



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:40 PM GMT

PDB ID : 4M9Z
Title : Crystal structure of CED-4 bound CED-3 fragment
Authors : Huang, W.J.; Jinag, T.Y.; Choi, W.Y.; Wang, J.W.; Shi, Y.G.
Deposited on : 2013-08-15
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

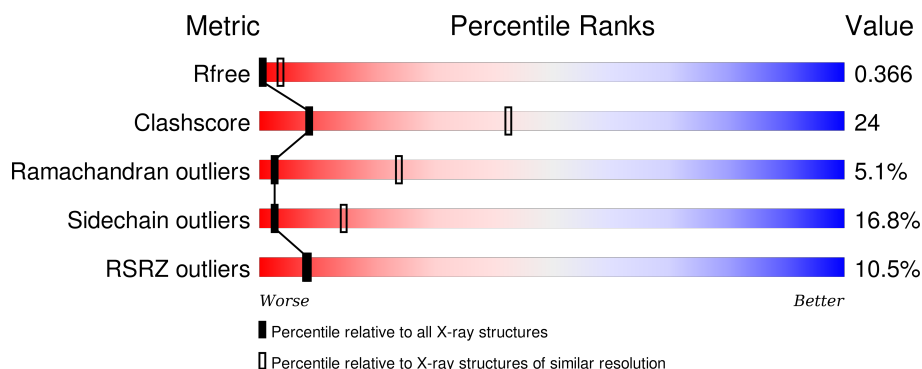
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 ≥ 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	<div> <div>5%</div> <div>44% 39% 9% 7%</div> </div>
1	B	549	<div> <div>10%</div> <div>40% 43% 10% 7%</div> </div>
1	C	549	<div> <div>8%</div> <div>42% 42% 9% 7%</div> </div>
1	D	549	<div> <div>14%</div> <div>41% 41% 10% 7%</div> </div>
2	E	8	<div> <div>25% 38% 13% 25%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	8	
2	G	8	
2	H	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	601	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16687 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			
1	C	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	D	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			

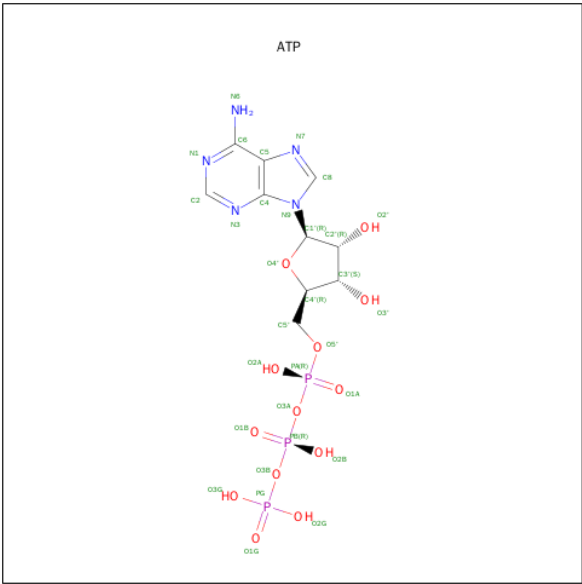
- Molecule 2 is a protein called CED-3 fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	Se	0	0	0
			50	35	7	7	1			
2	F	5	Total	C	N	O	Se	0	0	0
			46	33	6	6	1			
2	G	5	Total	C	N	O	Se	0	0	0
			46	33	6	6	1			
2	H	6	Total	C	N	O	Se	0	0	0
			53	38	7	7	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		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

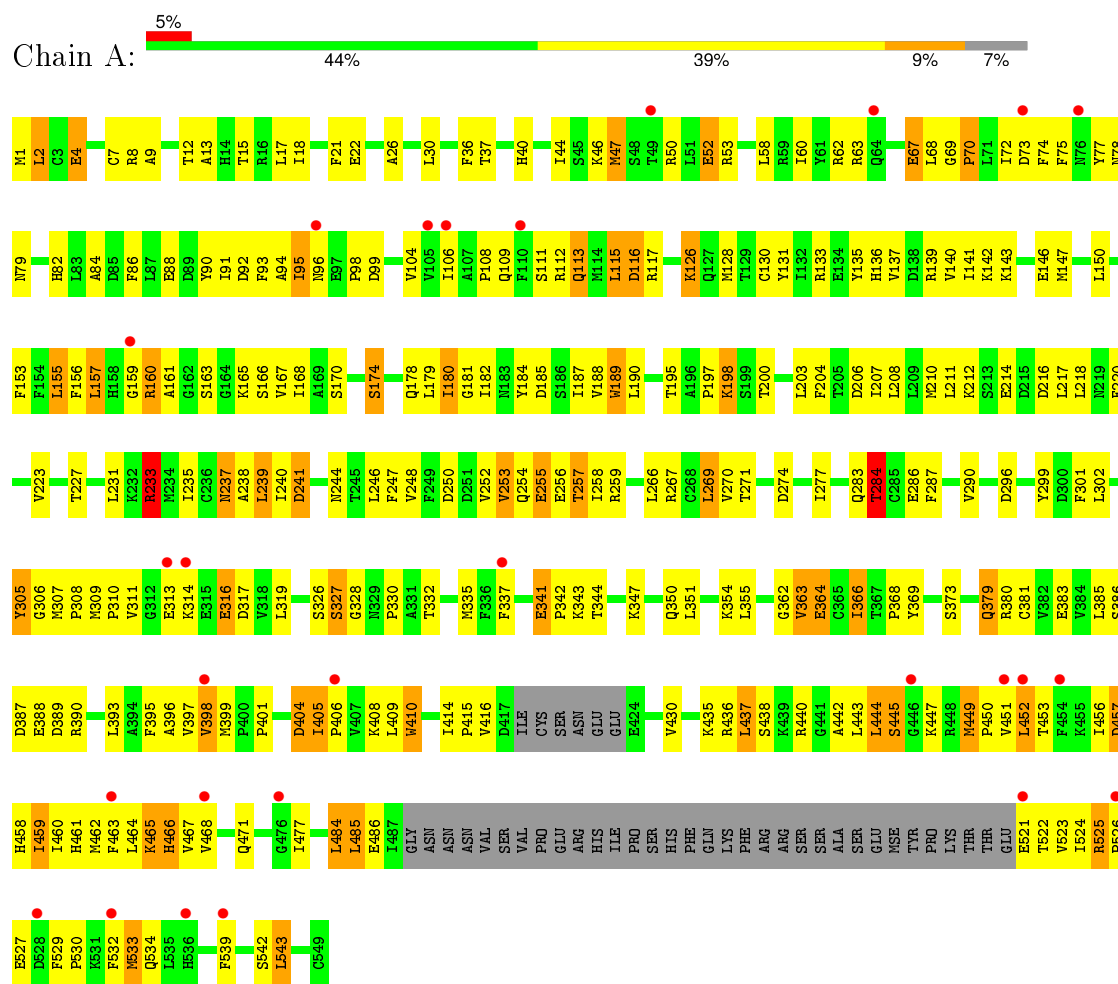


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

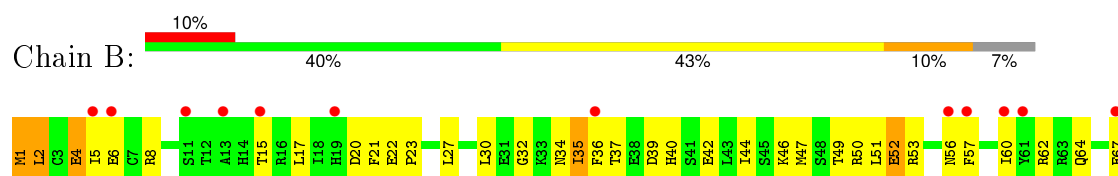
3 Residue-property plots

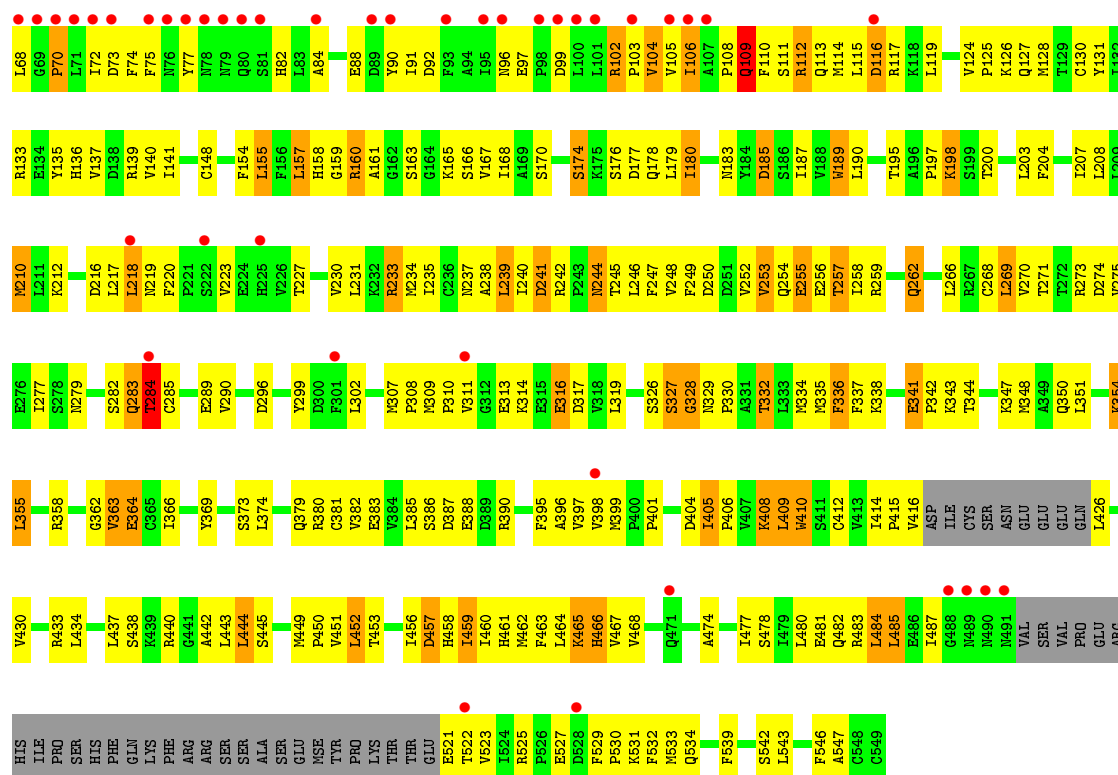
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

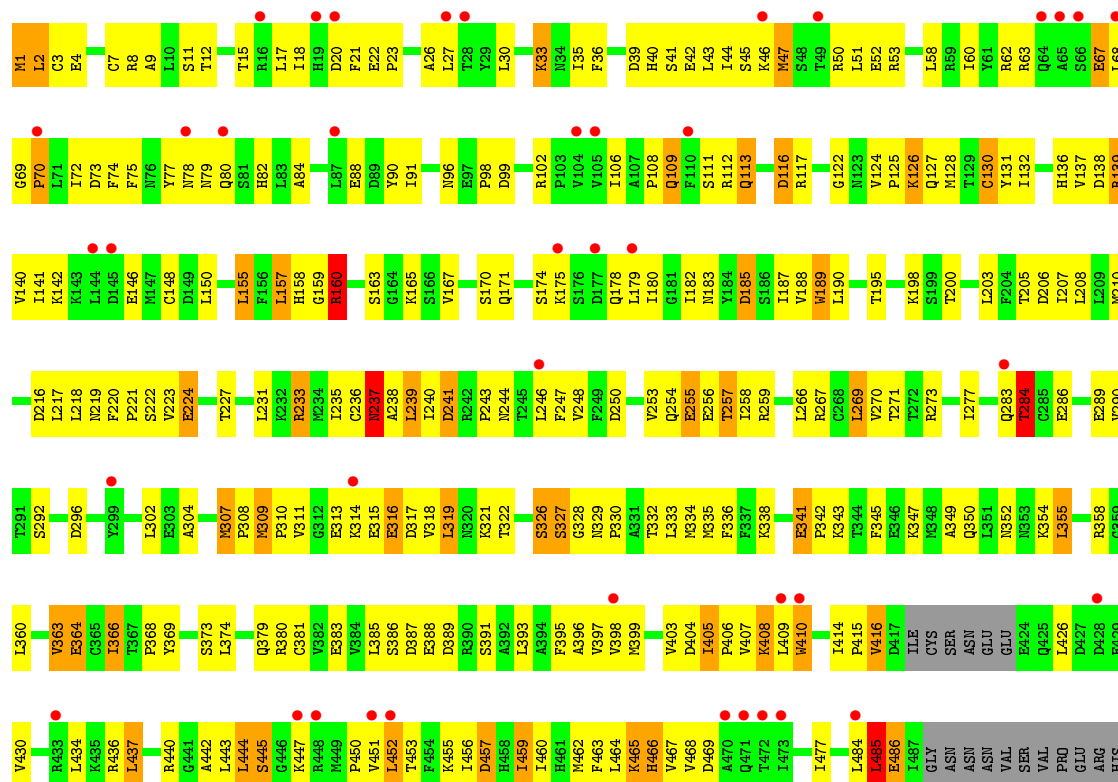
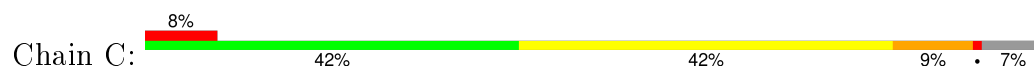


