



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:51 am GMT

PDB ID : 4M0L  
Title : Gamma subunit of the translation initiation factor 2 from *Sulfolobus solfataricus* complexed with GDP  
Authors : Nikonov, O.S.; Stolboushkina, E.A.; Arkhipova, V.I.; Gabdulkhakov, A.G.; Nikulin, A.D.; Lazopulo, A.M.; Lazopulo, S.M.; Garber, M.B.; Nikonov, S.V.  
Deposited on : 2013-08-01  
Resolution : 2.60 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

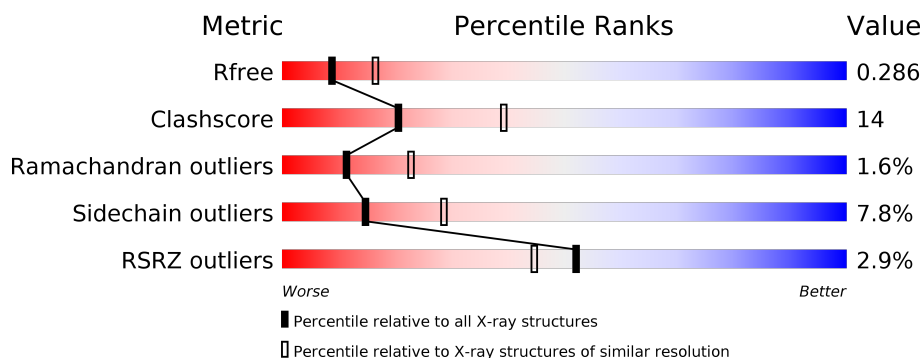
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	415	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>• •</div> </div> </div>
1	B	415	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div> </div>
1	C	415	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	D	415	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>29%</div> <div>5% •</div> </div> </div>
1	E	415	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>5% •</div> </div> </div>
1	F	415	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>5%</div> </div> </div>

## 2 Entry composition [i](#)

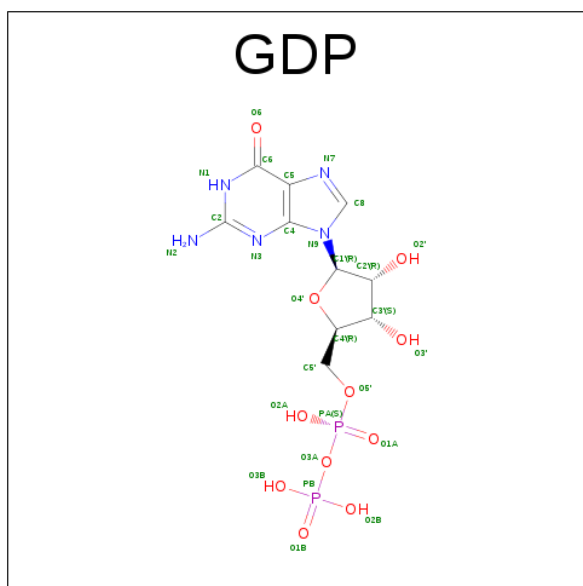
There are 5 unique types of molecules in this entry. The entry contains 19444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3197	2050	543	592	12			
1	B	396	Total	C	N	O	S	0	0	0
			3068	1970	521	565	12			
1	C	406	Total	C	N	O	S	0	0	0
			3148	2020	536	581	11			
1	D	405	Total	C	N	O	S	0	0	0
			3138	2014	533	580	11			
1	E	405	Total	C	N	O	S	0	0	0
			3138	2014	533	580	11			
1	F	414	Total	C	N	O	S	0	0	0
			3212	2058	548	594	12			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			5	4	1		

