



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 PM GMT

PDB ID : 4M9Y  
Title : Crystal structure of CED-4 bound CED-3 fragment  
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Deposited on : 2013-08-15  
Resolution : 4.20 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

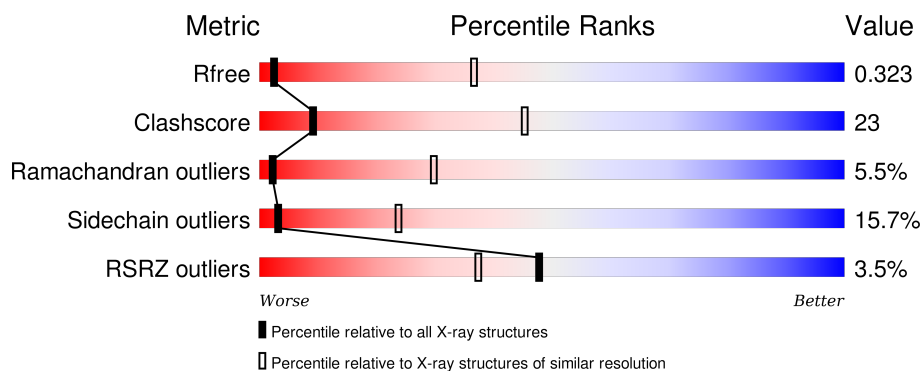
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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))
$R_{free}$	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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.

Mol	Chain	Length	Quality of chain
1	A	549	
1	B	549	
2	C	8	
2	D	8	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	B	602	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8349 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 Cell death protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	B	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			

- Molecule 2 is a protein called CED-3 fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	Se	0	0	0
			57	40	8	8	1			
2	D	5	Total	C	N	O	Se	0	0	0
			46	33	6	6	1			

- 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'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