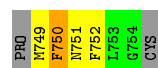
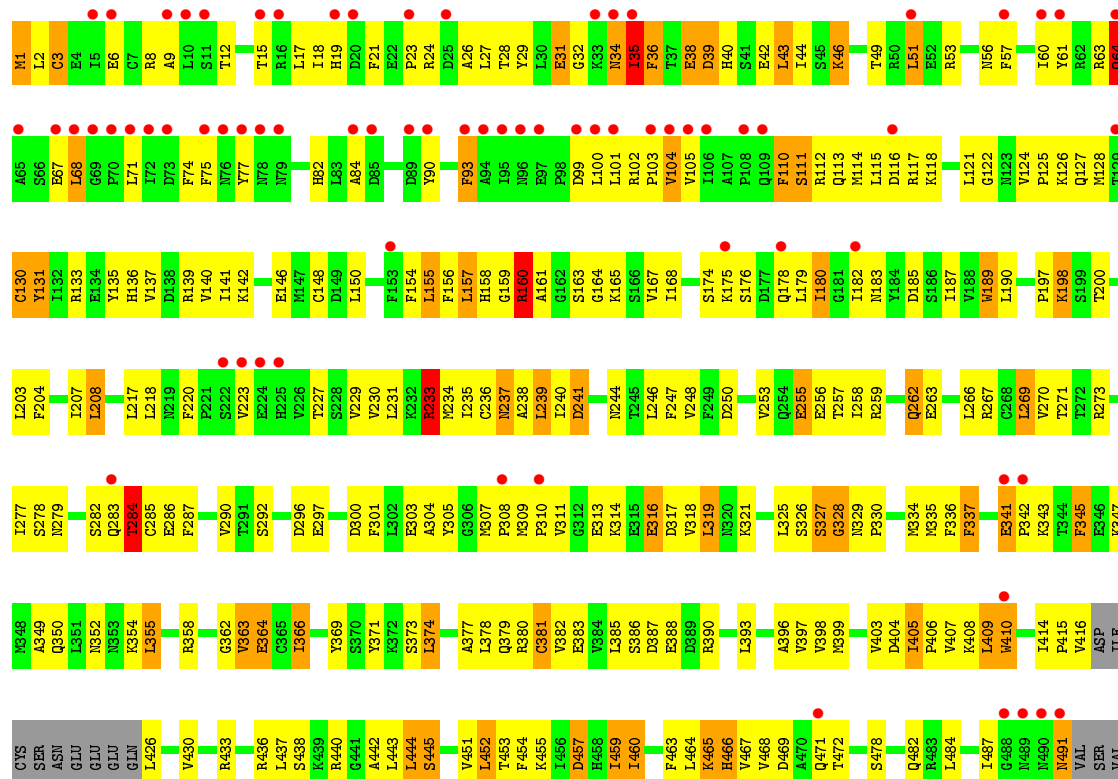
• Molecule 1: Cell death protein 4

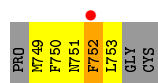




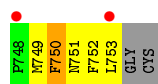
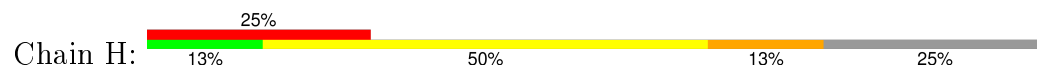
• Molecule 1: Cell death protein 4







- Molecule 2: CED-3 fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.17Å 178.17Å 200.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.21 – 3.40 44.33 – 3.40	Depositor EDS
% Data completeness (in resolution range)	57.0 (43.21-3.40) 78.5 (44.33-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.270 , 0.327 0.309 , 0.366	Depositor DCC
R_{free} test set	1759 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 35224 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16687	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2870e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	0.33	0/4147	0.73	3/5577 (0.1%)
1	B	0.33	0/4153	0.73	2/5585 (0.0%)
1	C	0.31	0/4147	0.70	1/5577 (0.0%)
1	D	0.31	0/4153	0.71	3/5585 (0.1%)
2	E	0.28	0/51	0.52	0/66
2	F	0.31	0/47	0.50	0/61
2	G	0.30	0/47	0.65	0/61
2	H	0.33	0/54	0.73	0/69
All	All	0.32	0/16799	0.72	9/22581 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	LEU	CB-CG-CD2	-8.71	96.19	111.00
1	D	484	LEU	CA-CB-CG	6.41	130.04	115.30
1	A	306	GLY	N-CA-C	5.88	127.79	113.10
1	D	160	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	484	LEU	CA-CB-CG	5.79	128.62	115.30
1	C	160	ARG	NE-CZ-NH1	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	233	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	336	PHE	CB-CG-CD1	-5.06	117.26	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	TYR	Mainchain
1	B	284	THR	Mainchain

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	4108	199	1
1	B	4094	0	4116	197	1
1	C	4088	0	4108	207	0
1	D	4094	0	4116	205	0
2	E	50	0	46	1	0
2	F	46	0	43	2	0
2	G	46	0	43	4	0
2	H	53	0	51	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	1	0
4	D	31	0	12	2	0
All	All	16687	0	16679	799	1