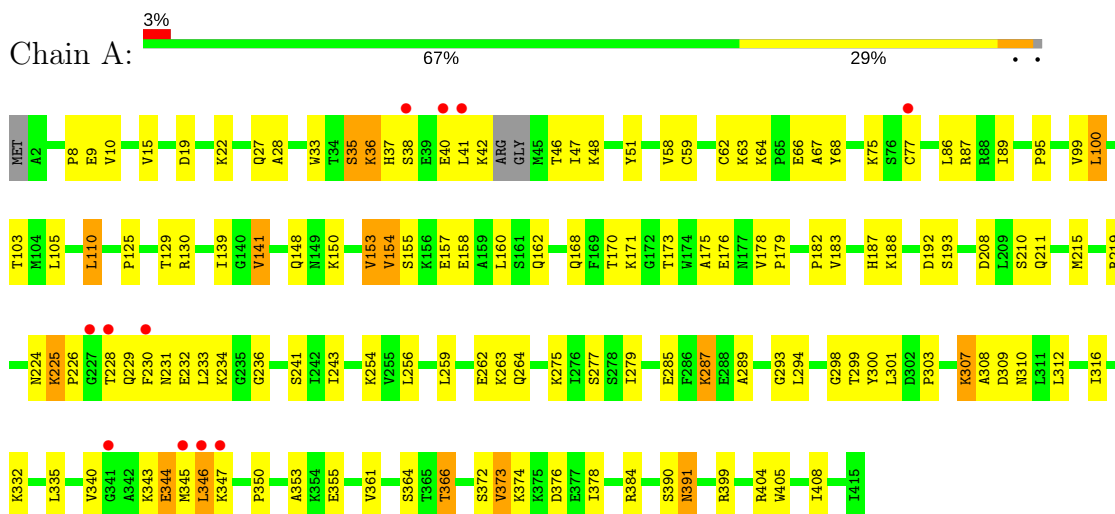
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	73	Total	O	0	0
			73	73		
5	C	77	Total	O	0	0
			77	77		
5	D	65	Total	O	0	0
			65	65		
5	E	51	Total	O	0	0
			51	51		
5	F	27	Total	O	0	0
			27	27		

