E401	A325
	K489	D402	T326
	N490		G327
	G491	Y405	A328
	V492	A406	S329
		A407	I330
	P495	G408	V331
	I496	G409	S332
	R497		T333
	V498	T412	I334
	G499		
	K500	E415	I337
	Q501	I416	S338
	A502		S339
	I503	L420	S340
		R421	D341
	T507	S422	L342
			G343
	A510		

## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: MG, ADP, AF3

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	0.49	0/3812	0.74	2/5139 (0.0%)
2	B	0.52	0/3834	0.74	1/5166 (0.0%)
All	All	0.50	0/7646	0.74	3/10305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	244	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	57	ASP	N-CA-C	5.18	125.00	111.00
1	A	160	SER	N-CA-C	5.15	124.91	111.00

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	3784	884	3935	191	0
2	B	3798	858	3892	195	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	374	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 24.

All (374) 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
1:A:163:ASN:HD21	2:B:127:ARG:HH22	1.32	0.78
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:H	1:A:478:LEU:HD23	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
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:87:GLN:HG2	2:B:95:THR:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:37:VAL:HG13	2:B:96:THR:HG23	1.75	0.69
1:A:154:ILE:HD13	1:A:492:VAL:HG23	1.73	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:275:GLN:O	1:A:279:LYS:HG2	1.97	0.65
1:A:163:ASN:ND2	2:B:127:ARG:HH22	1.94	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:219:VAL:HB	2:B:359:THR:HG23	1.81	0.62
2:B:64:VAL:HG22	2:B:95:THR:CG2	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:ALA:HB1	2:B:80:MET:HE1	1.83	0.60
1:A:50:MET:HE2	1:A:60:ILE:HD11	1.83	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:291:GLN:OE1	1:A:315:LYS:HD3	2.03	0.59
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:487:MET:HE3	2:B:492:VAL:HG21	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:212:GLN:HG3	2:B:214:ILE:HD11	1.85	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: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:412:GLU:OE2	1:A:498:LYS:HE3	2.05	0.57
1:A:48:ASP:OD1	1:A:62:ASN:HB2	2.03	0.57
2:B:301:HIS:CE1	2:B:305:ARG:HD2	2.39	0.57
2:B:239:LEU:HD22	2:B:328:ALA:HB3	1.86	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
1:A:289:LEU:HD23	1:A:321:LEU:HD13	1.88	0.56
1:A:61:SER:HB2	1:A:386:ARG:NH1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:HIS:CD2	2:B:120:THR:H	2.20	0.54
2:B:64:VAL:HA	2:B:84:SER:OG	2.06	0.54
1:A:196:ASN:HD21	1:A:323:LYS:HE2	1.72	0.54
1:A:192:VAL:HG21	1:A:396:ALA:HB1	1.89	0.54
1:A:286:ASN:C	1:A:307:ILE:HG23	2.28	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
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: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
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:CG	2:B:347:ARG:HH11	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:217:VAL:HG22	1:A:357:MET:HE2	1.93	0.51
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: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:406:TRP:O	1:A:410:ALA:HB3	2.10	0.50
1:A:255:GLN:NE2	2:B:256:ARG:HB2	2.26	0.50
2:B:490:ASN:N	2:B:490:ASN:HD22	2.08	0.50
2:B:47:ASP:OD1	2:B:61:ASN:HB2	2.12	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:224:HIS:CE1	1:A:226:LYS:HB2	2.47	0.50
1:A:25:ARG:O	1:A:29:GLU:HG2	2.12	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
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:NZ	1:A:253:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ALA:HB1	2:B:80:MET:CE	2.43	0.49
1:A:397:ILE:HG12	1:A:496:ARG:NH2	2.28	0.49
2:B:195:PHE:C	2:B:197:ASN:H	2.16	0.49
1:A:206:SER:C	1:A:208:ASN:H	2.16	0.49
2:B:58:VAL:HG11	2:B:69:GLU:HG2	1.93	0.49
1:A:305:GLU:HA	1:A:305:GLU:OE1	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: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