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 (799) 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:484:LEU:HD11	1:A:533:MSE:HG2	1.46	0.98
1:C:63:ARG:HE	1:C:240:ILE:HD11	1.31	0.93
1:D:160:ARG:HH11	1:D:160:ARG:HG3	1.34	0.91
1:C:160:ARG:HH11	1:C:160:ARG:HG3	1.35	0.91
1:D:364:GLU:HB2	1:D:373:SER:HB3	1.55	0.89
1:A:63:ARG:HE	1:A:240:ILE:HD11	1.38	0.88
1:C:47:MSE:HB2	1:C:53:ARG:HG3	1.57	0.87
1:A:302:LEU:HD13	1:A:319:LEU:HD11	1.59	0.82
1:A:47:MSE:HB2	1:A:53:ARG:HG3	1.60	0.82
1:B:20:ASP:OD2	1:B:82:HIS:NE2	2.12	0.82
1:D:160:ARG:NH1	1:D:442:ALA:O	2.15	0.79
1:D:150:LEU:O	1:D:267:ARG:NH1	2.18	0.77
1:C:364:GLU:HB2	1:C:373:SER:HB3	1.67	0.77
1:D:366:ILE:HD12	1:D:366:ILE:H	1.50	0.76
1:A:366:ILE:HD12	1:A:366:ILE:H	1.51	0.76
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.67	0.75
1:B:366:ILE:HD12	1:B:366:ILE:H	1.52	0.75
1:C:366:ILE:H	1:C:366:ILE:HD12	1.50	0.74
1:A:449:MSE:HE2	1:A:450:PRO:HA	1.69	0.74
1:C:75:PHE:HB2	1:C:84:ALA:HB2	1.70	0.74
1:A:364:GLU:HB2	1:A:373:SER:HB3	1.70	0.73
1:B:165:LYS:HG2	1:B:290:VAL:HG21	1.70	0.73
1:D:347:LYS:NZ	1:D:350:GLN:OE1	2.22	0.73
1:B:190:LEU:HD12	1:B:207:ILE:HG13	1.71	0.73
1:D:122:GLY:HA3	1:D:187:ILE:HG23	1.71	0.73
1:A:165:LYS:HG2	1:A:290:VAL:HG21	1.69	0.72
1:C:160:ARG:NH1	1:C:442:ALA:O	2.23	0.71
1:B:406:PRO:HA	1:B:453:THR:HG22	1.73	0.71
1:C:128:MSE:HE3	1:D:282:SER:HB2	1.72	0.71
1:C:90:TYR:HE2	1:C:106:ILE:HD11	1.55	0.71
1:D:443:LEU:HD23	1:D:460:ILE:HD11	1.71	0.71
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.55	0.70
1:B:302:LEU:HD13	1:B:319:LEU:HD11	1.72	0.70
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.73	0.70
1:B:135:TYR:O	1:B:139:ARG:HG3	1.90	0.70
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.73	0.69
1:C:406:PRO:HA	1:C:453:THR:HG22	1.74	0.69
1:C:128:MSE:HG3	1:C:167:VAL:HG22	1.73	0.69
1:A:386:SER:OG	1:A:388:GLU:OE1	2.10	0.69
1:A:96:ASN:O	1:A:98:PRO:HD3	1.91	0.69
1:B:478:SER:O	1:B:482:GLN:HG2	1.93	0.69
1:C:8:ARG:HG2	1:C:8:ARG:HH11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:VAL:HG21	1:A:468:VAL:HG21	1.75	0.68
1:D:341:GLU:HB2	1:D:342:PRO:HD3	1.75	0.68
1:C:58:LEU:O	1:C:62:ARG:HG3	1.93	0.68
1:D:478:SER:O	1:D:482:GLN:HG2	1.93	0.68
2:H:750:PHE:HB3	2:H:753:LEU:HD21	1.73	0.68
1:C:96:ASN:O	1:C:98:PRO:HD3	1.94	0.67
1:D:255:GLU:O	1:D:259:ARG:HG3	1.94	0.67
1:B:230:VAL:HG12	1:B:234:MSE:HE2	1.76	0.67
1:C:195:THR:O	1:C:254:GLN:NE2	2.28	0.67
1:D:8:ARG:NH1	1:D:90:TYR:OH	2.27	0.66
1:C:484:LEU:HD11	1:C:533:MSE:HG2	1.76	0.66
1:D:230:VAL:HG12	1:D:234:MSE:HE2	1.78	0.66
1:C:67:GLU:HG2	1:C:69:GLY:H	1.59	0.66
1:B:216:ASP:OD1	1:B:219:ASN:ND2	2.26	0.66
1:C:255:GLU:O	1:C:259:ARG:HG3	1.97	0.65
1:D:165:LYS:HG2	1:D:290:VAL:HG21	1.78	0.65
1:C:126:LYS:NZ	1:D:283:GLN:HG3	2.12	0.65
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.79	0.65
1:C:355:LEU:HD21	1:C:363:VAL:HB	1.77	0.65
1:B:92:ASP:OD1	1:B:96:ASN:ND2	2.29	0.64
1:D:463:PHE:O	1:D:467:VAL:HB	1.98	0.64
1:A:447:LYS:HE2	1:A:450:PRO:HD2	1.78	0.64
1:A:90:TYR:HE2	1:A:106:ILE:HD11	1.61	0.64
1:C:314:LYS:HA	1:C:317:ASP:HB2	1.79	0.64
1:C:165:LYS:HG2	1:C:290:VAL:HG21	1.79	0.64
1:C:397:VAL:HG21	1:C:468:VAL:HG21	1.80	0.64
1:D:40:HIS:HA	1:D:43:LEU:HB2	1.80	0.64
1:C:141:ILE:HD12	1:C:175:LYS:HE2	1.80	0.63
1:C:309:MSE:HG3	1:C:310:PRO:HD2	1.81	0.63
1:C:335:MSE:HE3	1:C:364:GLU:HA	1.80	0.63
1:D:43:LEU:O	1:D:56:ASN:ND2	2.32	0.63
1:A:190:LEU:HD12	1:A:207:ILE:HG13	1.79	0.63
1:B:385:LEU:O	1:B:390:ARG:NH2	2.32	0.62
1:B:397:VAL:HG21	1:B:468:VAL:HG21	1.80	0.62
1:B:464:LEU:O	1:B:468:VAL:HG22	1.98	0.62
1:A:67:GLU:HG2	1:A:69:GLY:H	1.64	0.62
1:C:136:HIS:O	1:C:140:VAL:HG23	2.00	0.62
1:B:335:MSE:HE3	1:B:364:GLU:HA	1.81	0.62
1:C:160:ARG:HB3	1:C:163:SER:HB3	1.81	0.62
1:D:128:MSE:HG3	1:D:167:VAL:HG22	1.81	0.62
1:A:128:MSE:HE3	1:B:282:SER:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:ASP:HB2	2:H:749:MSE:HA	1.80	0.62
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.81	0.62
1:D:49:THR:HG22	1:D:51:LEU:H	1.63	0.62
1:D:309:MSE:HG3	1:D:310:PRO:HD2	1.82	0.62
1:B:487:ILE:O	1:B:531:LYS:NZ	2.33	0.61
1:C:341:GLU:HB2	1:C:342:PRO:HD3	1.82	0.61
1:A:464:LEU:O	1:A:468:VAL:HG22	2.00	0.61
1:C:525:ARG:HD3	1:C:535:LEU:HD13	1.82	0.61
1:C:44:ILE:O	1:C:53:ARG:HG2	2.00	0.61
1:D:141:ILE:HD12	1:D:175:LYS:HE3	1.81	0.61
1:A:58:LEU:O	1:A:62:ARG:HG3	2.00	0.61
1:B:47:MSE:HB2	1:B:53:ARG:HG3	1.81	0.61
1:B:8:ARG:HG2	1:B:8:ARG:HH11	1.63	0.61
1:C:190:LEU:HD12	1:C:207:ILE:HG13	1.82	0.61
1:C:452:LEU:H	1:C:452:LEU:HD23	1.65	0.61
1:B:379:GLN:O	1:B:383:GLU:HG3	2.00	0.61
1:A:452:LEU:H	1:A:452:LEU:HD23	1.64	0.61
1:C:464:LEU:O	1:C:468:VAL:HG22	2.01	0.61
1:D:114:MSE:HG3	1:D:180:ILE:HB	1.83	0.61
1:A:92:ASP:OD1	1:A:96:ASN:ND2	2.29	0.61
1:D:397:VAL:HG21	1:D:468:VAL:HG21	1.82	0.60
1:B:299:TYR:HA	1:B:302:LEU:HD12	1.83	0.60
1:B:395:PHE:HD2	1:B:415:PRO:HD3	1.66	0.60
1:C:469:ASP:HB2	2:G:749:MSE:HA	1.83	0.60
1:D:464:LEU:O	1:D:468:VAL:HG22	2.02	0.60
1:C:327:SER:HB2	1:C:459:ILE:HG13	1.83	0.60
1:C:160:ARG:NH1	1:C:160:ARG:HG3	2.13	0.60
1:B:204:PHE:HA	1:B:207:ILE:HD12	1.83	0.60
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.83	0.60
1:D:160:ARG:NH1	1:D:160:ARG:HG3	2.10	0.60
1:A:128:MSE:HG3	1:A:167:VAL:HG22	1.83	0.60
1:B:47:MSE:HE3	1:B:52:GLU:HG2	1.84	0.60
1:A:410:TRP:HD1	1:A:414:ILE:HD13	1.66	0.60
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.84	0.60
1:C:178:GLN:HA	1:C:182:ILE:HB	1.83	0.60
1:D:386:SER:OG	1:D:388:GLU:OE1	2.20	0.60
1:C:447:LYS:HE2	1:C:450:PRO:HD2	1.84	0.59
1:A:36:PHE:HD2	1:A:40:HIS:HB3	1.66	0.59
1:A:309:MSE:HG3	1:A:310:PRO:HD2	1.84	0.59
1:D:452:LEU:HD23	1:D:452:LEU:H	1.67	0.59
1:C:443:LEU:HD23	1:C:460:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:NE	1:D:297:GLU:OE1	2.33	0.59
1:B:108:PRO:O	1:B:109:GLN:HB2	2.01	0.59
1:D:233:ARG:HH11	1:D:233:ARG:HG3	1.68	0.59
1:D:465:LYS:HD3	1:D:466:HIS:CE1	2.37	0.59
1:A:4:GLU:OE2	1:A:267:ARG:NH2	2.36	0.59
1:C:414:ILE:HG21	1:C:430:VAL:HG13	1.83	0.59
1:A:157:LEU:HD22	1:A:290:VAL:HG22	1.85	0.59
1:B:309:MSE:HG3	1:B:310:PRO:HD2	1.84	0.59
1:B:102:ARG:HG3	1:B:103:PRO:CD	2.33	0.59
1:A:90:TYR:CE2	1:A:106:ILE:HD11	2.38	0.59
1:A:385:LEU:O	1:A:390:ARG:NH2	2.36	0.59
1:A:335:MSE:HE3	1:A:364:GLU:HA	1.83	0.59
1:C:137:VAL:O	1:C:141:ILE:HG13	2.02	0.59
1:C:150:LEU:O	1:C:267:ARG:NH1	2.34	0.59
1:A:214:GLU:HG3	1:B:237:ASN:CG	2.23	0.58
1:A:457:ASP:OD1	1:A:457:ASP:N	2.35	0.58
1:D:342:PRO:O	1:D:343:LYS:HB3	2.02	0.58
1:C:216:ASP:HA	1:C:219:ASN:HB2	1.85	0.58
1:B:111:SER:O	1:B:115:LEU:HB3	2.03	0.58
1:A:395:PHE:HD2	1:A:415:PRO:HD3	1.68	0.58
1:A:342:PRO:O	1:A:343:LYS:HB3	2.04	0.58
1:C:465:LYS:HD3	1:C:466:HIS:CE1	2.38	0.58
1:B:437:LEU:HB3	1:B:444:LEU:HD22	1.86	0.58
1:C:397:VAL:HG22	1:C:464:LEU:HB3	1.84	0.58
1:C:465:LYS:HD3	1:C:466:HIS:HE1	1.69	0.58
1:B:30:LEU:HB3	1:B:36:PHE:CD1	2.39	0.58
1:D:385:LEU:O	1:D:390:ARG:NH2	2.37	0.58
1:B:47:MSE:HE2	1:B:56:ASN:HD21	1.69	0.57
1:A:437:LEU:HB3	1:A:444:LEU:HD22	1.84	0.57
1:B:443:LEU:HD23	1:B:460:ILE:HD11	1.86	0.57
1:A:72:ILE:HG21	1:A:88:GLU:HG3	1.85	0.57
2:G:750:PHE:O	2:G:752:PHE:N	2.37	0.57
1:A:414:ILE:HG21	1:A:430:VAL:HG13	1.86	0.57
1:D:24:ARG:HG3	1:D:27:LEU:HD12	1.85	0.57
2:E:750:PHE:O	2:E:752:PHE:N	2.37	0.57
1:C:395:PHE:HD2	1:C:415:PRO:HD3	1.69	0.57
1:D:436:ARG:O	1:D:440:ARG:HG3	2.04	0.57
1:A:379:GLN:O	1:A:383:GLU:HG3	2.05	0.57
1:C:527:GLU:HA	1:C:530:PRO:HG3	1.87	0.57
1:D:250:ASP:HA	1:D:271:THR:OG1	2.05	0.57
1:C:388:GLU:O	1:C:391:SER:OG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:MSE:HG3	1:B:167:VAL:HG22	1.85	0.57
1:A:63:ARG:HE	1:A:240:ILE:CD1	2.13	0.57
1:D:335:MSE:HE3	1:D:364:GLU:HA	1.86	0.56
1:B:4:GLU:HG3	1:B:5:ILE:N	2.19	0.56
1:A:150:LEU:O	1:A:267:ARG:NH1	2.39	0.56
1:A:247:PHE:HE2	1:A:266:LEU:HD22	1.69	0.56
1:B:302:LEU:HD23	1:B:337:PHE:CE1	2.41	0.56
1:D:283:GLN:HG2	1:D:284:THR:H	1.70	0.56
1:B:342:PRO:O	1:B:343:LYS:HB3	2.04	0.56
1:D:354:LYS:HD3	1:D:362:GLY:O	2.04	0.56
1:A:160:ARG:HG2	1:A:161:ALA:H	1.69	0.56
1:D:111:SER:O	1:D:115:LEU:HB3	2.05	0.56
1:C:159:GLY:N	1:C:165:LYS:HD3	2.21	0.56
1:A:406:PRO:HA	1:A:453:THR:HG22	1.87	0.56
1:A:91:ILE:O	1:A:95:ILE:HG13	2.05	0.56
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.88	0.56
1:C:233:ARG:HH11	1:C:233:ARG:HG3	1.70	0.56
1:B:529:PHE:HB3	1:B:532:PHE:CZ	2.40	0.56
1:D:406:PRO:HA	1:D:453:THR:HG22	1.86	0.56
1:A:79:ASN:ND2	1:B:36:PHE:O	2.38	0.56
1:C:126:LYS:HZ3	1:D:283:GLN:HG3	1.70	0.56
1:A:438:SER:O	1:A:442:ALA:HA	2.05	0.56
1:A:233:ARG:HH11	1:A:233:ARG:HG3	1.71	0.56
1:C:326:SER:O	1:C:328:GLY:N	2.39	0.55
1:B:452:LEU:HD23	1:B:452:LEU:H	1.71	0.55
1:A:465:LYS:HD3	1:A:466:HIS:CE1	2.41	0.55
1:B:1:MSE:HA	1:B:62:ARG:O	2.06	0.55
1:D:155:LEU:HB3	1:D:269:LEU:HD23	1.88	0.55
1:A:415:PRO:O	1:A:416:VAL:HG23	2.06	0.55
2:F:750:PHE:HB3	2:F:753:LEU:HA	1.88	0.55
1:B:274:ASP:OD2	1:B:440:ARG:NH1	2.40	0.55
1:D:255:GLU:HB3	1:D:277:ILE:HG22	1.88	0.55
1:A:257:THR:HG22	1:A:258:ILE:N	2.22	0.55
1:A:354:LYS:HD3	1:A:362:GLY:O	2.07	0.55
1:B:410:TRP:HD1	1:B:414:ILE:HD13	1.72	0.55
1:D:457:ASP:N	1:D:457:ASP:OD1	2.39	0.55
1:C:273:ARG:NH2	1:C:380:ARG:HH21	2.05	0.55
1:D:160:ARG:HB3	1:D:163:SER:HB3	1.86	0.55
1:C:532:PHE:HB2	1:C:534:GLN:HG2	1.88	0.55
1:A:250:ASP:HA	1:A:271:THR:OG1	2.06	0.55
1:A:397:VAL:O	1:A:461:HIS:NE2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PRO:O	1:C:343:LYS:HB3	2.07	0.55
1:C:457:ASP:N	1:C:457:ASP:OD1	2.40	0.54
1:B:529:PHE:N	1:B:530:PRO:HD3	2.22	0.54
1:D:487:ILE:O	1:D:531:LYS:NZ	2.40	0.54
1:D:537:GLN:O	1:D:541:ASP:N	2.38	0.54
1:C:36:PHE:HD2	1:C:40:HIS:HB3	1.72	0.54
1:A:178:GLN:O	1:A:182:ILE:HB	2.07	0.54
1:C:250:ASP:HA	1:C:271:THR:OG1	2.08	0.54
1:D:42:GLU:O	1:D:46:LYS:NZ	2.26	0.54
1:D:347:LYS:O	1:D:350:GLN:HB2	2.06	0.54
1:D:405:ILE:HG13	1:D:409:LEU:HB3	1.90	0.54
1:D:113:GLN:O	1:D:118:LYS:HG3	2.08	0.54
1:B:72:ILE:HG21	1:B:88:GLU:HG3	1.88	0.54
1:A:157:LEU:HD11	1:A:168:ILE:HG22	1.89	0.54
1:A:397:VAL:HG22	1:A:464:LEU:HB3	1.88	0.54
1:D:310:PRO:HA	1:D:345:PHE:HE2	1.72	0.54
1:C:407:VAL:HG23	1:C:452:LEU:O	2.07	0.54
1:B:250:ASP:HA	1:B:271:THR:OG1	2.07	0.54
1:D:326:SER:O	1:D:328:GLY:N	2.40	0.54
1:C:463:PHE:O	1:C:467:VAL:HB	2.08	0.54
1:B:458:HIS:HB3	1:B:462:MSE:HE2	1.90	0.54
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.73	0.54
1:A:44:ILE:O	1:A:53:ARG:HG2	2.08	0.53
1:B:23:PRO:HG2	1:B:53:ARG:C	2.29	0.53
1:C:90:TYR:CE2	1:C:106:ILE:HD11	2.40	0.53
1:B:415:PRO:O	1:B:416:VAL:HG23	2.08	0.53
1:A:389:ASP:HB3	1:A:437:LEU:HD21	1.89	0.53
1:B:457:ASP:N	1:B:457:ASP:OD1	2.40	0.53
1:A:521:GLU:C	1:A:523:VAL:H	2.12	0.53
1:D:136:HIS:O	1:D:140:VAL:HG23	2.08	0.53
1:C:354:LYS:O	1:C:358:ARG:HB2	2.09	0.53
1:B:112:ARG:HA	1:B:116:ASP:HB2	1.90	0.53
1:D:397:VAL:HG22	1:D:464:LEU:HB3	1.90	0.53
1:A:436:ARG:O	1:A:440:ARG:HG3	2.09	0.53
1:D:529:PHE:N	1:D:530:PRO:HD3	2.24	0.53
1:A:36:PHE:CD2	1:A:40:HIS:HB3	2.44	0.53
1:C:8:ARG:NH1	1:C:185:ASP:OD1	2.42	0.53
1:C:67:GLU:HG2	1:C:69:GLY:N	2.23	0.53
1:D:135:TYR:O	1:D:139:ARG:HG3	2.08	0.53
1:D:247:PHE:HE2	1:D:266:LEU:HD22	1.74	0.53
1:B:157:LEU:HD22	1:B:290:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:GLU:CB	1:D:342:PRO:HD3	2.39	0.53
1:A:189:TRP:CE3	1:A:248:VAL:HG11	2.44	0.52
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.91	0.52
1:B:257:THR:HG22	1:B:258:ILE:N	2.24	0.52
1:B:386:SER:OG	1:B:388:GLU:OE1	2.27	0.52
1:B:35:ILE:HD12	1:B:70:PRO:HG2	1.89	0.52
1:B:364:GLU:HB2	1:B:373:SER:HB3	1.90	0.52
1:A:443:LEU:HD23	1:A:460:ILE:HD11	1.91	0.52
1:A:93:PHE:HE2	1:A:104:VAL:HG11	1.75	0.52
1:C:122:GLY:HA3	1:C:187:ILE:HG23	1.91	0.52
1:B:527:GLU:OE1	1:B:527:GLU:N	2.42	0.52
1:C:436:ARG:O	1:C:440:ARG:HG3	2.08	0.52
1:B:157:LEU:HD11	1:B:168:ILE:CG2	2.39	0.52
1:B:109:GLN:C	1:B:111:SER:H	2.12	0.52
1:A:458:HIS:HB3	1:A:462:MSE:HE2	1.92	0.52
1:A:133:ARG:O	1:A:137:VAL:HG23	2.09	0.52