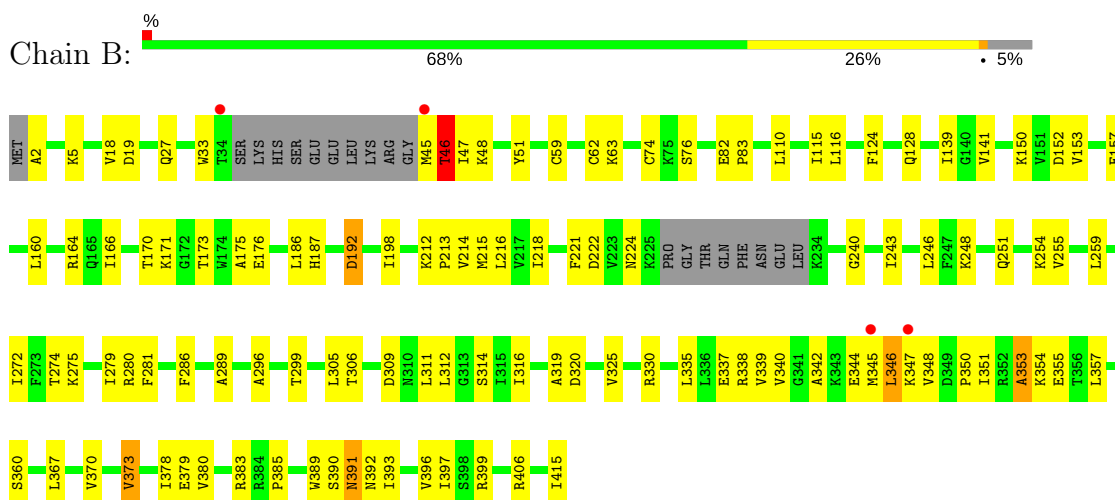
### 3 Residue-property plots

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

- Molecule 1: Translation initiation factor 2 subunit gamma

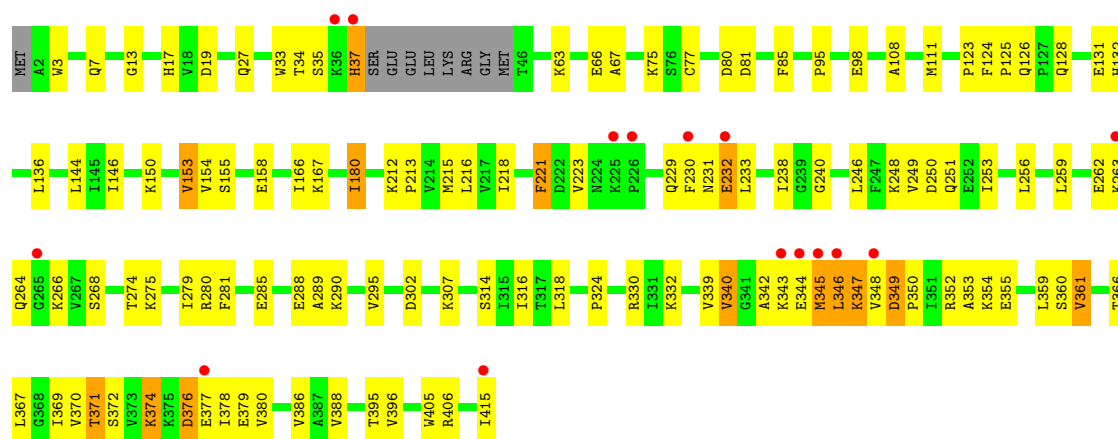


- Molecule 1: Translation initiation factor 2 subunit gamma

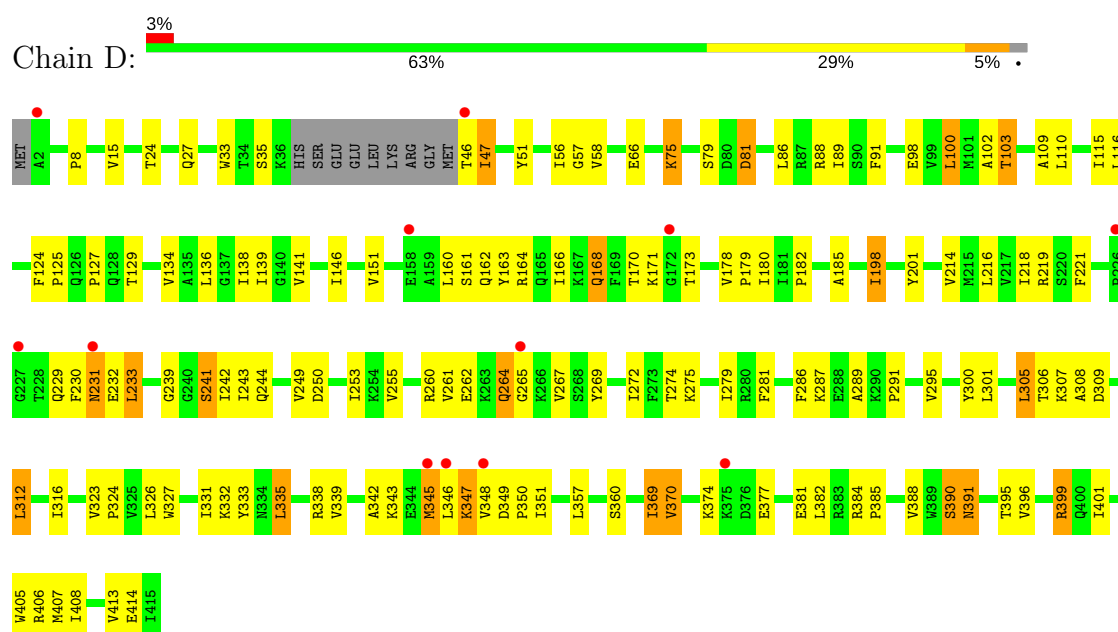


- Molecule 1: Translation initiation factor 2 subunit gamma

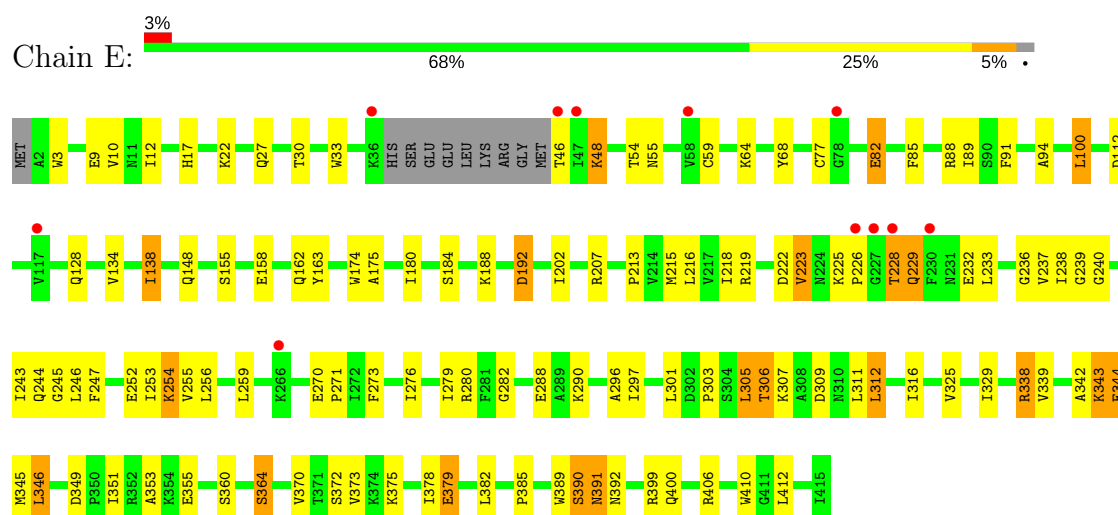




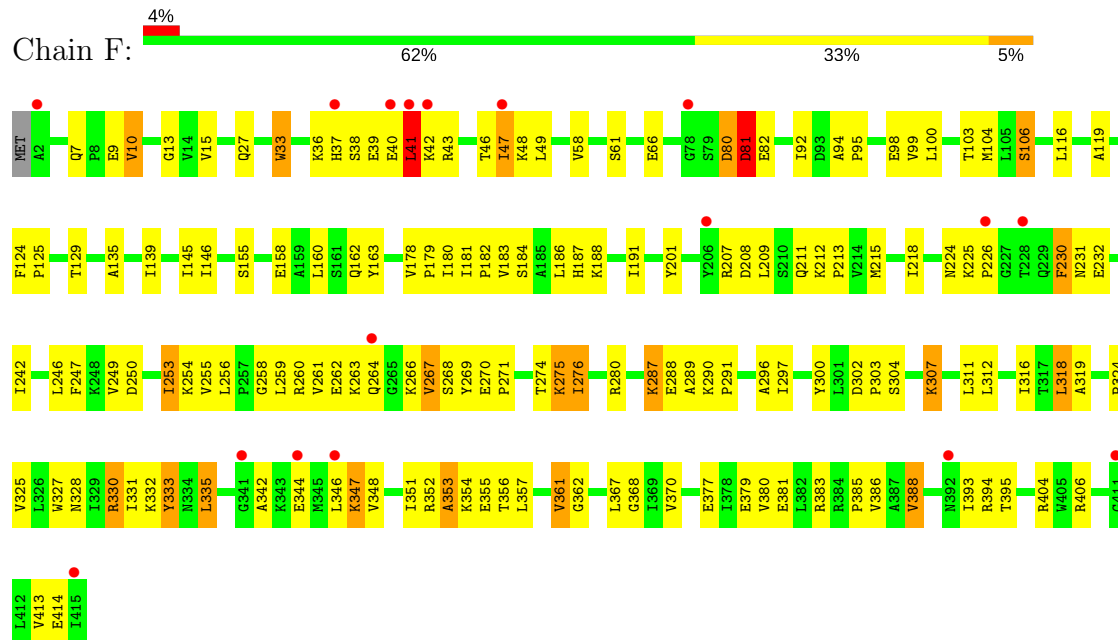
• Molecule 1: Translation initiation factor 2 subunit gamma



• Molecule 1: Translation initiation factor 2 subunit gamma



● Molecule 1: Translation initiation factor 2 subunit gamma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.05Å 106.55Å 156.30Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	19.81 – 2.60 19.81 – 2.56	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.81-2.60) 93.5 (19.81-2.56)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.234 , 0.286 0.233 , 0.286	Depositor DCC
$R_{free}$ test set	4216 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, PO4, MG

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	0.30	0/3255	0.49	0/4408
1	B	0.30	0/3122	0.48	0/4228
1	C	0.28	1/3206 (0.0%)	0.48	0/4344
1	D	0.28	0/3195	0.49	0/4329
1	E	0.26	0/3195	0.46	0/4329
1	F	0.29	0/3271	0.50	0/4430
All	All	0.28	1/19244 (0.0%)	0.49	0/26068

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	350	PRO	N-CD	5.40	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3197	0	3314	92	0
1	B	3068	0	3190	70	0
1	C	3148	0	3264	87	0
1	D	3138	0	3257	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3138	0	3258	79	0
1	F	3212	0	3331	116	0
2	A	28	0	12	3	0
2	B	28	0	12	1	0
2	C	28	0	12	1	0
2	D	28	0	12	0	0
2	E	28	0	12	2	0
2	F	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	E	5	0	0	0	0
5	A	70	0	0	0	0
5	B	73	0	0	1	0
5	C	77	0	0	0	0
5	D	65	0	0	0	0
5	E	51	0	0	2	0
5	F	27	0	0	1	0
All	All	19444	0	19686	539	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 14.