2:B:64:VAL:CG2	2:B:95:THR:HG21	2.32	0.48
1:A:261:LYS:HE2	1:A:261:LYS:CA	2.41	0.48
1:A:51:LEU:HD13	1:A:70:GLU:HB2	1.95	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:O	1:A:443:ILE:HD13	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: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
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:407:ALA:O	2:B:412:THR:HG22	2.14	0.47
2:B:158:THR:HG23	4:B:998:ADP:C8	2.50	0.47
2:B:136:VAL:O	2:B:140:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:130:ALA:HB2	1:A:434:ILE:HG23	1.96	0.46
1:A:78:ALA:O	1:A:82:VAL:HG23	2.15	0.46
2:B:221:LYS:HG3	2:B:314:VAL:HG22	1.97	0.46
2:B:492:VAL:O	2:B:492:VAL:HG23	2.14	0.46
1:A:405:LEU:HB3	1:A:411:VAL:HG22	1.97	0.46
1:A:256:ILE:HG23	1:A:261:LYS:HB2	1.97	0.46
2:B:199:GLN:O	2:B:371:SER:HA	2.14	0.46
2:B:51:VAL:HG13	2:B:57:ILE:HG12	1.95	0.46
1:A:154:ILE:HD13	1:A:492:VAL:CG2	2.44	0.46
1:A:69:LYS:HG2	1:A:86:LYS:HD3	1.97	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
2:B:149:LYS:HD2	2:B:177:TYR:CE2	2.50	0.46
1:A:308:TYR:OH	1:A:349:GLU:HB2	2.16	0.46
1:A:94:ASP:OD1	4:A:898:ADP:O2B	2.34	0.46
1:A:235:LYS:HB3	1:A:341:LEU:HD13	1.98	0.46
1:A:224:HIS:HE1	1:A:226:LYS:HB2	1.80	0.45
1:A:145:SER:HB3	1:A:404:PHE:HE2	1.81	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:O	1:A:491:VAL:HG23	2.16	0.45
1:A:409:GLY:CA	1:A:445:PRO:HG3	2.46	0.45
1:A:50:MET:O	2:B:519:VAL:HA	2.16	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ILE:HG12	2:B:311:VAL:HG22	1.99	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:472:ASN:O	2:B:474:THR:N	2.51	0.44
2:B:93:ASP:O	2:B:498:VAL:HG13	2.17	0.44
2:B:68:LYS:HE3	2:B:85:LYS:HG2	2.00	0.44
1:A:460:LEU:HA	1:A:460:LEU:HD23	1.82	0.43
2:B:23:MET:SD	2:B:113:ILE:HD13	2.58	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:HA	2:B:152:LEU:HD23	1.82	0.43
2:B:352:LYS:HD3	2:B:357:TYR:CZ	2.54	0.43
1:A:223:VAL:HG23	1:A:227:MET:HE1	2.00	0.43
1:A:57:ASP:HB3	1:A:58:ILE:H	1.59	0.43
2:B:137:ILE:HG22	2:B:496:ILE:CG1	2.49	0.43
2:B:77:ALA:O	2:B:81:VAL:HG23	2.19	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:284:VAL:HG22	2:B:339:SER:CA	2.49	0.43
1:A:58:ILE:HD11	2:B:75:PRO:HA	2.00	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:477:ASP:N	1:A:482:GLY:O	2.52	0.42
1:A:17:ARG:CG	1:A:519:ILE:HG12	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:ASP:O	2:B:300:GLN:HB2	2.19	0.42
2:B:457:PRO:O	2:B:461:LEU:HB2	2.20	0.42
1:A:58:ILE:HG21	2:B:79:MET:SD	2.59	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
2:B:50:LEU:HD13	2:B:69:GLU:HG2	2.02	0.42
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
1:A:197:ILE:HG21	1:A:392:ILE:HD13	2.02	0.41
2:B:91:VAL:HG21	2:B:498:VAL:HA	2.01	0.41
2:B:221:LYS:O	2:B:359:THR:HG22	2.19	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:69:LYS:CE	1:A:86:LYS:HG2	2.40	0.41
1:A:167:SER:O	1:A:170:PHE:HB3	2.21	0.41
1:A:242:ALA:HB2	1:A:292:LYS:HB3	2.02	0.41
1:A:230:VAL:HG23	1:A:348:GLU:HB3	2.02	0.41
1:A:324:ALA:O	1:A:363:CYS:HB3	2.20	0.41
2:B:215:ASN:O	2:B:362:THR:HG23	2.20	0.41
2:B:48:LYS:CG	2:B:66:ILE:HD13	2.46	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: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
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:147:ASP:O	2:B:148:GLU:C	2.59	0.41
2:B:204:GLN:HA	2:B:376:GLY:O	2.21	0.41
2:B:118:HIS:HD2	2:B:120:THR:N	2.11	0.41
2:B:303:LEU:HD13	2:B:310:ALA:CB	2.51	0.41
2:B:290:ILE:HD13	2:B:322:LEU:CD1	2.50	0.41
2:B:334:ILE:N	2:B:334:ILE:HD12	2.34	0.41
2:B:284:VAL:CG2	2:B:339:SER:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:CG2	1:A:357:MET:HE2	2.49	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
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.85	0.40
1:A:189:LYS:O	1:A:189:LYS:HD2	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
2:B:236:LYS:HB3	2:B:342:LEU:HD23	2.03	0.40
2:B:215:ASN:HA	2:B:370:VAL:HG23	2.04	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 ⓘ