1:A:165:LYS:N	4:A:602:ATP:O2B	2.42	0.52
1:C:102:ARG:HG2	1:C:182:ILE:HG22	1.92	0.52
1:C:216:ASP:H	1:C:218:LEU:HD23	1.74	0.52
1:C:26:ALA:HB2	1:C:74:PHE:CE1	2.45	0.52
1:A:255:GLU:O	1:A:259:ARG:HG3	2.10	0.52
1:D:1:MSE:O	1:D:2:LEU:HD23	2.10	0.52
2:H:749:MSE:O	2:H:750:PHE:HB2	2.10	0.52
1:B:231:LEU:HA	1:B:234:MSE:HE3	1.91	0.52
1:B:388:GLU:HB3	1:B:433:ARG:HH21	1.74	0.52
1:B:438:SER:O	1:B:442:ALA:HA	2.10	0.52
1:A:67:GLU:HG2	1:A:69:GLY:N	2.24	0.51
1:D:465:LYS:HD3	1:D:466:HIS:HE1	1.73	0.51
1:B:255:GLU:O	1:B:259:ARG:HG3	2.10	0.51
1:A:143:LYS:O	1:A:147:MSE:HG3	2.10	0.51
1:B:50:ARG:HA	1:B:53:ARG:HE	1.76	0.51
1:C:283:GLN:HG2	1:C:284:THR:H	1.74	0.51
1:D:532:PHE:C	1:D:534:GLN:H	2.13	0.51
1:A:532:PHE:HB2	1:A:534:GLN:HG2	1.91	0.51
1:C:41:SER:O	1:C:45:SER:OG	2.24	0.51
1:C:18:ILE:O	1:C:50:ARG:NH2	2.42	0.51
1:C:379:GLN:O	1:C:383:GLU:HG3	2.10	0.51
1:D:237:ASN:C	1:D:239:LEU:H	2.14	0.51
1:C:23:PRO:HG2	1:C:53:ARG:HB3	1.93	0.51
1:C:247:PHE:HE2	1:C:266:LEU:HD22	1.75	0.51
1:D:197:PRO:HD2	1:D:198:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD11	1:B:168:ILE:HG22	1.92	0.51
1:B:336:PHE:HE2	1:B:348:MSE:SE	2.44	0.51
1:D:437:LEU:HB3	1:D:444:LEU:HD22	1.93	0.51
1:A:247:PHE:CE2	1:A:266:LEU:HD13	2.46	0.51
1:C:313:GLU:O	1:C:316:GLU:HG3	2.09	0.51
1:C:72:ILE:HG13	1:C:88:GLU:HG3	1.91	0.51
1:C:9:ALA:HB2	1:C:90:TYR:CD1	2.46	0.51
1:B:397:VAL:HG22	1:B:464:LEU:HB3	1.93	0.51
1:D:388:GLU:HB3	1:D:433:ARG:HH21	1.74	0.51
1:B:158:HIS:CE1	1:B:289:GLU:HB2	2.45	0.51
1:A:111:SER:C	1:A:113:GLN:H	2.14	0.51
1:B:47:MSE:HE2	1:B:56:ASN:ND2	2.26	0.51
1:B:197:PRO:HD2	1:B:198:LYS:HE2	1.92	0.51
1:D:204:PHE:HA	1:D:207:ILE:HD12	1.92	0.51
1:A:40:HIS:ND1	1:A:60:ILE:HD13	2.26	0.51
1:B:4:GLU:O	1:B:8:ARG:HB2	2.11	0.51
1:B:160:ARG:NH1	1:B:442:ALA:O	2.44	0.51
1:D:75:PHE:HB3	1:D:84:ALA:HB2	1.92	0.51
1:C:102:ARG:HG2	1:C:182:ILE:CG2	2.40	0.51
1:B:170:SER:O	1:B:174:SER:HB2	2.11	0.51
1:D:415:PRO:O	1:D:416:VAL:HG23	2.11	0.51
1:D:257:THR:HG22	1:D:258:ILE:N	2.26	0.51
1:B:414:ILE:HG21	1:B:430:VAL:HG13	1.93	0.51
1:C:188:VAL:HB	1:C:247:PHE:CD1	2.47	0.50
1:D:200:THR:HG21	1:D:256:GLU:HB3	1.93	0.50
1:C:158:HIS:CE1	1:C:289:GLU:HB2	2.46	0.50
1:C:347:LYS:HA	1:C:350:GLN:HB2	1.93	0.50
1:B:189:TRP:CE3	1:B:248:VAL:HG11	2.46	0.50
1:A:47:MSE:HB2	1:A:53:ARG:CG	2.37	0.50
1:B:47:MSE:HB3	1:B:52:GLU:HB3	1.93	0.50
2:F:751:ASN:ND2	2:F:751:ASN:O	2.44	0.50
1:A:136:HIS:O	1:A:140:VAL:HG23	2.11	0.50
1:D:159:GLY:N	1:D:165:LYS:HD3	2.26	0.50
1:A:111:SER:O	1:A:113:GLN:N	2.44	0.50
1:B:160:ARG:HG2	1:B:161:ALA:H	1.76	0.50
1:A:216:ASP:H	1:A:218:LEU:HD23	1.76	0.50
1:D:397:VAL:O	1:D:399:MSE:N	2.44	0.50
1:D:314:LYS:HA	1:D:317:ASP:HB2	1.94	0.50
1:B:463:PHE:O	1:B:467:VAL:HB	2.12	0.50
1:D:355:LEU:HD21	1:D:363:VAL:HB	1.92	0.50
1:C:165:LYS:N	4:C:602:ATP:O2B	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:THR:HG22	1:C:258:ILE:N	2.26	0.50
1:D:164:GLY:HA3	4:D:602:ATP:H2	1.75	0.50
1:B:49:THR:HG22	1:B:51:LEU:H	1.77	0.50
1:A:188:VAL:HB	1:A:247:PHE:CD1	2.46	0.50
1:C:142:LYS:O	1:C:146:GLU:HG3	2.12	0.50
1:C:189:TRP:CE3	1:C:248:VAL:HG11	2.46	0.50
1:A:135:TYR:O	1:A:139:ARG:HG3	2.12	0.50
1:A:410:TRP:CD1	1:A:414:ILE:HD13	2.47	0.49
1:C:219:ASN:O	1:C:221:PRO:HD3	2.12	0.49
1:C:125:PRO:O	1:C:170:SER:OG	2.29	0.49
1:C:150:LEU:HD11	1:C:284:THR:HG21	1.93	0.49
1:C:529:PHE:N	1:C:530:PRO:HD3	2.27	0.49
1:A:465:LYS:HD3	1:A:466:HIS:HE1	1.77	0.49
1:D:235:ILE:O	1:D:239:LEU:HB2	2.11	0.49
1:B:136:HIS:O	1:B:140:VAL:HG23	2.12	0.49
1:B:302:LEU:HD23	1:B:337:PHE:HE1	1.77	0.49
1:A:190:LEU:CD1	1:A:207:ILE:HG13	2.42	0.49
1:D:178:GLN:HB3	1:D:183:ASN:OD1	2.13	0.49
1:B:332:THR:O	1:B:336:PHE:HB2	2.12	0.49
1:C:132:ILE:HG23	1:C:137:VAL:HG21	1.93	0.49
1:B:158:HIS:CD2	1:B:275:VAL:HG13	2.47	0.49
1:B:158:HIS:HE1	1:B:289:GLU:HB2	1.77	0.49
1:D:397:VAL:C	1:D:399:MSE:H	2.15	0.49
1:B:410:TRP:CD1	1:B:414:ILE:HD13	2.47	0.49
1:B:195:THR:O	1:B:254:GLN:NE2	2.46	0.49
1:B:56:ASN:O	1:B:60:ILE:HB	2.12	0.49
1:A:299:TYR:HA	1:A:302:LEU:HD12	1.95	0.49
1:D:178:GLN:HA	1:D:182:ILE:HB	1.94	0.49
1:B:355:LEU:HD21	1:B:363:VAL:HB	1.95	0.49
1:B:332:THR:HG23	1:B:374:LEU:HB2	1.95	0.49
1:C:524:ILE:HG13	1:C:525:ARG:N	2.27	0.49
1:D:157:LEU:HD11	1:D:168:ILE:HG22	1.95	0.49
1:B:114:MSE:SE	1:B:177:ASP:HA	2.62	0.49
1:C:21:PHE:CD1	1:C:75:PHE:HE1	2.30	0.49
1:A:166:SER:HA	1:A:271:THR:HG21	1.94	0.49
1:C:343:LYS:O	1:C:343:LYS:HG2	2.14	0.48
1:D:527:GLU:N	1:D:527:GLU:OE1	2.45	0.48
1:B:252:VAL:HG11	1:B:258:ILE:HD13	1.94	0.48
1:D:378:LEU:HA	1:D:381:CYS:HB2	1.94	0.48
1:C:40:HIS:O	1:C:44:ILE:HG13	2.13	0.48
1:D:135:TYR:CZ	1:D:139:ARG:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:HG22	1:A:269:LEU:HB3	1.95	0.48
1:B:521:GLU:C	1:B:523:VAL:H	2.16	0.48
1:C:163:SER:C	1:C:330:PRO:HG2	2.34	0.48
1:C:527:GLU:OE1	1:C:527:GLU:N	2.46	0.48
1:B:314:LYS:HA	1:B:317:ASP:HB2	1.95	0.48
1:B:23:PRO:HG2	1:B:53:ARG:O	2.13	0.48
1:D:327:SER:HB2	1:D:459:ILE:HD11	1.94	0.48
1:B:307:MSE:SE	1:B:308:PRO:HD2	2.64	0.48
1:C:525:ARG:HA	1:C:526:PRO:HD3	1.64	0.48
1:A:393:LEU:HB2	1:A:437:LEU:HD11	1.94	0.48
1:C:155:LEU:HB3	1:C:269:LEU:HD23	1.96	0.48
1:A:206:ASP:O	1:A:210:MSE:HG2	2.13	0.48
1:D:318:VAL:O	1:D:321:LYS:HB3	2.13	0.48
1:A:302:LEU:HD23	1:A:337:PHE:CE1	2.49	0.48
1:C:138:ASP:OD1	1:C:175:LYS:NZ	2.38	0.48
1:D:189:TRP:CE3	1:D:248:VAL:HG11	2.47	0.48
1:A:137:VAL:O	1:A:141:ILE:HG13	2.14	0.48
1:A:170:SER:O	1:A:174:SER:HB2	2.13	0.48
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.14	0.48
1:A:8:ARG:NH1	1:A:8:ARG:HG2	2.28	0.48
1:D:399:MSE:HE3	1:D:410:TRP:CD1	2.49	0.48
1:B:341:GLU:CB	1:B:342:PRO:HD3	2.44	0.48
1:C:47:MSE:HB2	1:C:53:ARG:CG	2.36	0.48
1:D:190:LEU:CD1	1:D:207:ILE:HG13	2.43	0.48
1:C:44:ILE:HD11	1:C:60:ILE:HD12	1.96	0.48
1:B:166:SER:HA	1:B:271:THR:HG21	1.96	0.48
1:C:269:LEU:HD22	1:C:270:VAL:H	1.79	0.48
1:C:334:MSE:HE3	1:C:334:MSE:HA	1.95	0.48
1:D:334:MSE:HA	1:D:334:MSE:HE3	1.96	0.48
1:D:44:ILE:HG23	1:D:56:ASN:HB3	1.94	0.48
1:D:319:LEU:HD12	1:D:345:PHE:CE1	2.48	0.48
1:A:252:VAL:CG2	1:A:257:THR:HG21	2.44	0.48
1:B:154:PHE:HE2	1:B:262:GLN:HG3	1.78	0.48
1:C:240:ILE:HG13	1:C:241:ASP:OD1	2.14	0.47
1:A:160:ARG:NH1	1:A:442:ALA:O	2.46	0.47
1:C:315:GLU:HA	1:C:318:VAL:HG23	1.96	0.47
1:C:206:ASP:O	1:C:210:MSE:HG2	2.14	0.47
1:B:114:MSE:HG3	1:B:180:ILE:HB	1.96	0.47
1:D:110:PHE:HA	1:D:110:PHE:HD1	1.60	0.47
1:A:181:GLY:N	1:A:184:TYR:O	2.31	0.47
1:A:47:MSE:HE2	1:A:52:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ARG:HH11	1:D:233:ARG:CG	2.27	0.47
1:D:329:ASN:HA	1:D:330:PRO:HD2	1.75	0.47
1:A:187:ILE:HD13	1:A:246:LEU:HB3	1.96	0.47
1:A:195:THR:O	1:A:254:GLN:NE2	2.47	0.47
1:D:233:ARG:HA	1:D:236:CYS:SG	2.55	0.47
1:C:222:SER:OG	1:C:224:GLU:OE1	2.26	0.47
1:D:414:ILE:HG21	1:D:430:VAL:HG13	1.96	0.47
1:D:259:ARG:O	1:D:263:GLU:HG3	2.15	0.47
1:A:135:TYR:CZ	1:A:139:ARG:HD2	2.49	0.47
1:B:114:MSE:O	1:B:119:LEU:HG	2.14	0.47
1:D:154:PHE:HE2	1:D:262:GLN:HG3	1.79	0.47
1:C:30:LEU:HD21	1:C:70:PRO:O	2.14	0.47
1:C:200:THR:HG21	1:C:256:GLU:HB3	1.96	0.47
1:B:336:PHE:CD1	1:B:363:VAL:HG21	2.50	0.47
1:C:126:LYS:HD3	1:D:283:GLN:HE21	1.79	0.47
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.28	0.47
1:B:88:GLU:HA	1:B:91:ILE:HG22	1.96	0.47
1:B:88:GLU:O	1:B:91:ILE:HG22	2.15	0.47
1:A:255:GLU:HB3	1:A:277:ILE:HG22	1.96	0.47
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.96	0.47
1:C:158:HIS:HE1	1:C:289:GLU:HB2	1.80	0.47
1:C:444:LEU:HD12	1:C:444:LEU:HA	1.74	0.47
1:D:380:ARG:HA	1:D:383:GLU:HG3	1.97	0.47
1:A:44:ILE:HD11	1:A:60:ILE:HD12	1.97	0.47
1:C:407:VAL:HG21	1:C:452:LEU:HD12	1.96	0.47
1:B:133:ARG:O	1:B:137:VAL:HG23	2.15	0.47
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.55	0.47
1:A:401:PRO:HB2	1:A:458:HIS:CE1	2.50	0.47
1:C:410:TRP:HD1	1:C:414:ILE:HD13	1.80	0.47
1:C:235:ILE:O	1:C:239:LEU:HB2	2.14	0.47
1:A:326:SER:O	1:A:328:GLY:N	2.48	0.47
1:A:269:LEU:HD22	1:A:270:VAL:H	1.80	0.46
1:C:88:GLU:HA	1:C:91:ILE:HG22	1.97	0.46
1:D:307:MSE:SE	1:D:308:PRO:HD2	2.65	0.46
1:A:283:GLN:HG2	1:A:284:THR:H	1.79	0.46
1:D:472:THR:HG21	2:H:749:MSE:HE2	1.96	0.46
1:A:2:LEU:HG	1:A:62:ARG:HA	1.96	0.46
1:B:257:THR:HG22	1:B:258:ILE:HD12	1.97	0.46
1:B:329:ASN:HA	1:B:330:PRO:HD2	1.76	0.46
1:B:354:LYS:HD3	1:B:362:GLY:O	2.15	0.46
1:B:283:GLN:O	1:B:285:CYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLU:OE1	1:A:527:GLU:N	2.47	0.46
1:D:44:ILE:HD11	1:D:60:ILE:HD12	1.96	0.46
1:D:248:VAL:HG22	1:D:269:LEU:HD12	1.98	0.46
1:A:252:VAL:HG21	1:A:257:THR:HG21	1.98	0.46
1:C:393:LEU:HB2	1:C:437:LEU:HD11	1.97	0.46
1:C:163:SER:O	1:C:330:PRO:HG2	2.15	0.46
1:C:443:LEU:HA	1:C:460:ILE:HG12	1.96	0.46
1:D:137:VAL:O	1:D:141:ILE:HG13	2.16	0.46
1:C:527:GLU:C	1:C:530:PRO:HD3	2.36	0.46
1:B:406:PRO:CA	1:B:453:THR:HG22	2.44	0.46
1:D:343:LYS:HG2	1:D:343:LYS:O	2.16	0.46
1:A:385:LEU:HD23	1:A:440:ARG:HH21	1.81	0.46
1:D:131:TYR:HE2	1:D:300:ASP:HB2	1.81	0.46
1:B:481:GLU:HA	1:B:484:LEU:CD2	2.46	0.46
1:D:371:TYR:CD2	1:D:377:ALA:HB2	2.51	0.46
1:C:111:SER:C	1:C:113:GLN:H	2.19	0.46
1:B:242:ARG:HB3	1:B:245:THR:OG1	2.16	0.46
1:A:347:LYS:HA	1:A:350:GLN:HB2	1.97	0.46
1:A:302:LEU:CD1	1:A:319:LEU:HD11	2.40	0.46
1:D:247:PHE:CE2	1:D:266:LEU:HD13	2.51	0.46
1:C:130:CYS:O	1:C:304:ALA:HB1	2.15	0.46
1:B:39:ASP:HA	1:B:42:GLU:HB2	1.97	0.46
1:C:368:PRO:HD3	1:D:279:ASN:O	2.16	0.46
1:A:30:LEU:HD21	1:A:70:PRO:O	2.15	0.46
1:A:404:ASP:OD1	1:A:447:LYS:HD3	2.15	0.46
1:B:252:VAL:HG22	1:B:257:THR:HG21	1.98	0.46
1:A:471:GLN:HE21	1:D:471:GLN:HG3	1.80	0.46
1:C:237:ASN:O	1:C:240:ILE:HG23	2.16	0.46
1:D:409:LEU:HA	1:D:409:LEU:HD22	1.77	0.46
1:C:178:GLN:HB3	1:C:183:ASN:OD1	2.16	0.46
1:A:471:GLN:HG3	1:D:471:GLN:NE2	2.31	0.46
1:B:465:LYS:HD3	1:B:466:HIS:CE1	2.51	0.46
1:A:347:LYS:O	1:A:347:LYS:HD3	2.15	0.45
1:B:408:LYS:HD2	1:B:408:LYS:HA	1.73	0.45
1:B:109:GLN:C	1:B:111:SER:N	2.68	0.45
1:B:189:TRP:CD1	1:B:189:TRP:C	2.90	0.45
1:D:142:LYS:O	1:D:146:GLU:HG3	2.17	0.45
1:B:32:GLY:C	1:B:34:ASN:H	2.19	0.45
1:C:109:GLN:HE21	1:C:109:GLN:HB2	1.53	0.45
1:D:491:ASN:N	1:D:491:ASN:OD1	2.50	0.45
1:A:116:ASP:N	1:A:116:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:PRO:O	1:C:27:LEU:HG	2.17	0.45
1:A:106:ILE:HG21	1:A:182:ILE:HA	1.99	0.45
1:B:253:VAL:HG11	1:B:380:ARG:HD3	1.98	0.45
1:A:78:ASN:HA	1:B:37:THR:HG21	1.98	0.45
1:C:329:ASN:HA	1:C:330:PRO:HD2	1.82	0.45
1:A:98:PRO:O	1:A:99:ASP:HB2	2.17	0.45
1:D:36:PHE:HE2	1:D:44:ILE:HD12	1.82	0.45
1:C:386:SER:OG	1:C:388:GLU:OE1	2.34	0.45
1:C:111:SER:O	1:C:113:GLN:N	2.50	0.45
1:D:28:THR:O	1:D:32:GLY:N	2.49	0.45
1:B:399:MSE:HE1	1:B:409:LEU:O	2.15	0.45
1:A:395:PHE:O	1:A:398:VAL:HG22	2.17	0.45
1:D:354:LYS:O	1:D:358:ARG:HB2	2.17	0.45
1:B:35:ILE:CD1	1:B:70:PRO:HG2	2.47	0.45
1:B:137:VAL:O	1:B:141:ILE:HG13	2.17	0.45
1:D:61:TYR:HE2	1:D:68:LEU:HD22	1.81	0.45
1:A:21:PHE:CG	1:A:22:GLU:N	2.84	0.45
1:B:327:SER:HB2	1:B:459:ILE:HG13	1.97	0.45
1:A:37:THR:H	1:A:40:HIS:HB2	1.81	0.45
1:C:248:VAL:HG22	1:C:269:LEU:HD12	1.98	0.45
1:A:156:PHE:HB2	1:A:287:PHE:CD2	2.52	0.45
1:C:397:VAL:C	1:C:399:MSE:H	2.19	0.45
1:D:403:VAL:HG12	1:D:405:ILE:HG22	1.99	0.45
1:D:100:LEU:HA	1:D:100:LEU:HD12	1.77	0.45
1:A:18:ILE:O	1:A:50:ARG:NH2	2.49	0.45
1:C:233:ARG:NH1	1:C:237:ASN:OD1	2.49	0.45
1:C:126:LYS:O	1:C:126:LYS:HE2	2.18	0.45
1:A:351:LEU:HD13	1:A:363:VAL:HG23	1.99	0.45
1:B:105:VAL:HG22	1:B:110:PHE:CE2	2.52	0.45
1:C:167:VAL:O	1:C:171:GLN:HG3	2.17	0.44
1:B:218:LEU:HG	1:B:219:ASN:N	2.33	0.44
1:B:23:PRO:O	1:B:27:LEU:HG	2.17	0.44
1:A:405:ILE:HA	1:A:406:PRO:HD3	1.71	0.44
1:A:368:PRO:HB2	4:A:602:ATP:O2'	2.17	0.44
1:D:124:VAL:HA	1:D:125:PRO:HD3	1.85	0.44
1:D:39:ASP:N	1:D:39:ASP:OD1	2.47	0.44
1:D:158:HIS:HE1	1:D:287:PHE:HB3	1.82	0.44
1:B:49:THR:HG22	1:B:50:ARG:N	2.31	0.44
1:D:405:ILE:HA	1:D:406:PRO:HD3	1.77	0.44
1:A:341:GLU:CB	1:A:342:PRO:HD3	2.47	0.44