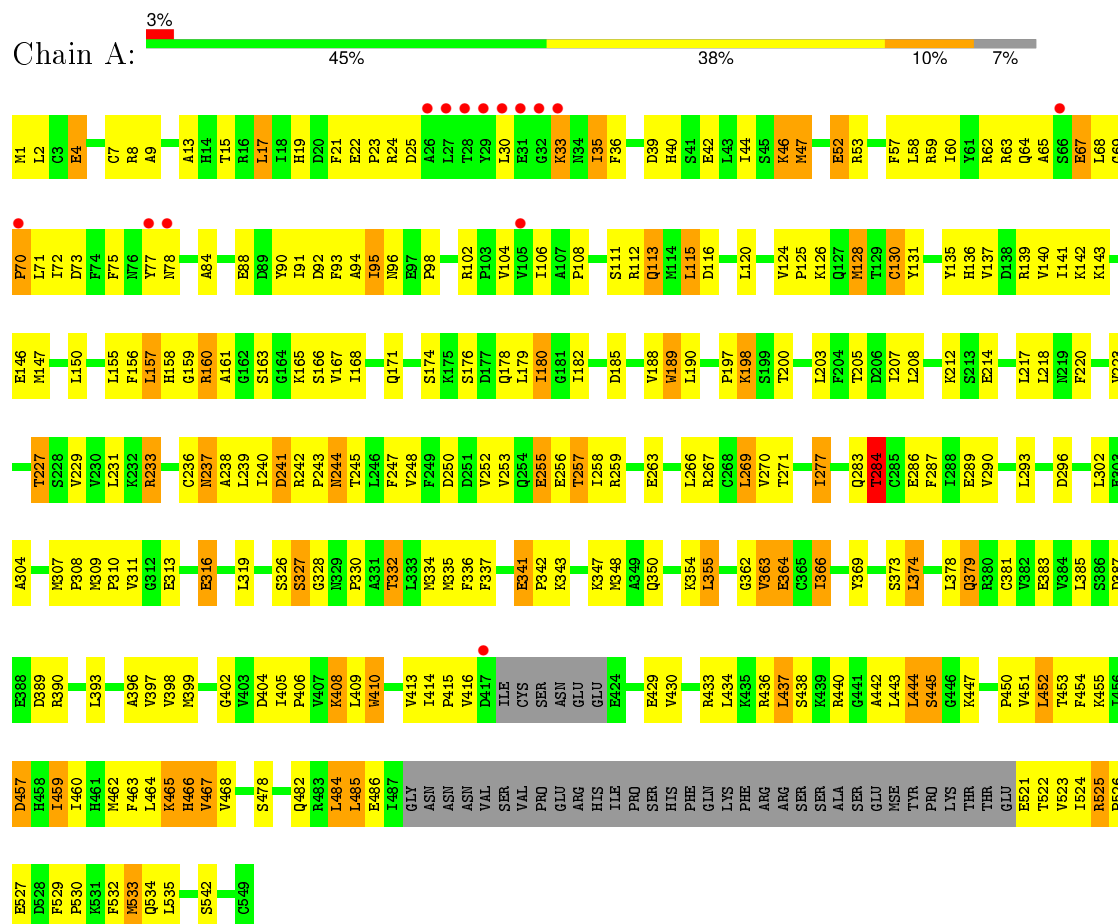


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

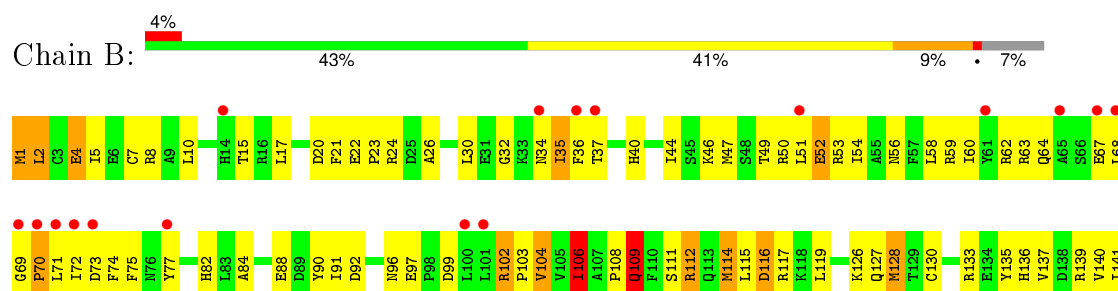
### 3 Residue-property plots

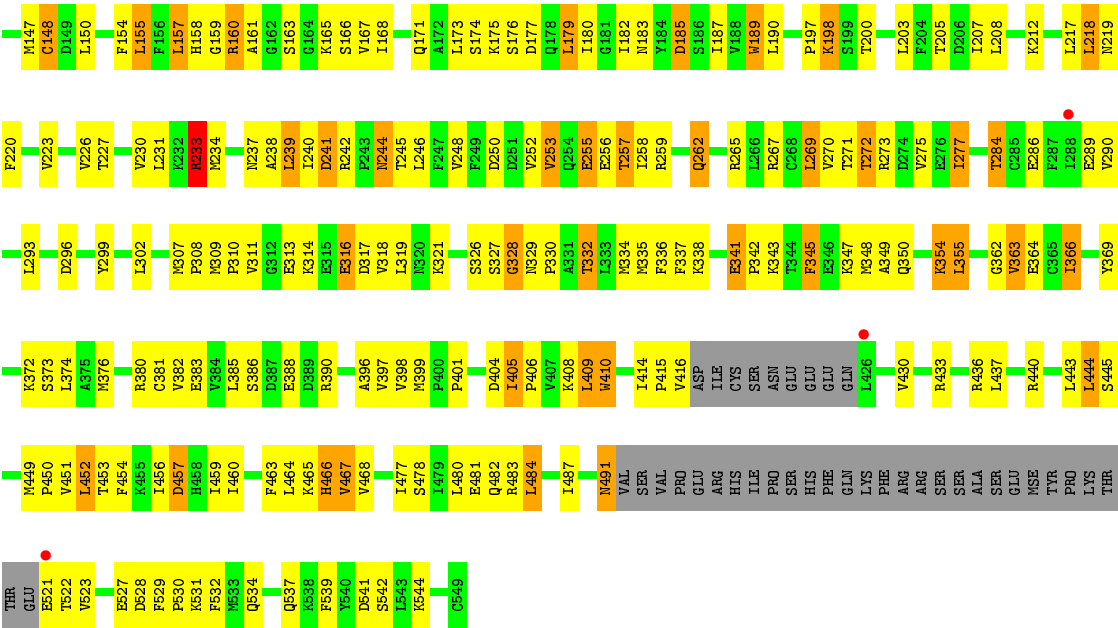
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

#### • Molecule 1: Cell death protein 4

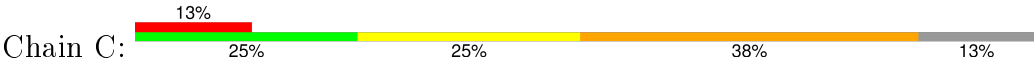


#### • Molecule 1: Cell death protein 4

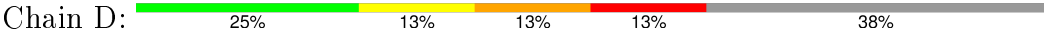




● Molecule 2: CED-3 fragment



● Molecule 2: CED-3 fragment



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.13Å 181.13Å 202.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.93 – 4.20 42.93 – 4.20	Depositor EDS
% Data completeness (in resolution range)	77.3 (42.93-4.20) 95.6 (42.93-4.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.34 (at 4.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.247 , 0.300 0.285 , 0.323	Depositor DCC
$R_{free}$ test set	575 reflections (4.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	266.1	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 256.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 12022 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	272.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ATP

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	0.37	0/4147	0.72	0/5577
1	B	0.38	0/4153	0.76	2/5585 (0.0%)
2	C	1.01	1/58 (1.7%)	1.11	1/74 (1.4%)
2	D	0.37	0/46	0.61	0/58
All	All	0.38	1/8404 (0.0%)	0.74	3/11294 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	748	PRO	CB-CG	6.67	1.83	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	749	LEU	CA-CB-CG	6.06	129.24	115.30
1	B	484	LEU	CA-CB-CG	5.81	128.66	115.30
1	B	233	ARG	NE-CZ-NH1	5.29	122.95	120.30

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	4088	0	4107	180	0
1	B	4094	0	4115	205	0
2	C	57	0	54	2	0
2	D	46	0	43	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	4	0
All	All	8349	0	8343	384	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 23.