All (539) 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:C:339:VAL:HG12	1:C:342:ALA:HB2	1.14	1.14
1:F:263:LYS:HE3	1:F:264:GLN:HG2	1.29	1.09
1:F:94:ALA:HB2	1:F:100:LEU:HD13	1.30	1.08
1:B:373:VAL:HG23	1:B:378:ILE:HG22	1.38	0.99
1:A:35:SER:CB	1:A:36:LYS:HA	1.94	0.97
1:E:344:GLU:N	1:E:344:GLU:OE2	2.00	0.94
1:F:262:GLU:HG3	1:F:267:VAL:HB	1.53	0.90
1:F:94:ALA:CB	1:F:100:LEU:HD13	2.02	0.89
1:F:263:LYS:CE	1:F:264:GLN:HG2	2.04	0.88
1:E:338:ARG:HD2	1:E:345:MET:HA	1.53	0.88
1:D:115:ILE:HD11	1:D:198:ILE:HD11	1.57	0.86
1:C:352:ARG:HG2	1:C:355:GLU:OE1	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:HG12	1:C:342:ALA:CB	2.02	0.85
1:D:179:PRO:O	1:D:180:ILE:HG22	1.76	0.85
1:C:339:VAL:CG1	1:C:342:ALA:HB2	2.04	0.84
1:B:216:LEU:HG	1:B:243:ILE:HD11	1.59	0.84
1:E:232:GLU:O	1:E:233:LEU:HG	1.77	0.84
1:F:15:VAL:HG12	1:F:100:LEU:HD21	1.59	0.84
1:A:225:LYS:HG3	1:A:226:PRO:HD2	1.61	0.82
1:F:37:HIS:CD2	1:F:38:SER:H	1.97	0.82
1:B:338:ARG:HE	1:B:345:MET:HG3	1.45	0.81
1:A:219:ARG:HH21	1:A:294:LEU:HD11	1.46	0.81
1:A:35:SER:HB3	1:A:36:LYS:HG2	1.63	0.80
1:A:41:LEU:HD11	1:D:35:SER:HB3	1.62	0.80
1:D:338:ARG:HB3	1:D:345:MET:O	1.80	0.80
1:F:262:GLU:HA	1:F:266:LYS:O	1.82	0.80
1:C:374:LYS:HB2	1:C:377:GLU:O	1.82	0.79
1:F:249:VAL:HA	1:F:276:ILE:HD11	1.66	0.77
1:A:225:LYS:HG3	1:A:226:PRO:CD	2.15	0.77
1:D:347:LYS:NZ	1:D:348:VAL:H	1.83	0.76
1:A:229:GLN:HB2	1:A:233:LEU:HD23	1.67	0.75
1:D:229:GLN:HB3	1:D:231:ASN:HD21	1.50	0.75
1:A:87:ARG:HE	1:A:89:ILE:HD11	1.52	0.75
1:E:192:ASP:OD1	1:E:192:ASP:N	2.19	0.74
1:B:218:ILE:HG12	1:B:240:GLY:HA2	1.69	0.74
1:A:35:SER:HB3	1:A:36:LYS:HA	1.69	0.74
1:B:110:LEU:HD11	1:B:243:ILE:HD13	1.68	0.74
1:A:332:LYS:NZ	1:A:376:ASP:OD2	2.21	0.73
1:F:7:GLN:NE2	1:F:290:LYS:O	2.22	0.73
1:C:75:LYS:NZ	1:C:80:ASP:OD1	2.20	0.73
1:D:347:LYS:HZ3	1:D:347:LYS:HA	1.54	0.73
1:D:347:LYS:HZ2	1:D:348:VAL:H	1.35	0.71
1:F:81:ASP:N	1:F:81:ASP:OD1	2.22	0.71
1:F:230:PHE:HD1	1:F:231:ASN:H	1.37	0.71
1:D:218:ILE:HG22	1:D:219:ARG:HG3	1.71	0.71
1:D:390:SER:OG	1:D:391:ASN:N	2.24	0.71
1:E:252:GLU:HG2	5:E:639:HOH:O	1.89	0.71
1:E:351:ILE:HD12	1:E:351:ILE:N	2.06	0.71
1:F:325:VAL:HG12	1:F:385:PRO:HB2	1.72	0.70
1:F:49:LEU:HD21	1:F:103:THR:HG21	1.74	0.70
1:A:15:VAL:HG12	1:A:100:LEU:HD11	1.74	0.70
1:D:229:GLN:HB3	1:D:231:ASN:ND2	2.07	0.70
2:E:501:GDP:H8	2:E:501:GDP:H5"	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:ASN:HB3	1:E:412:LEU:HB3	1.75	0.69