1:D:444:LEU:HB3	1:D:445:SER:H	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ILE:HD11	1:B:543:LEU:HG	2.00	0.44
1:C:116:ASP:OD1	1:C:116:ASP:N	2.51	0.44
1:C:233:ARG:HH11	1:C:233:ARG:CG	2.29	0.44
1:D:269:LEU:HD22	1:D:270:VAL:H	1.82	0.44
1:D:135:TYR:CE1	1:D:139:ARG:HD2	2.52	0.44
1:C:247:PHE:CE2	1:C:266:LEU:HD13	2.53	0.44
1:D:190:LEU:HD12	1:D:207:ILE:HG13	1.98	0.44
1:D:17:LEU:O	1:D:21:PHE:HB3	2.17	0.44
1:A:163:SER:C	1:A:330:PRO:HG2	2.38	0.44
1:C:21:PHE:CG	1:C:22:GLU:N	2.86	0.44
1:D:443:LEU:HA	1:D:460:ILE:HG12	2.00	0.44
1:C:466:HIS:N	1:C:466:HIS:ND1	2.65	0.44
1:B:233:ARG:CG	1:B:233:ARG:HH11	2.30	0.44
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.81	0.44
1:B:525:ARG:HD3	1:B:525:ARG:HA	1.76	0.44
1:A:40:HIS:O	1:A:44:ILE:HG13	2.18	0.44
1:B:44:ILE:HD13	1:B:57:PHE:HA	1.99	0.44
1:C:210:MSE:HE1	1:D:233:ARG:HD3	1.99	0.44
1:A:247:PHE:CD2	1:A:266:LEU:HD13	2.52	0.44
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.99	0.44
1:D:237:ASN:O	1:D:239:LEU:N	2.51	0.44
1:B:347:LYS:HA	1:B:350:GLN:HB2	1.99	0.44
1:C:4:GLU:OE2	1:C:267:ARG:NH2	2.50	0.44
1:A:444:LEU:HA	1:A:444:LEU:HD12	1.72	0.44
1:A:72:ILE:C	1:A:74:PHE:H	2.21	0.44
1:A:88:GLU:HA	1:A:91:ILE:HG22	2.00	0.44
1:C:434:LEU:HD22	1:C:444:LEU:HD21	1.98	0.44
1:D:23:PRO:HG2	1:D:53:ARG:HB3	1.99	0.44
1:D:21:PHE:CE2	1:D:23:PRO:HG3	2.52	0.44
1:A:307:MSE:SE	1:A:308:PRO:HD2	2.67	0.44
1:A:126:LYS:HD3	1:B:283:GLN:OE1	2.18	0.44
1:A:163:SER:O	1:A:330:PRO:HG2	2.18	0.44
1:B:449:MSE:HE3	1:B:450:PRO:HA	2.00	0.44
1:C:477:ILE:HG21	1:C:544:LYS:HE3	1.99	0.44
1:B:319:LEU:HA	1:B:348:MSE:HE1	1.99	0.43
1:A:255:GLU:CB	1:A:277:ILE:HG22	2.48	0.43
1:D:75:PHE:CB	1:D:84:ALA:HB2	2.48	0.43
1:B:334:MSE:HE2	1:B:338:LYS:CD	2.48	0.43
1:A:463:PHE:O	1:A:467:VAL:HB	2.18	0.43
1:B:2:LEU:HB3	1:B:6:GLU:HB2	2.00	0.43
1:C:1:MSE:HE2	1:C:2:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:GLU:CB	1:C:342:PRO:HD3	2.46	0.43
1:B:44:ILE:O	1:B:53:ARG:HG2	2.18	0.43
1:A:343:LYS:HG2	1:A:343:LYS:O	2.18	0.43
1:B:481:GLU:O	1:B:484:LEU:HG	2.17	0.43
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.82	0.43
1:B:187:ILE:HD13	1:B:246:LEU:HB3	2.00	0.43
1:C:426:LEU:HA	1:C:426:LEU:HD23	1.76	0.43
1:A:235:ILE:O	1:A:239:LEU:HB2	2.18	0.43
1:B:92:ASP:O	1:B:96:ASN:HB2	2.18	0.43
1:A:395:PHE:CD2	1:A:415:PRO:HD3	2.50	0.43
1:D:437:LEU:HA	1:D:437:LEU:HD23	1.77	0.43
1:A:527:GLU:C	1:A:530:PRO:HD3	2.39	0.43
1:C:485:LEU:HD12	1:C:486:GLU:H	1.83	0.43
1:A:92:ASP:C	1:A:94:ALA:H	2.22	0.43
1:C:334:MSE:HG3	1:C:338:LYS:HD3	1.99	0.43
1:A:301:PHE:CE1	1:A:305:TYR:HE2	2.36	0.43
1:D:161:ALA:O	1:D:374:LEU:HD21	2.19	0.43
1:B:190:LEU:HA	1:B:190:LEU:HD23	1.83	0.43
1:D:283:GLN:C	1:D:285:CYS:H	2.22	0.43
1:D:525:ARG:HA	1:D:526:PRO:HD3	1.73	0.43
1:D:31:GLU:OE1	1:D:38:GLU:HG2	2.18	0.43
1:B:399:MSE:HE3	1:B:405:ILE:HD11	2.01	0.43
1:B:532:PHE:C	1:B:534:GLN:H	2.22	0.43
1:B:72:ILE:C	1:B:74:PHE:H	2.21	0.43
1:D:237:ASN:C	1:D:239:LEU:N	2.72	0.43
1:B:185:ASP:N	1:B:244:ASN:O	2.51	0.43
1:D:93:PHE:N	1:D:93:PHE:HD1	2.17	0.43
1:A:159:GLY:N	1:A:165:LYS:HD3	2.34	0.43
1:C:460:ILE:O	1:C:464:LEU:HG	2.18	0.43
1:C:383:GLU:HG2	2:G:753:LEU:HD13	1.99	0.43
1:A:529:PHE:N	1:A:530:PRO:HD3	2.34	0.43
1:D:231:LEU:HA	1:D:234:MSE:HE3	2.00	0.43
1:D:133:ARG:O	1:D:137:VAL:HG23	2.18	0.43
1:C:190:LEU:HD21	1:D:229:VAL:HG21	2.00	0.43
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.72	0.43
1:D:165:LYS:H	1:D:165:LYS:HG3	1.64	0.43
1:D:303:GLU:HA	1:D:309:MSE:HE1	2.01	0.43
1:A:248:VAL:HG22	1:A:269:LEU:HD12	2.00	0.43
1:A:529:PHE:HB3	1:A:532:PHE:CZ	2.53	0.43
1:C:72:ILE:HG21	1:C:88:GLU:CD	2.39	0.43
1:A:216:ASP:H	1:A:218:LEU:CD2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LEU:HA	1:C:155:LEU:HD23	1.88	0.43
1:D:6:GLU:O	1:D:9:ALA:HB3	2.19	0.43
1:C:75:PHE:HB3	1:C:80:GLN:O	2.18	0.43
1:D:460:ILE:HA	1:D:460:ILE:HD12	1.75	0.43
1:D:237:ASN:O	1:D:240:ILE:HG23	2.19	0.43
1:C:20:ASP:HB2	1:D:63:ARG:HB3	2.01	0.43
1:A:204:PHE:HB3	1:A:231:LEU:HD21	2.01	0.43
1:D:444:LEU:HD12	1:D:444:LEU:HA	1.76	0.42
1:D:527:GLU:C	1:D:530:PRO:HD3	2.38	0.42
1:A:187:ILE:HD12	1:A:246:LEU:O	2.18	0.42
1:B:326:SER:O	1:B:328:GLY:N	2.51	0.42
2:H:752:PHE:HB3	2:H:753:LEU:HA	2.01	0.42
1:A:150:LEU:HD13	1:A:153:PHE:HB3	2.01	0.42
1:B:460:ILE:HD12	1:B:460:ILE:HA	1.85	0.42
1:D:426:LEU:HA	1:D:426:LEU:HD23	1.78	0.42
1:A:247:PHE:HD2	1:A:266:LEU:HB3	1.84	0.42
1:C:187:ILE:HD13	1:C:246:LEU:HB3	2.01	0.42
1:B:178:GLN:HB3	1:B:183:ASN:OD1	2.19	0.42
1:D:157:LEU:O	1:D:165:LYS:HD2	2.20	0.42
1:C:456:ILE:HG13	1:C:460:ILE:CG2	2.49	0.42
1:A:444:LEU:HB3	1:A:445:SER:H	1.61	0.42
1:C:529:PHE:HB3	1:C:532:PHE:CZ	2.53	0.42
1:D:327:SER:HB2	1:D:459:ILE:CD1	2.50	0.42
1:B:412:CYS:O	1:B:483:ARG:NH1	2.51	0.42
1:D:313:GLU:O	1:D:316:GLU:HG3	2.20	0.42
1:A:13:ALA:HB2	1:A:86:PHE:CE1	2.54	0.42
1:A:26:ALA:HA	1:A:74:PHE:CE1	2.55	0.42
1:D:24:ARG:HA	1:D:27:LEU:HB2	2.01	0.42
1:C:532:PHE:C	1:C:534:GLN:H	2.21	0.42
1:D:93:PHE:N	1:D:93:PHE:CD1	2.87	0.42
1:C:462:MSE:HE3	1:C:462:MSE:HB2	1.92	0.42
1:B:343:LYS:O	1:B:343:LYS:HG2	2.18	0.42
1:A:532:PHE:C	1:A:534:GLN:H	2.22	0.42
1:C:189:TRP:CD1	1:C:189:TRP:C	2.93	0.42
1:D:35:ILE:O	1:D:64:GLN:HG3	2.19	0.42
1:B:474:ALA:HB2	1:B:547:ALA:HB1	2.01	0.42
1:D:121:LEU:HD23	1:D:121:LEU:HA	1.82	0.42
1:C:124:VAL:HA	1:C:125:PRO:HD3	1.82	0.42
1:D:100:LEU:HB3	1:D:101:LEU:H	1.71	0.42
1:A:435:LYS:HD3	1:A:435:LYS:HA	1.90	0.42
1:C:385:LEU:HD22	1:C:389:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:CB	1:B:277:ILE:HG22	2.50	0.42
1:B:163:SER:C	1:B:330:PRO:HG2	2.40	0.42
1:C:403:VAL:HG12	1:C:405:ILE:HG22	2.02	0.42
1:C:139:ARG:HD3	1:C:139:ARG:C	2.40	0.42
1:A:368:PRO:HD3	1:B:279:ASN:O	2.18	0.42
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.79	0.42
1:C:157:LEU:O	1:C:165:LYS:HD2	2.19	0.42
1:D:405:ILE:HG12	1:D:410:TRP:CE3	2.55	0.42
1:B:235:ILE:O	1:B:239:LEU:HB2	2.20	0.42
1:A:86:PHE:HE2	1:A:109:GLN:HE22	1.67	0.42
1:B:200:THR:HG21	1:B:256:GLU:HB3	2.02	0.42
1:B:212:LYS:HA	1:B:212:LYS:HE2	2.02	0.42
1:C:23:PRO:HG2	1:C:53:ARG:CB	2.50	0.42
1:C:255:GLU:HB3	1:C:277:ILE:HG22	2.02	0.42
1:C:460:ILE:HD12	1:C:460:ILE:HA	1.76	0.42
1:C:443:LEU:O	1:C:460:ILE:HG21	2.20	0.42
1:B:237:ASN:C	1:B:239:LEU:H	2.22	0.42
1:D:385:LEU:HD11	1:D:437:LEU:HD21	2.01	0.42
1:D:529:PHE:HB3	1:D:532:PHE:CZ	2.55	0.42
1:D:240:ILE:HG13	1:D:241:ASP:OD1	2.19	0.42
1:C:188:VAL:HB	1:C:247:PHE:HD1	1.84	0.42
1:C:33:LYS:HD3	1:C:70:PRO:HG3	2.01	0.42
1:B:354:LYS:O	1:B:358:ARG:HB2	2.20	0.42
1:C:307:MSE:SE	1:C:308:PRO:HD2	2.70	0.42
1:B:456:ILE:HD13	1:B:461:HIS:HD2	1.84	0.42
1:C:237:ASN:HD22	1:C:237:ASN:HA	1.66	0.41
1:D:165:LYS:N	4:D:602:ATP:O2B	2.53	0.41
1:D:44:ILE:HD13	1:D:57:PHE:HD1	1.84	0.41
1:D:292:SER:HB3	1:D:328:GLY:HA3	2.02	0.41
1:B:401:PRO:HB2	1:B:458:HIS:CE1	2.54	0.41
1:D:154:PHE:CE2	1:D:262:GLN:HG3	2.54	0.41
1:B:481:GLU:HA	1:B:484:LEU:HG	2.01	0.41
1:A:211:LEU:HD11	1:A:239:LEU:HD23	2.02	0.41
1:A:524:ILE:HD12	1:A:525:ARG:H	1.85	0.41
1:B:131:TYR:HD1	4:B:602:ATP:HN62	1.67	0.41
1:C:302:LEU:HD13	1:C:319:LEU:HD21	2.01	0.41
1:B:351:LEU:HD13	1:B:363:VAL:HG23	2.02	0.41
1:A:397:VAL:O	1:A:399:MSE:N	2.52	0.41
1:C:126:LYS:HB3	1:C:126:LYS:HE2	1.87	0.41
1:C:347:LYS:HD3	1:C:347:LYS:O	2.19	0.41
1:C:189:TRP:CD2	1:C:248:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ILE:HG13	1:B:241:ASP:N	2.35	0.41
1:C:349:ALA:HA	1:C:352:ASN:HD22	1.85	0.41
1:D:156:PHE:CE2	1:D:278:SER:HB3	2.56	0.41
1:C:126:LYS:HZ2	1:D:283:GLN:HG3	1.82	0.41
1:D:29:TYR:CD2	1:D:74:PHE:HB2	2.55	0.41
1:C:39:ASP:HA	1:C:42:GLU:HB2	2.02	0.41
1:D:337:PHE:C	1:D:337:PHE:CD1	2.94	0.41
1:A:1:MSE:HG2	1:A:63:ARG:HA	2.02	0.41
1:A:449:MSE:HB2	1:A:449:MSE:HE2	1.73	0.41
1:B:336:PHE:CE2	1:B:348:MSE:SE	3.23	0.41
1:A:456:ILE:HD13	1:A:461:HIS:HD2	1.86	0.41
1:D:105:VAL:HG22	1:D:110:PHE:CE2	2.55	0.41
1:C:333:LEU:O	1:C:336:PHE:HB2	2.21	0.41
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.67	0.41
1:D:438:SER:O	1:D:442:ALA:HA	2.20	0.41
1:D:343:LYS:HB3	1:D:343:LYS:HE3	1.78	0.41
1:B:40:HIS:O	1:B:44:ILE:HG13	2.21	0.41
1:B:8:ARG:HD3	1:B:90:TYR:OH	2.21	0.41
1:B:269:LEU:HD22	1:B:270:VAL:H	1.86	0.41
1:D:208:LEU:HD23	1:D:235:ILE:HA	2.02	0.41
1:A:237:ASN:C	1:A:239:LEU:H	2.23	0.41
1:B:273:ARG:NE	4:B:602:ATP:O3G	2.46	0.41
1:B:21:PHE:CG	1:B:22:GLU:N	2.89	0.41
1:B:485:LEU:HD23	1:B:485:LEU:HA	1.86	0.41
1:A:314:LYS:HA	1:A:317:ASP:HB2	2.02	0.41
1:A:157:LEU:HD11	1:A:168:ILE:CG2	2.50	0.41
1:C:128:MSE:HG3	1:C:167:VAL:CG2	2.45	0.41
1:C:9:ALA:HA	1:C:12:THR:HG22	2.02	0.41
1:D:393:LEU:HD11	1:D:443:LEU:HD13	2.03	0.41
1:A:274:ASP:O	1:A:277:ILE:HG12	2.20	0.41
1:D:110:PHE:O	1:D:112:ARG:N	2.54	0.41
1:B:247:PHE:CE2	1:B:266:LEU:HD22	2.56	0.41
1:B:249:PHE:HE2	1:B:268:CYS:HG	1.66	0.41
1:D:407:VAL:HG22	1:D:454:PHE:HE1	1.84	0.41
1:A:313:GLU:O	1:A:316:GLU:HG3	2.20	0.41
1:B:313:GLU:O	1:B:316:GLU:HG3	2.21	0.41
1:B:159:GLY:N	1:B:165:LYS:HD3	2.35	0.41
1:D:283:GLN:HG2	1:D:284:THR:N	2.35	0.41
1:D:466:HIS:ND1	1:D:466:HIS:N	2.67	0.41
1:B:444:LEU:HD12	1:B:444:LEU:HA	1.72	0.41
1:A:437:LEU:HA	1:A:437:LEU:HD22	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ALA:HB2	1:D:74:PHE:CE2	2.56	0.41
1:C:39:ASP:O	1:C:43:LEU:HD13	2.20	0.41
1:D:301:PHE:CE1	1:D:305:TYR:HE1	2.39	0.41
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.71	0.41
1:C:257:THR:HG22	1:C:258:ILE:HD12	2.03	0.41
1:C:30:LEU:HA	1:C:30:LEU:HD23	1.82	0.41
1:C:434:LEU:HA	1:C:437:LEU:HB2	2.02	0.41
1:C:445:SER:HB3	1:C:455:LYS:O	2.21	0.41
1:C:408:LYS:HA	1:C:408:LYS:HD2	1.76	0.41
1:B:207:ILE:O	1:B:210:MSE:N	2.54	0.41
1:A:157:LEU:HD22	1:A:290:VAL:CG2	2.49	0.41
1:C:395:PHE:CD2	1:C:415:PRO:HD3	2.51	0.41
1:C:322:THR:O	1:C:326:SER:OG	2.37	0.41
1:A:527:GLU:HA	1:A:530:PRO:HG3	2.02	0.41
1:D:104:VAL:HB	1:D:105:VAL:H	1.63	0.41
1:D:337:PHE:C	1:D:337:PHE:HD1	2.23	0.41
1:B:124:VAL:HA	1:B:125:PRO:HD3	1.90	0.41
1:C:406:PRO:CA	1:C:453:THR:HG22	2.47	0.41
1:D:399:MSE:HG3	1:D:410:TRP:NE1	2.36	0.41
1:A:189:TRP:CD1	1:A:189:TRP:C	2.94	0.41
1:D:110:PHE:C	1:D:112:ARG:H	2.23	0.41
1:C:444:LEU:HB3	1:C:445:SER:H	1.55	0.41
1:A:347:LYS:O	1:A:350:GLN:HB2	2.21	0.41
1:B:347:LYS:HD3	1:B:347:LYS:O	2.20	0.41
1:C:205:THR:HA	1:C:231:LEU:HD11	2.02	0.41
1:D:445:SER:HB3	1:D:455:LYS:O	2.22	0.40
1:C:292:SER:HB3	1:C:328:GLY:HA3	2.03	0.40
1:C:385:LEU:HD23	1:C:440:ARG:HH21	1.86	0.40
1:B:154:PHE:CE2	1:B:262:GLN:HG3	2.55	0.40
1:A:9:ALA:HA	1:A:12:THR:HG22	2.04	0.40
1:D:187:ILE:HD13	1:D:246:LEU:HB3	2.04	0.40
1:C:415:PRO:O	1:C:416:VAL:HG13	2.21	0.40
1:A:93:PHE:CE2	1:A:104:VAL:HG11	2.56	0.40
1:A:253:VAL:HG11	1:A:380:ARG:HD3	2.03	0.40
1:C:240:ILE:HG13	1:C:241:ASP:N	2.37	0.40
1:B:409:LEU:HA	1:B:409:LEU:HD22	1.85	0.40
1:D:157:LEU:HD22	1:D:290:VAL:HG22	2.02	0.40
1:B:430:VAL:O	1:B:434:LEU:HG	2.21	0.40
1:A:189:TRP:CD2	1:A:248:VAL:HG11	2.55	0.40
1:A:212:LYS:HA	1:A:212:LYS:HE2	2.03	0.40
1:D:325:LEU:HA	1:D:325:LEU:HD23	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:HG13	1:A:241:ASP:OD1	2.22	0.40
1:B:409:LEU:HD21	1:B:530:PRO:HB3	2.02	0.40
1:D:255:GLU:CB	1:D:277:ILE:HG22	2.51	0.40
1:B:395:PHE:CD2	1:B:415:PRO:HD3	2.52	0.40
1:A:466:HIS:N	1:A:466:HIS:ND1	2.69	0.40
1:D:273:ARG:HD2	1:D:381:CYS:SG	2.60	0.40
1:C:318:VAL:O	1:C:321:LYS:HB3	2.20	0.40
1:D:32:GLY:C	1:D:34:ASN:H	2.24	0.40
1:C:307:MSE:HA	1:C:308:PRO:HD3	1.85	0.40
1:D:130:CYS:O	1:D:304:ALA:HB1	2.22	0.40
1:C:7:CYS:HB3	1:C:243:PRO:HG3	2.02	0.40
1:D:349:ALA:HA	1:D:352:ASN:HB2	2.03	0.40
1:C:233:ARG:HA	1:C:236:CYS:SG	2.62	0.40
2:G:752:PHE:O	2:G:753:LEU:HG	2.22	0.40
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.86	0.40
1:D:487:ILE:HG22	1:D:531:LYS:HG2	2.03	0.40
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.89	0.40
1:A:115:LEU:HD21	1:A:180:ILE:O	2.21	0.40
1:A:477:ILE:HD11	1:A:543:LEU:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:O	1:B:113:GLN:NE2[3_545]	2.19	0.01