All (384) 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)
2:C:748:PRO:CB	2:C:748:PRO:CG	1.83	1.48
1:A:484:LEU:HD11	1:A:533:MSE:HG2	1.52	0.89
1:A:63:ARG:HE	1:A:240:ILE:HD11	1.41	0.84
1:B:200:THR:HG21	1:B:256:GLU:HB3	1.65	0.79
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.66	0.78
1:B:72:ILE:HG21	1:B:88:GLU:HG3	1.65	0.76
1:B:165:LYS:HG2	1:B:290:VAL:HG21	1.68	0.76
1:A:366:ILE:HD12	1:A:366:ILE:H	1.52	0.74
1:A:150:LEU:O	1:A:267:ARG:NH1	2.20	0.74
1:B:190:LEU:HD12	1:B:207:ILE:HG13	1.67	0.74
1:B:230:VAL:HG12	1:B:234:MSE:HE2	1.70	0.74
1:A:47:MSE:HB2	1:A:53:ARG:HG3	1.70	0.73
1:B:478:SER:O	1:B:482:GLN:HG2	1.89	0.72
1:A:128:MSE:HG3	1:A:167:VAL:HG22	1.72	0.71
1:B:366:ILE:H	1:B:366:ILE:HD12	1.54	0.70
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.74	0.70
1:A:8:ARG:HH11	1:A:8:ARG:HG2	1.55	0.70
1:B:273:ARG:NE	4:B:602:ATP:O3G	2.22	0.70
1:B:154:PHE:HE2	1:B:262:GLN:HG3	1.56	0.69
1:A:335:MSE:HE3	1:A:364:GLU:HA	1.74	0.69
1:B:383:GLU:HG2	2:D:753:MSE:HG2	1.73	0.69
1:B:20:ASP:OD2	1:B:82:HIS:NE2	2.27	0.68
1:A:67:GLU:HG2	1:A:69:GLY:H	1.58	0.67
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.75	0.67
1:B:92:ASP:OD1	1:B:96:ASN:ND2	2.28	0.67
1:B:24:ARG:HH22	1:B:53:ARG:HH11	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HG21	1:A:88:GLU:HG3	1.76	0.67
1:B:147:MSE:HE1	1:B:286:GLU:HG2	1.75	0.67
1:A:447:LYS:HE2	1:A:450:PRO:HD2	1.77	0.66
1:B:23:PRO:HG2	1:B:53:ARG:C	2.16	0.66
1:A:96:ASN:O	1:A:98:PRO:HD3	1.95	0.66
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.77	0.66
1:A:354:LYS:HD3	1:A:362:GLY:O	1.96	0.66
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.79	0.65
1:B:457:ASP:N	1:B:457:ASP:OD1	2.29	0.65
1:B:8:ARG:HG2	1:B:8:ARG:HH11	1.60	0.65
1:B:487:ILE:O	1:B:531:LYS:NZ	2.30	0.64
1:B:114:MSE:SE	1:B:177:ASP:HA	2.46	0.64
1:A:190:LEU:HD12	1:A:207:ILE:HG13	1.80	0.63
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.38	0.63
1:B:50:ARG:HA	1:B:53:ARG:HE	1.64	0.63
1:B:386:SER:OG	1:B:388:GLU:OE1	2.16	0.63
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.80	0.63
1:B:197:PRO:HD2	1:B:198:LYS:HE2	1.81	0.63
1:A:452:LEU:H	1:A:452:LEU:HD23	1.64	0.62
1:B:385:LEU:O	1:B:390:ARG:NH2	2.32	0.62
1:A:24:ARG:HE	1:A:53:ARG:NH1	1.98	0.61
1:B:24:ARG:HH22	1:B:53:ARG:NH1	1.98	0.61
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.82	0.61
1:B:148:CYS:HB2	1:B:183:ASN:HB3	1.81	0.61
1:B:128:MSE:HG3	1:B:167:VAL:HG22	1.82	0.61
1:B:47:MSE:HB2	1:B:53:ARG:HG3	1.83	0.61
1:B:342:PRO:O	1:B:343:LYS:HB3	1.99	0.61
1:B:452:LEU:H	1:B:452:LEU:HD23	1.66	0.61
1:B:158:HIS:HE1	1:B:289:GLU:HB2	1.66	0.60
1:B:372:LYS:H	1:B:376:MSE:HE2	1.66	0.60
1:A:309:MSE:HG3	1:A:310:PRO:HD2	1.84	0.60
1:B:114:MSE:O	1:B:119:LEU:HG	2.02	0.59
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.83	0.59
1:B:414:ILE:HG21	1:B:430:VAL:HG13	1.83	0.59
1:B:109:GLN:C	1:B:111:SER:H	2.05	0.59
1:A:532:PHE:HB2	1:A:534:GLN:HG2	1.84	0.59
1:B:226:VAL:HG13	1:B:230:VAL:HB	1.85	0.59
1:B:4:GLU:HG3	1:B:5:ILE:N	2.17	0.59
1:A:47:MSE:HE2	1:A:52:GLU:HG2	1.84	0.59
1:A:342:PRO:O	1:A:343:LYS:HB3	2.03	0.59
1:A:326:SER:O	1:A:328:GLY:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:VAL:HG11	1:B:380:ARG:HD3	1.84	0.59
1:A:464:LEU:O	1:A:468:VAL:HG22	2.03	0.59
1:B:406:PRO:HA	1:B:453:THR:HG22	1.83	0.59
1:A:336:PHE:HE1	1:A:348:MSE:SE	2.36	0.59
1:A:165:LYS:HG2	1:A:290:VAL:HG21	1.86	0.58
1:A:463:PHE:O	1:A:467:VAL:HB	2.03	0.58
1:B:135:TYR:O	1:B:139:ARG:HG3	2.04	0.58
1:A:526:PRO:HD2	1:A:529:PHE:HD2	1.68	0.57
1:A:58:LEU:O	1:A:62:ARG:HG3	2.03	0.57
1:A:437:LEU:HB3	1:A:444:LEU:HD22	1.86	0.57
1:B:231:LEU:HA	1:B:234:MSE:HE3	1.86	0.57
1:A:135:TYR:CZ	1:A:139:ARG:HD2	2.40	0.57
1:B:112:ARG:HA	1:B:116:ASP:HB2	1.86	0.57
2:C:750:PHE:O	2:C:752:PHE:N	2.38	0.57
1:B:443:LEU:HD23	1:B:460:ILE:HD11	1.86	0.56
1:A:252:VAL:HG21	1:A:257:THR:HG21	1.87	0.56
1:A:255:GLU:O	1:A:259:ARG:HG3	2.05	0.56
1:A:364:GLU:HB2	1:A:373:SER:HB3	1.87	0.56
1:B:135:TYR:CZ	1:B:139:ARG:HD2	2.40	0.56
1:B:355:LEU:HD21	1:B:363:VAL:HB	1.87	0.56
1:B:102:ARG:HG3	1:B:103:PRO:CD	2.35	0.56
1:A:178:GLN:O	1:A:182:ILE:HB	2.06	0.56
1:A:313:GLU:O	1:A:316:GLU:HG3	2.05	0.56
1:A:67:GLU:HG2	1:A:69:GLY:N	2.20	0.56
2:D:751:ASN:O	2:D:751:ASN:ND2	2.38	0.56
1:B:4:GLU:O	1:B:8:ARG:HB2	2.06	0.56
1:B:527:GLU:N	1:B:527:GLU:OE1	2.39	0.55
1:B:302:LEU:HD13	1:B:319:LEU:HD11	1.88	0.55
1:B:397:VAL:HG21	1:B:468:VAL:HG21	1.89	0.55
1:A:415:PRO:O	1:A:416:VAL:HG23	2.07	0.55
1:A:250:ASP:HA	1:A:271:THR:OG1	2.06	0.55
1:B:250:ASP:HA	1:B:271:THR:OG1	2.07	0.55
1:A:457:ASP:OD1	1:A:457:ASP:N	2.40	0.55
1:B:108:PRO:O	1:B:109:GLN:HB2	2.06	0.55
1:A:159:GLY:N	1:A:165:LYS:HD3	2.22	0.55
1:A:269:LEU:HD22	1:A:270:VAL:H	1.72	0.55
1:A:233:ARG:HH11	1:A:233:ARG:HG3	1.72	0.54
1:A:247:PHE:HE2	1:A:266:LEU:HD22	1.73	0.54
1:B:436:ARG:O	1:B:440:ARG:HG3	2.08	0.54
1:B:273:ARG:CZ	1:B:380:ARG:HH21	2.20	0.54
1:B:47:MSE:HE3	1:B:52:GLU:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:HD23	1:A:460:ILE:HD11	1.90	0.54
1:A:334:MSE:HA	1:A:334:MSE:HE3	1.88	0.54
1:B:257:THR:HG22	1:B:258:ILE:HD12	1.89	0.54
1:B:309:MSE:HG3	1:B:310:PRO:HD2	1.88	0.54
1:B:257:THR:HG22	1:B:258:ILE:N	2.22	0.54
1:A:44:ILE:O	1:A:53:ARG:HG2	2.08	0.54
1:B:464:LEU:O	1:B:468:VAL:HG22	2.08	0.54
1:B:310:PRO:HA	1:B:345:PHE:HE2	1.71	0.54
1:A:160:ARG:HG2	1:A:161:ALA:H	1.73	0.54
1:A:247:PHE:CD2	1:A:266:LEU:HD13	2.43	0.53
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.73	0.53
1:B:24:ARG:NH2	1:B:53:ARG:HH11	2.06	0.53
1:B:158:HIS:CE1	1:B:289:GLU:HB2	2.41	0.53
1:B:166:SER:HA	1:B:271:THR:HG21	1.91	0.53
1:A:214:GLU:HG3	1:B:237:ASN:ND2	2.24	0.53
1:A:128:MSE:HG3	1:A:167:VAL:CG2	2.37	0.53
1:A:36:PHE:HE2	1:A:44:ILE:HD12	1.74	0.53
1:A:90:TYR:HE2	1:A:106:ILE:HD11	1.73	0.53