### 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	501/545 (92%)	450 (90%)	41 (8%)	10 (2%)	8	42
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	49	83
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	16	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP

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Mol	Chain	Res	Type
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 [i](#)

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%)	375 (91%)	36 (9%)	11	39
2	B	410/446 (92%)	376 (92%)	34 (8%)	12	43
All	All	821/888 (92%)	751 (92%)	70 (8%)	12	42

All (70) 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	92	VAL
1	A	102	LEU
1	A	122	VAL
1	A	135	ARG
1	A	143	GLU
1	A	156	LEU
1	A	162	LYS
1	A	166	LEU

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Mol	Chain	Res	Type
1	A	189	LYS
1	A	223	VAL
1	A	230	VAL
1	A	240	ASP
1	A	251	GLU
1	A	253	LYS
1	A	296	ASP
1	A	305	GLU
1	A	311	ARG
1	A	333	LEU
1	A	354	ASP
1	A	361	MET
1	A	380	VAL
1	A	388	LEU
1	A	393	ARG
1	A	443	ILE
1	A	464	LYS
1	A	466	ASP
1	A	467	ASP
1	A	478	LEU
1	A	496	ARG
1	A	513	LEU
1	A	516	ASP
2	B	24	LYS
2	B	54	LEU
2	B	58	VAL
2	B	67	LEU
2	B	79	MET
2	B	87	GLN
2	B	106	LEU
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	209	ASP
2	B	239	LEU
2	B	248	LYS
2	B	250	GLU
2	B	305	ARG
2	B	339	SER

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Mol	Chain	Res	Type
2	B	340	SER
2	B	347	ARG
2	B	366	ASN
2	B	391	ASP
2	B	396	VAL
2	B	412	THR
2	B	425	GLN
2	B	430	ARG
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	514	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	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	292	GLN
2	B	300	GLN
2	B	301	HIS

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Mol	Chain	Res	Type
2	B	366	ASN
2	B	394	HIS
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 carbohydrates 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	25,29,29	1.24	4 (16%)	25,45,45	2.33	3 (12%)
5	AF3	A	899	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	998	3,5	25,29,29	1.24	4 (16%)	25,45,45	2.38	2 (8%)
5	AF3	B	999	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-

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	-	0/12/32/32	0/3/3/3
5	AF3	A	899	3,4,6	-	0/0/0/0	0/0/0/0
4	ADP	B	998	3,5	-	0/12/32/32	0/3/3/3
5	AF3	B	999	3,4,6	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	998	ADP	C8-N9	-3.13	1.33	1.36
4	A	898	ADP	C8-N9	-2.80	1.33	1.36
4	A	898	ADP	C5-N7	-2.43	1.31	1.39
4	B	998	ADP	C5-N7	-2.22	1.31	1.39
4	A	898	ADP	O4'-C1'	2.17	1.44	1.41
4	B	998	ADP	O4'-C1'	2.39	1.44	1.41
4	B	998	ADP	PB-O2B	2.46	1.64	1.54
4	A	898	ADP	PB-O2B	2.59	1.65	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	ADP	N3-C2-N1	-11.04	119.41	128.86
4	A	898	ADP	N3-C2-N1	-10.61	119.79	128.86
4	A	898	ADP	C4-C5-N7	-2.84	106.67	109.41
4	B	998	ADP	C4-C5-N7	-2.68	106.82	109.41
4	A	898	ADP	C4'-O4'-C1'	-2.08	107.66	109.83

There are no chirality outliers.

There are no torsion outliers.

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

## 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.