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	504/549 (92%)	404 (80%)	77 (15%)	23 (5%)	3 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	505/549 (92%)	406 (80%)	73 (14%)	26 (5%)	2	24
1	C	504/549 (92%)	406 (81%)	72 (14%)	26 (5%)	2	23
1	D	505/549 (92%)	405 (80%)	76 (15%)	24 (5%)	3	25
2	E	4/8 (50%)	2 (50%)	1 (25%)	1 (25%)	0	0
2	F	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	G	3/8 (38%)	1 (33%)	0	2 (67%)	0	0
2	H	4/8 (50%)	1 (25%)	2 (50%)	1 (25%)	0	0
All	All	2032/2228 (91%)	1626 (80%)	302 (15%)	104 (5%)	2	24

All (104) 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
2	E	751	ASN
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	C	127	GLN
1	C	327	SER
1	C	341	GLU
1	C	398	VAL
1	C	445	SER
1	D	35	ILE
1	D	127	GLN
1	D	284	THR
1	D	327	SER
1	D	341	GLU
1	D	398	VAL
1	D	445	SER
1	A	112	ARG
1	A	238	ALA
1	A	244	ASN
1	A	396	ALA

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Mol	Chain	Res	Type
1	A	465	LYS
1	A	522	THR
1	B	244	ASN
1	B	396	ALA
1	B	465	LYS
1	B	522	THR
1	C	112	ARG
1	C	160	ARG
1	C	244	ASN
1	C	396	ALA
1	C	465	LYS
1	C	522	THR
2	G	751	ASN
1	D	104	VAL
1	D	160	ARG
1	D	208	LEU
1	D	244	ASN
1	D	465	LYS
1	D	522	THR
2	H	750	PHE
1	A	2	LEU
1	A	73	ASP
1	A	160	ARG
1	A	208	LEU
1	A	284	THR
1	B	2	LEU
1	B	104	VAL
1	B	160	ARG
1	B	208	LEU
1	B	238	ALA
1	B	284	THR
2	F	751	ASN
1	C	2	LEU
1	C	73	ASP
1	C	208	LEU
1	C	238	ALA
1	C	284	THR
1	C	486	GLU
1	D	111	SER
1	D	238	ALA
1	D	396	ALA
1	A	485	LEU