1:A:257:THR:HG22	1:A:258:ILE:N	2.23	0.53
1:B:335:MSE:HE3	1:B:364:GLU:HA	1.91	0.53
1:B:409:LEU:HD21	1:B:530:PRO:HB3	1.92	0.52
1:B:332:THR:O	1:B:336:PHE:HB2	2.08	0.52
1:B:529:PHE:N	1:B:530:PRO:HD3	2.24	0.52
1:B:165:LYS:N	4:B:602:ATP:O2B	2.42	0.52
1:B:529:PHE:HB3	1:B:532:PHE:CZ	2.45	0.52
1:A:465:LYS:HD3	1:A:466:HIS:CE1	2.44	0.52
1:A:521:GLU:C	1:A:523:VAL:H	2.13	0.52
1:B:269:LEU:HD22	1:B:270:VAL:H	1.74	0.52
1:A:393:LEU:HB2	1:A:437:LEU:HD11	1.91	0.52
1:B:233:ARG:NH1	1:B:237:ASN:HD21	2.08	0.52
1:B:135:TYR:CE1	1:B:139:ARG:HD2	2.44	0.52
1:A:283:GLN:HG2	1:A:284:THR:H	1.73	0.52
1:B:56:ASN:O	1:B:60:ILE:HB	2.10	0.52
1:B:388:GLU:HB3	1:B:433:ARG:HH21	1.74	0.52
1:B:22:GLU:OE2	1:B:24:ARG:NH1	2.43	0.52
1:B:109:GLN:C	1:B:111:SER:N	2.62	0.52
1:A:406:PRO:HA	1:A:453:THR:HG22	1.92	0.52
1:A:33:LYS:HD3	1:A:70:PRO:HG3	1.91	0.51
1:B:167:VAL:O	1:B:171:GLN:HG3	2.11	0.51
1:B:354:LYS:HD3	1:B:362:GLY:O	2.10	0.51
1:A:4:GLU:OE2	1:A:267:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:MSE:HE2	1:B:338:LYS:CD	2.41	0.51
1:A:242:ARG:HB3	1:A:245:THR:OG1	2.11	0.51
1:A:436:ARG:O	1:A:440:ARG:HG3	2.09	0.51
1:B:154:PHE:CE2	1:B:262:GLN:HG3	2.42	0.51
1:B:189:TRP:CE3	1:B:248:VAL:HG11	2.46	0.51
1:A:17:LEU:HD23	1:A:21:PHE:CD2	2.45	0.51
1:B:521:GLU:C	1:B:523:VAL:H	2.13	0.51
1:A:135:TYR:O	1:A:139:ARG:HG3	2.10	0.51
1:B:242:ARG:HB3	1:B:245:THR:OG1	2.11	0.51
1:B:313:GLU:O	1:B:316:GLU:HG3	2.10	0.51
1:B:173:LEU:HD23	1:B:179:LEU:HD23	1.92	0.50
1:B:491:ASN:OD1	1:B:491:ASN:N	2.44	0.50
1:B:166:SER:OG	1:B:250:ASP:OD1	2.28	0.50
1:A:430:VAL:O	1:A:434:LEU:HG	2.12	0.50
1:A:355:LEU:HD21	1:A:363:VAL:HB	1.93	0.50
1:B:35:ILE:HD12	1:B:70:PRO:HG2	1.93	0.50
1:A:341:GLU:CB	1:A:342:PRO:HD3	2.41	0.50
1:A:160:ARG:HB3	1:A:163:SER:HB3	1.93	0.50
1:B:415:PRO:O	1:B:416:VAL:HG23	2.12	0.50
1:A:212:LYS:HA	1:A:212:LYS:HE2	1.94	0.50
1:A:137:VAL:O	1:A:141:ILE:HG13	2.12	0.50
1:A:25:ASP:HB3	1:A:78:ASN:ND2	2.27	0.50
1:B:23:PRO:HG2	1:B:53:ARG:O	2.11	0.50
1:B:364:GLU:HB2	1:B:373:SER:HB3	1.94	0.50
1:B:136:HIS:O	1:B:140:VAL:HG23	2.12	0.50
1:B:293:LEU:HG	1:B:330:PRO:HD3	1.94	0.50
1:B:449:MSE:HE3	1:B:450:PRO:HA	1.92	0.49
1:B:326:SER:O	1:B:328:GLY:N	2.45	0.49
1:B:437:LEU:HB3	1:B:444:LEU:HD22	1.93	0.49
1:A:293:LEU:HG	1:A:330:PRO:HD3	1.94	0.49
1:A:30:LEU:HD21	1:A:70:PRO:O	2.11	0.49
1:B:1:MSE:HA	1:B:62:ARG:O	2.12	0.49
1:A:156:PHE:HB2	1:A:287:PHE:CD2	2.47	0.49
1:A:120:LEU:HD13	1:B:265:ARG:HB2	1.94	0.49
1:A:19:HIS:HD2	1:B:1:MSE:SE	2.45	0.49
1:B:318:VAL:HG11	1:B:349:ALA:HB2	1.94	0.49
1:A:102:ARG:HG2	1:A:182:ILE:CG2	2.42	0.49
1:A:136:HIS:O	1:A:140:VAL:HG23	2.12	0.49
1:A:91:ILE:O	1:A:95:ILE:HG13	2.12	0.49
1:B:341:GLU:CB	1:B:342:PRO:HD3	2.43	0.49
1:A:255:GLU:HB3	1:A:277:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MSE:O	1:A:150:LEU:HB2	2.12	0.49
1:B:255:GLU:O	1:B:259:ARG:HG3	2.13	0.48
1:A:478:SER:O	1:A:482:GLN:HG2	2.12	0.48
1:B:137:VAL:O	1:B:141:ILE:HG13	2.13	0.48
1:B:30:LEU:HB3	1:B:36:PHE:CD1	2.48	0.48
1:A:332:THR:O	1:A:336:PHE:HB2	2.13	0.48
1:A:527:GLU:OE1	1:A:527:GLU:N	2.44	0.48
1:A:402:GLY:HA2	1:A:455:LYS:HD2	1.96	0.48
1:A:158:HIS:NE2	1:A:289:GLU:HB2	2.29	0.48
1:A:163:SER:O	1:A:330:PRO:HG2	2.13	0.48
1:A:462:MSE:HB2	1:A:462:MSE:HE3	1.69	0.48
1:B:410:TRP:CZ3	1:B:454:PHE:HB2	2.49	0.48
1:B:343:LYS:O	1:B:343:LYS:HG2	2.14	0.48
1:B:44:ILE:O	1:B:53:ARG:HG2	2.13	0.47
1:A:233:ARG:HA	1:A:236:CYS:SG	2.54	0.47
1:A:247:PHE:CE2	1:A:266:LEU:HD13	2.49	0.47
1:B:88:GLU:O	1:B:91:ILE:HG22	2.14	0.47
1:A:205:THR:HA	1:A:231:LEU:HD11	1.94	0.47
1:B:111:SER:O	1:B:115:LEU:HB3	2.15	0.47
1:B:2:LEU:HB2	1:B:7:CYS:SG	2.54	0.47
1:B:218:LEU:HG	1:B:219:ASN:N	2.30	0.47
1:B:273:ARG:NH2	1:B:380:ARG:HH21	2.12	0.47
1:B:537:GLN:O	1:B:541:ASP:N	2.44	0.47
1:A:525:ARG:HD3	1:A:535:LEU:HD13	1.95	0.47
1:A:529:PHE:N	1:A:530:PRO:HD3	2.30	0.47
1:B:463:PHE:O	1:B:467:VAL:HB	2.15	0.47
1:B:106:ILE:O	1:B:106:ILE:HG23	2.14	0.47
1:B:32:GLY:C	1:B:34:ASN:H	2.18	0.47
1:A:142:LYS:O	1:A:146:GLU:HG3	2.14	0.47
1:A:397:VAL:HG22	1:A:464:LEU:HB3	1.96	0.47
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.76	0.47
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.97	0.47
1:B:177:ASP:O	1:B:182:ILE:HD13	2.14	0.47
1:B:133:ARG:O	1:B:137:VAL:HG23	2.15	0.47
1:A:116:ASP:OD1	1:A:116:ASP:N	2.48	0.47
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.29	0.46
1:B:248:VAL:HG22	1:B:269:LEU:HD12	1.98	0.46
1:A:46:LYS:H	1:A:46:LYS:HG3	1.54	0.46
1:B:59:ARG:HH11	1:B:63:ARG:HH22	1.63	0.46
1:B:40:HIS:HD2	1:B:60:ILE:HG23	1.80	0.46
1:A:465:LYS:HD3	1:A:466:HIS:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.96	0.46
1:B:158:HIS:CD2	1:B:275:VAL:HG13	2.50	0.46
1:A:527:GLU:C	1:A:530:PRO:HD3	2.36	0.46
1:B:49:THR:HG22	1:B:50:ARG:N	2.30	0.46
1:B:157:LEU:HD11	1:B:168:ILE:HG22	1.97	0.46
1:A:167:VAL:HG11	4:A:602:ATP:C5	2.50	0.46
1:A:397:VAL:O	1:A:399:MSE:N	2.47	0.46
1:A:269:LEU:HD22	1:A:270:VAL:N	2.31	0.46
1:B:88:GLU:HA	1:B:91:ILE:HG22	1.97	0.46
1:B:481:GLU:O	1:B:484:LEU:HG	2.15	0.46
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.80	0.46
1:A:102:ARG:HG2	1:A:182:ILE:HG22	1.98	0.46
1:B:329:ASN:HA	1:B:330:PRO:HD2	1.77	0.46
1:A:21:PHE:CG	1:A:22:GLU:N	2.84	0.46
1:B:159:GLY:N	1:B:165:LYS:HD3	2.32	0.45
1:A:252:VAL:CG2	1:A:257:THR:HG21	2.45	0.45
1:A:307:MSE:HA	1:A:308:PRO:HD3	1.80	0.45
1:B:318:VAL:O	1:B:321:LYS:HB3	2.17	0.45
1:A:444:LEU:HB3	1:A:445:SER:H	1.57	0.45
1:B:163:SER:O	1:B:330:PRO:HG2	2.17	0.45
1:B:233:ARG:CG	1:B:233:ARG:HH11	2.29	0.45
1:A:167:VAL:O	1:A:171:GLN:HG3	2.16	0.45
1:A:25:ASP:HB3	1:A:78:ASN:HD21	1.81	0.45
1:B:252:VAL:CG2	1:B:257:THR:HG21	2.47	0.45
1:B:35:ILE:O	1:B:64:GLN:HB2	2.17	0.45
1:B:128:MSE:HG3	1:B:167:VAL:CG2	2.47	0.45
1:A:459:ILE:H	1:A:459:ILE:HG13	1.37	0.45