1:B:346:LEU:HD22	1:F:209:LEU:HD22	1.74	0.69
1:D:260:ARG:HB2	1:D:269:TYR:CZ	2.27	0.69
1:F:318:LEU:HD12	1:F:318:LEU:H	1.56	0.69
1:A:215:MET:HB3	1:A:316:ILE:HB	1.74	0.69
1:D:179:PRO:O	1:D:180:ILE:CG2	2.41	0.68
1:E:351:ILE:HD12	1:E:351:ILE:H	1.58	0.68
1:D:168:GLN:OE1	1:D:171:LYS:NZ	2.26	0.68
1:D:24:THR:HG22	1:D:185:ALA:HB1	1.76	0.68
1:A:229:GLN:HB2	1:A:233:LEU:CD2	2.23	0.68
1:E:148:GLN:OE1	1:E:162:GLN:NE2	2.27	0.68
1:F:208:ASP:HB3	1:F:211:GLN:HE22	1.58	0.68
1:E:55:ASN:OD1	1:E:88:ARG:NH1	2.27	0.67
1:D:342:ALA:O	1:D:343:LYS:CB	2.43	0.67
1:D:342:ALA:O	1:D:343:LYS:HB3	1.96	0.66
1:F:353:ALA:O	1:F:355:GLU:N	2.26	0.66
1:E:391:ASN:OD1	1:E:392:ASN:N	2.27	0.66
1:D:216:LEU:HD23	1:D:243:ILE:HD11	1.79	0.65
1:C:229:GLN:CG	1:C:232:GLU:HB3	2.28	0.64
1:C:330:ARG:HG2	1:C:379:GLU:HG2	1.80	0.64
1:F:47:ILE:HD13	1:F:218:ILE:HG22	1.79	0.64
1:B:222:ASP:OD2	1:B:224:ASN:ND2	2.31	0.64
1:D:338:ARG:CB	1:D:345:MET:O	2.44	0.64
1:A:63:LYS:HE3	1:C:264:GLN:HA	1.80	0.64
1:B:339:VAL:HG13	1:B:342:ALA:HB2	1.80	0.64
1:D:360:SER:HB2	1:D:396:VAL:HG13	1.78	0.64
1:E:10:VAL:HG23	1:E:112:ASP:HB2	1.80	0.64
1:B:340:VAL:O	1:B:406:ARG:NH1	2.30	0.63
1:C:263:LYS:HD2	1:C:266:LYS:HE3	1.79	0.63
1:C:123:PRO:O	1:C:126:GLN:NE2	2.32	0.63
1:A:58:VAL:HG23	1:A:86:LEU:HD11	1.81	0.63
1:F:48:LYS:HB3	1:F:95:PRO:HG3	1.80	0.63
1:C:7:GLN:NE2	1:C:290:LYS:O	2.30	0.62
1:F:262:GLU:CG	1:F:267:VAL:HB	2.27	0.62
1:F:213:PRO:HG2	1:F:318:LEU:HD11	1.80	0.62
1:C:361:VAL:HG13	1:C:395:THR:HB	1.82	0.62
1:E:373:VAL:HG22	1:E:378:ILE:HG22	1.82	0.62
1:F:287:LYS:H	1:F:287:LYS:HD3	1.65	0.61
1:C:360:SER:HB2	1:C:396:VAL:HG13	1.82	0.61
1:D:229:GLN:OE1	1:D:229:GLN:HA	2.00	0.61
1:D:102:ALA:HA	1:D:407:MET:HE3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ILE:O	1:C:180:ILE:HA	2.00	0.61
1:A:346:LEU:H	1:A:346:LEU:HD12	1.65	0.61
1:F:342:ALA:HB1	1:F:344:GLU:HG2	1.82	0.61
1:D:260:ARG:HB2	1:D:269:TYR:CE2	2.36	0.61
1:B:390:SER:OG	1:B:391:ASN:N	2.33	0.61
1:E:219:ARG:HE	1:E:239:GLY:HA3	1.66	0.61
1:F:324:PRO:HG2	1:F:388:VAL:HG13	1.83	0.60
1:F:40:GLU:O	1:F:41:LEU:HB2	2.01	0.60
1:D:146:ILE:CG2	1:D:180:ILE:HD13	2.31	0.60
1:E:232:GLU:C	1:E:233:LEU:HG	2.22	0.60
1:C:324:PRO:HG2	1:C:388:VAL:HG23	1.83	0.60
1:C:352:ARG:HG3	1:C:355:GLU:HB2	1.82	0.60
1:A:27:GLN:HG3	1:A:33:TRP:CE2	2.37	0.60
1:C:230:PHE:O	1:C:233:LEU:HD23	2.01	0.60
1:A:309:ASP:O	1:A:312:LEU:HB2	2.02	0.60
1:B:248:LYS:HE3	1:B:251:GLN:NE2	2.17	0.60