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Mol	Chain	Res	Type
1	B	73	ASP
1	B	176	SER
1	C	485	LEU
2	G	752	PHE
1	D	3	CYS
1	A	484	LEU
1	B	35	ILE
1	B	257	THR
1	B	328	GLY
1	B	354	LYS
1	D	34	ASN
1	D	102	ARG
1	D	237	ASN
1	A	237	ASN
1	A	257	THR
1	B	102	ARG
1	C	3	CYS
1	C	33	LYS
1	C	237	ASN
1	C	257	THR
1	D	64	GLN
1	B	106	ILE
1	B	311	VAL
1	C	108	PRO
1	D	311	VAL
1	A	70	PRO
1	A	108	PRO
1	A	311	VAL
1	B	70	PRO
1	C	70	PRO
1	C	311	VAL
1	D	103	PRO
1	D	328	GLY
1	C	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	20
1	B	464/483 (96%)	391 (84%)	73 (16%)	3	18
1	C	462/483 (96%)	379 (82%)	83 (18%)	2	11
1	D	464/483 (96%)	378 (82%)	86 (18%)	2	10
2	E	5/6 (83%)	3 (60%)	2 (40%)	0	1
2	F	5/6 (83%)	5 (100%)	0	100	100
2	G	5/6 (83%)	5 (100%)	0	100	100
2	H	6/6 (100%)	5 (83%)	1 (17%)	3	14
All	All	1873/1956 (96%)	1559 (83%)	314 (17%)	2	14

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	82	HIS
1	A	95	ILE
1	A	113	GLN
1	A	115	LEU
1	A	116	ASP
1	A	117	ARG
1	A	126	LYS
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

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Mol	Chain	Res	Type
1	A	217	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
1	A	284	THR
1	A	286	GLU
1	A	296	ASP
1	A	316	GLU
1	A	332	THR
1	A	344	THR
1	A	355	LEU
1	A	363	VAL
1	A	364	GLU
1	A	366	ILE
1	A	369	TYR
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	449	MSE
1	A	451	VAL
1	A	452	LEU
1	A	457	ASP
1	A	459	ILE
1	A	466	HIS
1	A	485	LEU
1	A	525	ARG
1	A	533	MSE
1	A	539	PHE
1	A	542	SER

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Mol	Chain	Res	Type
2	E	749	MSE
2	E	750	PHE
1	B	1	MSE
1	B	4	GLU
1	B	15	THR
1	B	17	LEU
1	B	46	LYS
1	B	52	GLU
1	B	64	GLN
1	B	67	GLU
1	B	68	LEU
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	116	ASP
1	B	117	ARG
1	B	126	LYS
1	B	130	CYS
1	B	148	CYS
1	B	155	LEU
1	B	157	LEU
1	B	174	SER
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	210	MSE
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

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Mol	Chain	Res	Type
1	B	255	GLU
1	B	262	GLN
1	B	269	LEU
1	B	283	GLN
1	B	284	THR
1	B	296	ASP
1	B	316	GLU
1	B	332	THR
1	B	344	THR
1	B	355	LEU
1	B	363	VAL
1	B	364	GLU
1	B	369	TYR
1	B	381	CYS
1	B	382	VAL
1	B	387	ASP
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	480	LEU
1	B	485	LEU
1	B	533	MSE
1	B	539	PHE
1	B	542	SER
1	B	546	PHE
1	C	1	MSE
1	C	11	SER
1	C	15	THR
1	C	17	LEU
1	C	46	LYS
1	C	47	MSE
1	C	51	LEU
1	C	52	GLU
1	C	67	GLU

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Mol	Chain	Res	Type
1	C	68	LEU
1	C	77	TYR
1	C	78	ASN
1	C	79	ASN
1	C	82	HIS
1	C	99	ASP
1	C	109	GLN
1	C	113	GLN
1	C	116	ASP
1	C	117	ARG
1	C	126	LYS
1	C	130	CYS
1	C	131	TYR
1	C	139	ARG
1	C	148	CYS
1	C	155	LEU
1	C	157	LEU
1	C	160	ARG
1	C	174	SER
1	C	179	LEU
1	C	180	ILE
1	C	185	ASP
1	C	189	TRP
1	C	198	LYS
1	C	203	LEU
1	C	217	LEU
1	C	220	PHE
1	C	223	VAL
1	C	224	GLU
1	C	227	THR
1	C	233	ARG
1	C	237	ASN
1	C	239	LEU
1	C	241	ASP
1	C	253	VAL
1	C	255	GLU
1	C	269	LEU
1	C	284	THR
1	C	286	GLU
1	C	296	ASP
1	C	307	MSE
1	C	309	MSE

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Mol	Chain	Res	Type
1	C	316	GLU
1	C	319	LEU
1	C	326	SER
1	C	332	THR
1	C	345	PHE
1	C	355	LEU
1	C	360	LEU
1	C	363	VAL
1	C	364	GLU
1	C	366	ILE
1	C	369	TYR
1	C	374	LEU
1	C	381	CYS
1	C	387	ASP
1	C	404	ASP
1	C	405	ILE
1	C	408	LYS
1	C	409	LEU
1	C	410	TRP
1	C	416	VAL
1	C	437	LEU
1	C	444	LEU
1	C	451	VAL
1	C	452	LEU
1	C	457	ASP
1	C	459	ILE
1	C	466	HIS
1	C	485	LEU
1	C	524	ILE
1	C	525	ARG
1	C	533	MSE
1	C	539	PHE
1	D	1	MSE
1	D	3	CYS
1	D	12	THR
1	D	15	THR
1	D	18	ILE
1	D	19	HIS
1	D	31	GLU
1	D	35	ILE
1	D	36	PHE
1	D	38	GLU