1:A:111:SER:O	1:A:113:GLN:N	2.50	0.45
1:A:7:CYS:HB3	1:A:243:PRO:HG3	1.99	0.44
1:B:8:ARG:HD3	1:B:90:TYR:OH	2.17	0.44
1:B:237:ASN:C	1:B:239:LEU:H	2.21	0.44
1:A:466:HIS:ND1	1:A:466:HIS:N	2.65	0.44
1:B:189:TRP:CD1	1:B:189:TRP:C	2.91	0.44
1:B:160:ARG:HG2	1:B:161:ALA:H	1.82	0.44
1:A:166:SER:OG	1:A:250:ASP:OD1	2.36	0.44
1:A:90:TYR:CE2	1:A:106:ILE:HD11	2.51	0.44
1:A:35:ILE:O	1:A:64:GLN:HB3	2.17	0.44
1:B:10:LEU:HD22	1:B:58:LEU:HD21	1.99	0.44
1:A:157:LEU:HD11	1:A:168:ILE:HG22	1.99	0.44
1:B:190:LEU:CD1	1:B:207:ILE:HG13	2.44	0.44
1:A:44:ILE:HD11	1:A:60:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:CYS:O	1:A:304:ALA:HB1	2.17	0.44
1:B:150:LEU:O	1:B:267:ARG:NH1	2.51	0.44
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.75	0.44
1:A:259:ARG:O	1:A:263:GLU:HG3	2.17	0.44
1:A:78:ASN:HA	1:B:37:THR:HG21	2.00	0.44
1:A:374:LEU:HD13	1:A:378:LEU:HG	1.99	0.44
1:B:314:LYS:HA	1:B:317:ASP:HB2	1.99	0.44
1:A:347:LYS:O	1:A:347:LYS:HD3	2.17	0.44
1:B:167:VAL:HG11	4:B:602:ATP:C6	2.53	0.43
1:A:23:PRO:HG2	1:A:53:ARG:C	2.38	0.43
1:A:44:ILE:HD13	1:A:57:PHE:HA	2.01	0.43
1:B:49:THR:HG22	1:B:50:ARG:H	1.83	0.43
1:A:139:ARG:NH2	1:A:143:LYS:HE3	2.33	0.43
1:A:189:TRP:CE3	1:A:248:VAL:HG11	2.53	0.43
1:A:379:GLN:O	1:A:383:GLU:HG3	2.18	0.43
1:A:406:PRO:HD3	1:A:524:ILE:HD11	1.99	0.43
1:B:401:PRO:HA	1:B:456:ILE:HG23	2.00	0.43
1:B:307:MSE:HA	1:B:308:PRO:HD3	1.77	0.43
1:A:521:GLU:O	1:A:523:VAL:N	2.51	0.43
1:B:187:ILE:HD13	1:B:246:LEU:HB3	2.00	0.43
1:B:185:ASP:N	1:B:244:ASN:O	2.44	0.43
1:B:334:MSE:HE3	1:B:337:PHE:HB2	2.01	0.43
1:A:8:ARG:NH1	1:A:8:ARG:HG2	2.30	0.43
1:B:484:LEU:HD13	1:B:531:LYS:O	2.18	0.43
1:B:444:LEU:HA	1:B:444:LEU:HD12	1.76	0.43
1:A:302:LEU:HD13	1:A:319:LEU:HD11	2.00	0.43
1:A:343:LYS:O	1:A:343:LYS:HG2	2.19	0.43
1:A:240:ILE:C	1:A:242:ARG:H	2.22	0.43
1:B:269:LEU:HD22	1:B:270:VAL:N	2.34	0.43
1:A:437:LEU:HA	1:A:437:LEU:HD22	1.85	0.43
1:B:477:ILE:HG21	1:B:544:LYS:HE2	2.01	0.43
1:B:163:SER:C	1:B:330:PRO:HG2	2.39	0.42
1:A:233:ARG:NH1	1:A:237:ASN:HD21	2.17	0.42
1:B:521:GLU:O	1:B:523:VAL:N	2.51	0.42
1:A:429:GLU:OE2	1:A:433:ARG:NH1	2.50	0.42
1:B:40:HIS:O	1:B:44:ILE:HG13	2.19	0.42
1:B:332:THR:HG23	1:B:374:LEU:HB2	2.02	0.42
1:B:212:LYS:HA	1:B:212:LYS:HE2	2.00	0.42
1:B:532:PHE:C	1:B:534:GLN:H	2.23	0.42
1:B:47:MSE:HB3	1:B:52:GLU:HB3	2.01	0.42
1:B:460:ILE:HA	1:B:460:ILE:HD12	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HH11	1:B:63:ARG:NH2	2.17	0.42
1:A:307:MSE:SE	1:A:308:PRO:HD2	2.69	0.42
1:A:115:LEU:HD21	1:A:180:ILE:HB	2.02	0.42
1:B:21:PHE:CG	1:B:22:GLU:N	2.87	0.42
1:B:388:GLU:H	1:B:388:GLU:CD	2.23	0.42
1:B:397:VAL:O	1:B:399:MSE:N	2.51	0.42
1:A:438:SER:O	1:A:442:ALA:HA	2.18	0.42
1:B:252:VAL:HG21	1:B:257:THR:HG21	2.02	0.42
1:B:239:LEU:HD22	1:B:242:ARG:HB2	2.00	0.42
1:A:408:LYS:HD2	1:A:408:LYS:HA	1.75	0.42
1:A:397:VAL:C	1:A:399:MSE:H	2.22	0.42
1:A:35:ILE:HG12	1:A:65:ALA:HA	2.02	0.42
1:B:26:ALA:HA	1:B:74:PHE:CE1	2.55	0.42
1:A:47:MSE:HB2	1:A:53:ARG:CG	2.45	0.42
1:A:13:ALA:O	1:A:17:LEU:HD12	2.20	0.42
1:A:347:LYS:HA	1:A:350:GLN:HB2	2.01	0.42
1:B:50:ARG:CA	1:B:53:ARG:HH21	2.33	0.42
1:A:410:TRP:CZ3	1:A:454:PHE:HB2	2.55	0.42
1:A:532:PHE:C	1:A:534:GLN:H	2.23	0.42
1:A:334:MSE:HE1	1:A:337:PHE:HD2	1.84	0.42
1:A:163:SER:C	1:A:330:PRO:HG2	2.40	0.42
1:B:69:GLY:O	1:B:71:LEU:N	2.52	0.42
1:B:343:LYS:HB3	1:B:343:LYS:HE3	1.86	0.41
1:B:336:PHE:HE1	1:B:348:MSE:SE	2.53	0.41
1:B:205:THR:HA	1:B:231:LEU:HD11	2.01	0.41
1:A:385:LEU:O	1:A:390:ARG:NH2	2.53	0.41
1:A:255:GLU:CB	1:A:277:ILE:HG22	2.50	0.41
1:B:299:TYR:HA	1:B:302:LEU:HD12	2.02	0.41
1:A:240:ILE:HG13	1:A:241:ASP:OD1	2.20	0.41
1:B:21:PHE:CD2	1:B:54:ILE:HG12	2.56	0.41
1:A:188:VAL:HB	1:A:247:PHE:CD1	2.55	0.41
1:B:332:THR:HA	1:B:335:MSE:SE	2.71	0.41
1:A:111:SER:C	1:A:113:GLN:H	2.23	0.41
1:B:49:THR:HB	1:B:52:GLU:OE1	2.20	0.41
1:B:527:GLU:C	1:B:530:PRO:HD3	2.41	0.41
1:B:397:VAL:HG22	1:B:464:LEU:HB3	2.03	0.41
1:A:59:ARG:HH11	1:A:63:ARG:NH1	2.18	0.41
1:B:72:ILE:C	1:B:74:PHE:H	2.24	0.41
1:B:272:THR:OG1	1:B:273:ARG:N	2.53	0.41
1:A:40:HIS:O	1:A:44:ILE:HG13	2.20	0.41
1:B:310:PRO:HA	1:B:345:PHE:CE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:MSE:HE2	1:B:338:LYS:HD2	2.02	0.41
1:B:147:MSE:O	1:B:150:LEU:HB2	2.20	0.41
1:B:308:PRO:HG2	1:B:343:LYS:HD3	2.03	0.41
1:B:309:MSE:HB2	1:B:309:MSE:HE2	1.92	0.41
1:A:93:PHE:CE2	1:A:104:VAL:HG11	2.55	0.41
1:B:483:ARG:O	1:B:487:ILE:HG13	2.20	0.41
1:B:374:LEU:HD13	1:B:374:LEU:O	2.21	0.41
1:B:165:LYS:HG3	1:B:165:LYS:H	1.66	0.41
1:B:21:PHE:CE2	1:B:23:PRO:HG3	2.56	0.41
1:A:243:PRO:O	1:A:244:ASN:C	2.59	0.41
1:B:414:ILE:HA	1:B:415:PRO:HD3	1.89	0.41
1:A:176:SER:OG	1:A:178:GLN:HB2	2.21	0.41
1:B:299:TYR:CZ	1:B:319:LEU:HD22	2.56	0.41
1:A:9:ALA:HB2	1:A:90:TYR:CD1	2.56	0.41
1:A:39:ASP:HA	1:A:42:GLU:HB2	2.02	0.41
1:B:347:LYS:O	1:B:350:GLN:HB2	2.20	0.41
1:B:466:HIS:N	1:B:466:HIS:ND1	2.69	0.41
1:A:165:LYS:HG2	1:A:290:VAL:CG2	2.49	0.41
1:A:413:VAL:HG23	1:A:414:ILE:HD12	2.02	0.41
1:B:334:MSE:HE2	1:B:338:LYS:HD3	2.01	0.40
1:A:385:LEU:HD22	1:A:389:ASP:HB3	2.03	0.40
1:A:248:VAL:HG22	1:A:269:LEU:HD12	2.04	0.40
1:A:71:LEU:O	1:A:71:LEU:HD13	2.21	0.40
1:A:227:THR:HB	1:A:229:VAL:HG12	2.03	0.40
1:A:92:ASP:C	1:A:94:ALA:H	2.24	0.40
1:B:330:PRO:HB3	4:B:602:ATP:N3	2.36	0.40
1:A:24:ARG:HE	1:A:53:ARG:HH11	1.68	0.40
1:A:36:PHE:CE2	1:A:44:ILE:HD12	2.54	0.40
1:B:237:ASN:O	1:B:240:ILE:HG23	2.21	0.40
1:A:42:GLU:OE1	1:A:46:LYS:HD3	2.21	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	504/549 (92%)	405 (80%)	74 (15%)	25 (5%)	3	31
1	B	505/549 (92%)	405 (80%)	73 (14%)	27 (5%)	2	30
2	C	5/8 (62%)	2 (40%)	1 (20%)	2 (40%)	0	0
2	D	3/8 (38%)	1 (33%)	0	2 (67%)	0	0
All	All	1017/1114 (91%)	813 (80%)	148 (15%)	56 (6%)	2	30