1:B:171:LYS:HD3	1:C:250:ASP:OD1	2.01	0.60
1:F:254:LYS:HD3	1:F:256:LEU:HD21	1.84	0.60
1:C:229:GLN:O	1:C:229:GLN:HG3	2.02	0.60
1:F:116:LEU:HD11	1:F:129:THR:HG23	1.83	0.60
1:D:351:ILE:HD13	1:D:399:ARG:NH2	2.16	0.59
1:B:115:ILE:HD11	1:B:198:ILE:HD11	1.83	0.59
1:E:351:ILE:CD1	1:E:351:ILE:H	2.16	0.59
1:F:230:PHE:CD1	1:F:231:ASN:N	2.71	0.59
1:C:332:LYS:NZ	1:C:376:ASP:OD2	2.36	0.59
1:E:372:SER:OG	1:E:379:GLU:OE1	2.21	0.59
1:A:345:MET:O	1:A:347:LYS:N	2.35	0.59
1:F:95:PRO:HG2	1:F:99:VAL:HG11	1.83	0.58
1:A:139:ILE:HG13	1:A:141:VAL:HG13	1.85	0.58
1:A:225:LYS:CG	1:A:226:PRO:HD2	2.32	0.58
1:F:356:THR:HA	1:F:368:GLY:O	2.03	0.58
1:D:146:ILE:O	1:D:180:ILE:HA	2.03	0.58
1:F:262:GLU:HG3	1:F:267:VAL:CB	2.31	0.58
1:A:308:ALA:O	1:A:309:ASP:HB2	2.03	0.58
1:D:24:THR:HG22	1:D:185:ALA:CB	2.34	0.57
1:E:238:ILE:HG21	1:E:316:ILE:HD11	1.84	0.57
2:E:501:GDP:C8	2:E:501:GDP:H5"	2.39	0.57
1:E:82:GLU:OE1	1:E:82:GLU:N	2.37	0.57
1:A:335:LEU:HD11	1:A:350:PRO:HA	1.85	0.57
1:B:320:ASP:OD1	1:B:320:ASP:N	2.32	0.57
1:C:154:VAL:HG13	1:C:158:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:LEU:HB2	1:B:383:ARG:HD3	1.85	0.57
1:C:229:GLN:HG3	1:C:232:GLU:HB3	1.87	0.57
1:F:370:VAL:HG22	1:F:380:VAL:HG22	1.87	0.57
1:C:229:GLN:HE21	1:C:232:GLU:HB2	1.69	0.57
1:D:103:THR:HB	1:D:109:ALA:HB2	1.86	0.57
1:D:399:ARG:HD2	1:D:408:ILE:HD13	1.87	0.57
1:A:59:CYS:HB3	1:A:62:CYS:SG	2.45	0.56
1:E:246:LEU:HD11	1:E:288:GLU:HB2	1.86	0.56
1:A:399:ARG:HG2	1:A:408:ILE:HG21	1.87	0.56
1:B:215:MET:HE3	1:B:316:ILE:HB	1.88	0.56
1:A:229:GLN:HB3	1:A:232:GLU:HB3	1.87	0.56
1:B:255:VAL:HG13	1:B:272:ILE:HG13	1.88	0.56
1:B:370:VAL:HG22	1:B:380:VAL:HG22	1.88	0.56
1:B:355:GLU:OE2	1:B:399:ARG:NE	2.36	0.56
1:E:223:VAL:HG13	1:E:237:VAL:HG11	1.86	0.56
1:F:94:ALA:HB2	1:F:100:LEU:CD1	2.21	0.56
1:B:360:SER:HB2	1:B:396:VAL:HG12	1.88	0.56
1:C:361:VAL:HG21	1:C:386:VAL:HG11	1.87	0.56
1:E:343:LYS:HE2	1:E:344:GLU:HG3	1.88	0.56
1:F:104:MET:O	1:F:139:ILE:HG21	2.06	0.56
1:C:274:THR:OG1	1:C:275:LYS:N	2.39	0.56
1:A:8:PRO:HG2	1:A:293:GLY:HA3	1.88	0.56
1:C:352:ARG:CG	1:C:355:GLU:HB2	2.36	0.56
1:E:389:TRP:CE3	1:E:390:SER:HB3	2.41	0.56
1:C:230:PHE:HA	1:C:233:LEU:HD23	1.89	0.55
1:C:229:GLN:HG2	1:C:232:GLU:HB3	1.87	0.55
1:D:127:PRO:HB3	1:D:338:ARG:HH22	1.71	0.55
1:A:171:LYS:HA	1:A:176:GLU:HG3	1.88	0.55
1:B:164:ARG:NH1	1:C:302:ASP:OD1	2.39	0.55
1:A:154:VAL:HG13	1:A:158:GLU:HB2	1.88	0.55