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Mol	Chain	Res	Type
1	D	39	ASP
1	D	43	LEU
1	D	46	LYS
1	D	51	LEU
1	D	64	GLN
1	D	67	GLU
1	D	68	LEU
1	D	71	LEU
1	D	77	TYR
1	D	82	HIS
1	D	93	PHE
1	D	99	ASP
1	D	110	PHE
1	D	116	ASP
1	D	117	ARG
1	D	126	LYS
1	D	130	CYS
1	D	131	TYR
1	D	148	CYS
1	D	155	LEU
1	D	157	LEU
1	D	160	ARG
1	D	174	SER
1	D	176	SER
1	D	179	LEU
1	D	180	ILE
1	D	185	ASP
1	D	189	TRP
1	D	198	LYS
1	D	203	LEU
1	D	217	LEU
1	D	218	LEU
1	D	220	PHE
1	D	223	VAL
1	D	227	THR
1	D	233	ARG
1	D	239	LEU
1	D	241	ASP
1	D	253	VAL
1	D	255	GLU
1	D	262	GLN
1	D	269	LEU

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Mol	Chain	Res	Type
1	D	284	THR
1	D	286	GLU
1	D	296	ASP
1	D	316	GLU
1	D	319	LEU
1	D	336	PHE
1	D	337	PHE
1	D	345	PHE
1	D	355	LEU
1	D	363	VAL
1	D	364	GLU
1	D	366	ILE
1	D	369	TYR
1	D	374	LEU
1	D	379	GLN
1	D	381	CYS
1	D	382	VAL
1	D	387	ASP
1	D	404	ASP
1	D	405	ILE
1	D	408	LYS
1	D	409	LEU
1	D	410	TRP
1	D	444	LEU
1	D	451	VAL
1	D	452	LEU
1	D	457	ASP
1	D	459	ILE
1	D	460	ILE
1	D	466	HIS
1	D	491	ASN
1	D	525	ARG
1	D	539	PHE
1	D	548	CYS
2	H	751	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	B	56	ASN
1	B	254	GLN

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Mol	Chain	Res	Type
1	C	254	GLN
1	D	171	GLN
1	D	283	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	ATP	A	602	3	24,33,33	0.95	1 (4%)	31,52,52	1.78	5 (16%)
4	ATP	B	602	3	24,33,33	0.97	1 (4%)	31,52,52	2.14	6 (19%)
4	ATP	C	602	3	24,33,33	0.99	1 (4%)	31,52,52	1.78	5 (16%)
4	ATP	D	602	3	24,33,33	1.00	1 (4%)	31,52,52	1.90	5 (16%)

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
4	ATP	C	602	3	-	0/18/38/38	0/3/3/3
4	ATP	D	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	C5-C4	3.16	1.47	1.40
4	B	602	ATP	C5-C4	3.17	1.47	1.40
4	C	602	ATP	C5-C4	3.19	1.47	1.40
4	D	602	ATP	C5-C4	3.19	1.47	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ATP	N3-C2-N1	-6.90	123.61	128.89
4	D	602	ATP	N3-C2-N1	-6.65	123.80	128.89
4	C	602	ATP	N3-C2-N1	-6.08	124.24	128.89
4	A	602	ATP	N3-C2-N1	-5.96	124.33	128.89
4	B	602	ATP	C2'-C1'-N9	-5.26	106.26	114.29
4	B	602	ATP	PA-O3A-PB	-4.45	120.23	132.73
4	D	602	ATP	PA-O3A-PB	-4.38	120.42	132.73
4	D	602	ATP	C2'-C1'-N9	-4.21	107.86	114.29
4	A	602	ATP	PA-O3A-PB	-3.94	121.65	132.73
4	C	602	ATP	PA-O3A-PB	-3.90	121.77	132.73
4	C	602	ATP	C2'-C1'-N9	-3.84	108.42	114.29
4	B	602	ATP	PB-O3B-PG	-3.56	120.73	132.67
4	A	602	ATP	C2'-C1'-N9	-3.52	108.91	114.29
4	B	602	ATP	C4-C5-N7	-3.02	106.70	109.48
4	A	602	ATP	PB-O3B-PG	-2.80	123.27	132.67
4	D	602	ATP	C4-C5-N7	-2.78	106.92	109.48
4	C	602	ATP	C4-C5-N7	-2.76	106.94	109.48
4	A	602	ATP	C4-C5-N7	-2.73	106.97	109.48
4	C	602	ATP	PB-O3B-PG	-2.69	123.65	132.67
4	D	602	ATP	PB-O3B-PG	-2.07	125.73	132.67
4	B	602	ATP	O4'-C1'-N9	2.14	112.58	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	2	0
4	B	602	ATP	2	0
4	C	602	ATP	1	0
4	D	602	ATP	2	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	493/549 (89%)	0.38	27 (5%) 29 26	55, 109, 155, 194	0
1	B	494/549 (89%)	0.67	54 (10%) 7 7	62, 108, 206, 225	0
1	C	493/549 (89%)	0.50	46 (9%) 11 11	67, 119, 159, 205	0
1	D	494/549 (89%)	0.80	77 (15%) 3 3	62, 122, 203, 247	0
2	E	5/8 (62%)	1.08	0 100 100	90, 98, 101, 110	0
2	F	4/8 (50%)	1.85	2 (50%) 0 0	90, 102, 105, 139	0
2	G	4/8 (50%)	1.48	1 (25%) 1 1	94, 100, 112, 131	0
2	H	5/8 (62%)	2.60	2 (40%) 0 0	95, 124, 153, 162	0
All	All	1992/2228 (89%)	0.60	209 (10%) 8 8	55, 116, 184, 247	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	TYR	9.3
1	D	72	ILE	9.2
1	D	68	LEU	8.3
1	B	106	ILE	8.0
1	B	100	LEU	7.2
1	B	68	LEU	6.9
1	D	70	PRO	6.1
1	B	72	ILE	6.0
1	B	75	PHE	6.0
1	B	69	GLY	5.9
1	D	101	LEU	5.5
1	B	77	TYR	5.5
2	H	753	LEU	5.5
1	D	71	LEU	5.5
1	C	66	SER	5.4
1	B	70	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	98	PRO	5.3
1	B	105	VAL	5.3
1	B	101	LEU	5.3
1	D	89	ASP	5.2
1	B	103	PRO	5.1
1	B	79	ASN	5.1
1	C	105	VAL	5.1
1	D	96	ASN	5.1
1	C	175	LYS	5.0
1	B	67	GLU	5.0
1	D	105	VAL	4.9
1	D	69	GLY	4.8
1	B	528	ASP	4.8
1	D	6	GLU	4.8
1	D	67	GLU	4.8
1	D	25	ASP	4.7
1	D	100	LEU	4.6
1	D	78	ASN	4.5
1	B	489	ASN	4.5
1	B	6	GLU	4.4
1	D	522	THR	4.4
1	A	105	VAL	4.3
1	B	491	ASN	4.3
1	B	78	ASN	4.3
1	D	109	GLN	4.1
1	D	76	ASN	4.1
1	D	60	ILE	4.0
1	C	484	LEU	4.0
2	F	753	LEU	4.0
1	D	222	SER	4.0
1	C	20	ASP	3.9
1	D	85	ASP	3.9
1	D	75	PHE	3.9
1	D	99	ASP	3.8
2	H	748	PRO	3.8
1	B	95	ILE	3.8
1	A	539	PHE	3.7
1	B	89	ASP	3.7
1	C	521	GLU	3.6
1	D	5	ILE	3.6
1	B	56	ASN	3.6
1	C	471	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	73	ASP	3.5
1	B	311	VAL	3.5
1	D	310	PRO	3.5
1	B	84	ALA	3.4
1	D	341	GLU	3.4
1	D	94	ALA	3.4
1	D	104	VAL	3.4
1	B	225	HIS	3.4
1	D	103	PRO	3.4
1	B	61	TYR	3.4
1	D	108	PRO	3.4
1	A	110	PHE	3.4
1	D	488	GLY	3.4
1	D	225	HIS	3.4
1	D	106	ILE	3.4
1	B	222	SER	3.3
1	D	10	LEU	3.3
1	D	64	GLN	3.3
1	D	84	ALA	3.3
1	D	178	GLN	3.3
1	C	314	LYS	3.2
1	B	76	ASN	3.2
1	B	71	LEU	3.2
1	C	447	LYS	3.2
1	C	27	LEU	3.2
1	D	410	TRP	3.1
1	D	491	ASN	3.1
1	C	522	THR	3.0
1	D	9	ALA	3.0
1	D	308	PRO	3.0
1	D	90	TYR	3.0
1	A	406	PRO	3.0
1	C	528	ASP	3.0
1	B	60	ILE	3.0
1	D	97	GLU	3.0
1	D	57	PHE	3.0
1	D	528	ASP	3.0
1	C	451	VAL	3.0
1	D	65	ALA	3.0
1	D	489	ASN	2.9
1	D	19	HIS	2.9
1	A	314	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	523	VAL	2.9
1	B	522	THR	2.9
1	A	528	ASP	2.9
1	B	11	SER	2.9
1	B	471	GLN	2.9
1	B	5	ILE	2.9
1	B	488	GLY	2.8
1	C	16	ARG	2.8
1	D	79	ASN	2.8
1	C	470	ALA	2.8
1	A	73	ASP	2.8
1	B	116	ASP	2.8
1	B	490	ASN	2.8
1	C	49	THR	2.8
1	B	96	ASN	2.7
1	C	179	LEU	2.7
1	C	145	ASP	2.7
1	B	93	PHE	2.7
1	A	476	GLY	2.7
1	D	342	PRO	2.7
1	C	539	PHE	2.7
1	D	20	ASP	2.7
1	C	433	ARG	2.6
1	B	57	PHE	2.6
1	A	76	ASN	2.6
1	B	80	GLN	2.6
1	C	65	ALA	2.6
1	D	23	PRO	2.6
1	A	454	PHE	2.6
1	D	471	GLN	2.6
1	D	34	ASN	2.6
1	C	409	LEU	2.5
1	C	532	PHE	2.6
1	C	473	ILE	2.5
1	D	95	ILE	2.5
1	A	451	VAL	2.5
1	A	337	PHE	2.5
1	B	284	THR	2.5
1	D	527	GLU	2.5
1	A	96	ASN	2.5
1	A	536	HIS	2.5
1	C	19	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLU	2.5
1	B	90	TYR	2.5
1	D	16	ARG	2.5
1	D	77	TYR	2.5
1	D	93	PHE	2.5
1	A	64	GLN	2.5
1	B	73	ASP	2.4
1	C	46	LYS	2.4
1	D	11	SER	2.4
2	G	752	PHE	2.4
1	A	446	GLY	2.4
1	D	129	THR	2.4
1	C	78	ASN	2.4
1	B	81	SER	2.3
1	D	153	PHE	2.3
1	D	33	LYS	2.3
1	B	36	PHE	2.3
1	B	398	VAL	2.3
1	D	283	GLN	2.3
1	A	521	GLU	2.3
1	C	70	PRO	2.3
1	B	19	HIS	2.3
1	B	301	PHE	2.3
1	A	452	LEU	2.3
1	A	468	VAL	2.3
1	D	175	LYS	2.2
1	D	182	ILE	2.2
1	C	410	TRP	2.2
1	D	524	ILE	2.2
1	D	521	GLU	2.2
1	C	472	THR	2.2
1	D	15	THR	2.2
1	D	490	ASN	2.2
1	C	177	ASP	2.2
1	C	28	THR	2.2
1	C	104	VAL	2.2
1	A	526	PRO	2.2
1	A	49	THR	2.2
1	A	159	GLY	2.2
1	C	428	ASP	2.2
1	D	35	ILE	2.1
1	B	13	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	68	LEU	2.1
1	C	110	PHE	2.1
1	D	51	LEU	2.1
1	C	299	TYR	2.1
1	C	87	LEU	2.1
1	C	144	LEU	2.1
1	B	107	ALA	2.1
1	C	448	ARG	2.1
1	A	532	PHE	2.1
2	F	752	PHE	2.1
1	A	463	PHE	2.1
1	B	15	THR	2.1
1	B	218	LEU	2.1
1	D	223	VAL	2.1
1	D	224	GLU	2.1
1	C	80	GLN	2.0
1	C	452	LEU	2.0
1	A	106	ILE	2.0
1	B	99	ASP	2.0
1	C	398	VAL	2.0
1	C	64	GLN	2.0
1	C	246	LEU	2.0
1	C	283	GLN	2.0
1	D	116	ASP	2.0
1	A	398	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	D	601	1/1	0.91	0.45	3.83	75,75,75,75	0
4	ATP	B	602	31/31	0.89	0.24	-0.11	60,75,88,102	0
4	ATP	D	602	31/31	0.89	0.23	-0.25	66,91,123,128	0
4	ATP	C	602	31/31	0.91	0.22	-0.42	68,91,117,119	0
4	ATP	A	602	31/31	0.92	0.21	-0.56	62,79,97,107	0
3	MG	A	601	1/1	0.93	0.21	-	60,60,60,60	0
3	MG	C	601	1/1	0.92	0.28	-	77,77,77,77	0
3	MG	B	601	1/1	0.95	0.30	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.