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	341	GLU
1	A	398	VAL
1	A	445	SER
1	A	486	GLU
1	B	109	GLN
1	B	127	GLN
1	B	327	SER
1	B	341	GLU
1	B	398	VAL
1	B	445	SER
1	A	112	ARG
1	A	208	LEU
1	A	238	ALA
1	A	244	ASN
1	A	396	ALA
1	A	465	LYS
1	A	522	THR
2	C	750	PHE
2	C	751	ASN
1	B	244	ASN
1	B	396	ALA
1	B	465	LYS
1	B	522	THR
1	A	2	LEU
1	A	73	ASP
1	A	160	ARG
1	A	284	THR
1	B	2	LEU
1	B	104	VAL

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Mol	Chain	Res	Type
1	B	160	ARG
1	B	208	LEU
1	B	238	ALA
1	B	284	THR
2	D	751	ASN
1	A	33	LYS
1	B	73	ASP
1	B	176	SER
1	A	237	ASN
1	A	484	LEU
1	A	485	LEU
1	B	35	ILE
1	B	241	ASP
1	B	257	THR
1	B	328	GLY
1	B	354	LYS
2	D	750	PHE
1	A	257	THR
1	B	102	ARG
1	A	70	PRO
1	A	108	PRO
1	B	311	VAL
1	A	311	VAL
1	B	70	PRO
1	B	106	ILE
1	A	35	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	462/483 (96%)	393 (85%)	69 (15%)	4	26
1	B	464/483 (96%)	389 (84%)	75 (16%)	3	22
2	C	6/6 (100%)	5 (83%)	1 (17%)	3	21
2	D	5/6 (83%)	3 (60%)	2 (40%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	937/978 (96%)	790 (84%)	147 (16%)	3 24

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	4	GLU
1	A	15	THR
1	A	17	LEU
1	A	46	LYS
1	A	47	MSE
1	A	52	GLU
1	A	67	GLU
1	A	68	LEU
1	A	77	TYR
1	A	95	ILE
1	A	113	GLN
1	A	115	LEU
1	A	126	LYS
1	A	128	MSE
1	A	130	CYS
1	A	131	TYR
1	A	155	LEU
1	A	157	LEU
1	A	174	SER
1	A	179	LEU
1	A	180	ILE
1	A	185	ASP
1	A	189	TRP
1	A	198	LYS
1	A	203	LEU
1	A	217	LEU
1	A	218	LEU
1	A	220	PHE
1	A	223	VAL
1	A	227	THR
1	A	233	ARG
1	A	239	LEU
1	A	241	ASP
1	A	253	VAL
1	A	255	GLU
1	A	269	LEU

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Mol	Chain	Res	Type
1	A	277	ILE
1	A	284	THR
1	A	286	GLU
1	A	296	ASP
1	A	316	GLU
1	A	332	THR
1	A	355	LEU
1	A	363	VAL
1	A	364	GLU
1	A	366	ILE
1	A	369	TYR
1	A	374	LEU
1	A	379	GLN
1	A	381	CYS
1	A	387	ASP
1	A	404	ASP
1	A	405	ILE
1	A	408	LYS
1	A	409	LEU
1	A	410	TRP
1	A	437	LEU
1	A	444	LEU
1	A	451	VAL
1	A	452	LEU
1	A	457	ASP
1	A	459	ILE
1	A	466	HIS
1	A	467	VAL
1	A	485	LEU
1	A	525	ARG
1	A	533	MSE
1	A	542	SER
2	C	749	LEU
1	B	1	MSE
1	B	4	GLU
1	B	15	THR
1	B	17	LEU
1	B	46	LYS
1	B	51	LEU
1	B	52	GLU
1	B	67	GLU
1	B	68	LEU

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Mol	Chain	Res	Type
1	B	77	TYR
1	B	97	GLU
1	B	99	ASP
1	B	104	VAL
1	B	106	ILE
1	B	109	GLN
1	B	112	ARG
1	B	114	MSE
1	B	116	ASP
1	B	117	ARG
1	B	126	LYS
1	B	128	MSE
1	B	130	CYS
1	B	148	CYS
1	B	155	LEU
1	B	157	LEU
1	B	174	SER
1	B	175	LYS
1	B	179	LEU
1	B	180	ILE
1	B	185	ASP
1	B	189	TRP
1	B	198	LYS
1	B	203	LEU
1	B	217	LEU
1	B	218	LEU
1	B	220	PHE
1	B	223	VAL
1	B	227	THR
1	B	233	ARG
1	B	239	LEU
1	B	241	ASP
1	B	253	VAL
1	B	255	GLU
1	B	262	GLN
1	B	269	LEU
1	B	272	THR
1	B	277	ILE
1	B	284	THR
1	B	296	ASP
1	B	316	GLU
1	B	332	THR

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Mol	Chain	Res	Type
1	B	345	PHE
1	B	355	LEU
1	B	363	VAL
1	B	366	ILE
1	B	369	TYR
1	B	381	CYS
1	B	382	VAL
1	B	404	ASP
1	B	405	ILE
1	B	408	LYS
1	B	409	LEU
1	B	410	TRP
1	B	444	LEU
1	B	451	VAL
1	B	452	LEU
1	B	457	ASP
1	B	459	ILE
1	B	466	HIS
1	B	467	VAL
1	B	480	LEU
1	B	491	ASN
1	B	528	ASP
1	B	539	PHE
1	B	542	SER
2	D	751	ASN
2	D	753	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	80	GLN
1	B	96	ASN
1	B	237	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ATP	A	602	3	24,33,33	1.06	2 (8%)	31,52,52	1.99	6 (19%)
4	ATP	B	602	3	24,33,33	1.06	2 (8%)	31,52,52	2.23	6 (19%)

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	ATP	A	602	3	-	0/18/38/38	0/3/3/3
4	ATP	B	602	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	ATP	O4'-C1'	2.13	1.43	1.41
4	B	602	ATP	O4'-C1'	2.14	1.43	1.41
4	B	602	ATP	C5-C4	3.36	1.48	1.40
4	A	602	ATP	C5-C4	3.47	1.48	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ATP	N3-C2-N1	-7.25	123.34	128.89
4	A	602	ATP	N3-C2-N1	-6.35	124.03	128.89
4	B	602	ATP	PA-O3A-PB	-5.81	116.40	132.73
4	A	602	ATP	C2'-C1'-N9	-4.50	107.41	114.29
4	B	602	ATP	C2'-C1'-N9	-4.47	107.46	114.29
4	A	602	ATP	PA-O3A-PB	-3.97	121.57	132.73
4	A	602	ATP	C4-C5-N7	-3.77	106.01	109.48
4	B	602	ATP	PB-O3B-PG	-3.45	121.10	132.67
4	A	602	ATP	PB-O3B-PG	-3.14	122.12	132.67
4	B	602	ATP	C4-C5-N7	-2.73	106.97	109.48
4	A	602	ATP	O3G-PG-O2G	2.00	115.00	107.38
4	B	602	ATP	O4'-C1'-N9	2.60	113.53	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	1	0
4	B	602	ATP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	493/549 (89%)	-0.07	14 (2%) 56 45	211, 266, 316, 339	0
1	B	494/549 (89%)	0.06	20 (4%) 42 32	219, 265, 341, 379	0
2	C	6/8 (75%)	0.10	1 (16%) 2 3	251, 260, 276, 280	0
2	D	4/8 (50%)	0.20	0 100 100	260, 267, 270, 285	0
All	All	997/1114 (89%)	-0.00	35 (3%) 48 37	211, 266, 330, 379	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	LEU	8.4
1	B	100	LEU	8.4
1	A	27	LEU	7.3
1	B	67	GLU	6.2
1	A	30	LEU	5.0
1	B	70	PRO	4.9
1	A	66	SER	4.7
1	A	26	ALA	4.7
1	B	69	GLY	4.7
1	A	29	TYR	4.1
1	B	61	TYR	4.1
1	B	73	ASP	4.0
1	A	28	THR	3.9
1	A	31	GLU	3.6
1	B	101	LEU	3.4
1	B	77	TYR	3.3
1	B	72	ILE	3.2
1	B	36	PHE	3.1
1	B	51	LEU	3.0
1	B	521	GLU	2.9
1	A	32	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	288	ILE	2.7
1	A	417	ASP	2.7
1	B	65	ALA	2.7
1	B	71	LEU	2.7
1	B	14	HIS	2.7
1	A	77	TYR	2.7
1	A	105	VAL	2.5
1	A	33	LYS	2.5
1	B	37	THR	2.4
2	C	754	GLY	2.3
1	B	34	ASN	2.2
1	A	70	PRO	2.2
1	B	426	LEU	2.2
1	A	78	ASN	2.2

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ATP	A	602	31/31	0.80	0.38	0.79	221,239,252,253	0
4	ATP	B	602	31/31	0.80	0.42	0.72	226,238,251,253	0
3	MG	B	601	1/1	0.97	0.40	-	218,218,218,218	0
3	MG	A	601	1/1	0.83	0.33	-	185,185,185,185	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.