1:D:345:MET:SD	1:D:345:MET:N	2.80	0.55
1:E:30:THR:HG22	1:E:54:THR:HB	1.88	0.55
1:A:35:SER:HB3	1:A:36:LYS:CA	2.37	0.55
1:C:280:ARG:NH1	1:C:285:GLU:OE1	2.40	0.55
1:C:67:ALA:HA	1:C:77:CYS:SG	2.46	0.55
1:B:45:MET:HG2	1:B:46:THR:HG22	1.88	0.55
1:F:261:VAL:O	1:F:261:VAL:HG23	2.06	0.55
1:E:225:LYS:HB3	1:E:226:PRO:HD2	1.89	0.55
1:F:212:LYS:HE2	1:F:318:LEU:HD13	1.87	0.55
1:A:22:LYS:N	2:A:501:GDP:O1B	2.34	0.55
1:C:352:ARG:NH1	1:C:354:LYS:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:LYS:HG2	1:F:288:GLU:HG2	1.88	0.55
1:A:355:GLU:OE1	1:A:399:ARG:NE	2.36	0.54
1:D:306:THR:O	1:D:308:ALA:N	2.40	0.54
1:F:215:MET:HB2	1:F:242:ILE:HG22	1.89	0.54
1:B:192:ASP:OD1	1:B:192:ASP:N	2.40	0.54
1:E:255:VAL:HG11	1:E:311:LEU:HD12	1.87	0.54
1:C:150:LYS:HG2	2:C:501:GDP:C6	2.43	0.54
1:F:357:LEU:O	1:F:368:GLY:N	2.35	0.54
1:A:259:LEU:HD21	1:D:75:LYS:HB3	1.90	0.54
1:B:344:GLU:OE1	1:B:344:GLU:N	2.40	0.54
1:C:370:VAL:HG11	1:C:378:ILE:HD11	1.90	0.54
1:F:215:MET:HA	1:F:242:ILE:HA	1.89	0.54
1:E:243:ILE:HG21	1:E:389:TRP:CH2	2.42	0.54
1:D:214:VAL:HG12	1:D:244:GLN:HG2	1.90	0.54
1:D:351:ILE:CD1	1:D:399:ARG:NH2	2.71	0.54
1:F:7:GLN:HE22	1:F:290:LYS:H	1.56	0.54
1:A:263:LYS:O	1:A:264:GLN:HG2	2.08	0.53
1:D:146:ILE:HG22	1:D:180:ILE:HD13	1.90	0.53
1:C:229:GLN:CG	1:C:232:GLU:CB	2.85	0.53
1:F:37:HIS:CG	1:F:38:SER:N	2.77	0.53
1:D:274:THR:OG1	1:D:275:LYS:N	2.42	0.53
1:F:290:LYS:HG2	1:F:291:PRO:HD2	1.91	0.53
1:C:230:PHE:O	1:C:233:LEU:CD2	2.57	0.53
1:C:370:VAL:HG22	1:C:380:VAL:HG22	1.91	0.53
1:D:347:LYS:HE3	1:D:349:ASP:OD2	2.09	0.53
1:A:307:LYS:HG3	1:A:308:ALA:N	2.23	0.53
1:E:329:ILE:HD13	1:E:382:LEU:HD11	1.91	0.53
1:F:361:VAL:HG13	1:F:395:THR:HB	1.91	0.52
1:A:35:SER:OG	1:A:36:LYS:HA	2.09	0.52
1:E:134:VAL:O	1:E:138:ILE:HG22	2.08	0.52
1:B:391:ASN:O	1:B:393:ILE:N	2.42	0.52
1:C:218:ILE:HG12	1:C:240:GLY:HA2	1.91	0.52
1:F:27:GLN:OE1	1:F:33:TRP:CE2	2.63	0.52
1:A:150:LYS:HG2	2:A:501:GDP:C6	2.44	0.52
1:B:338:ARG:NE	1:B:345:MET:HG3	2.20	0.52
1:B:373:VAL:CG2	1:B:378:ILE:HG22	2.26	0.52
1:A:219:ARG:HH21	1:A:294:LEU:CD1	2.18	0.52
1:B:344:GLU:HG2	1:B:346:LEU:HG	1.91	0.52
1:E:325:VAL:HG12	1:E:385:PRO:HB2	1.91	0.52
1:E:390:SER:OG	1:E:391:ASN:N	2.42	0.52
1:C:279:ILE:HG21	1:C:289:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:ILE:HD12	1:E:316:ILE:HG21	1.91	0.52
1:A:224:ASN:HD21	1:A:234:LYS:N	2.08	0.52
1:D:348:VAL:HG12	1:D:348:VAL:O	2.09	0.52
1:F:275:LYS:HB3	1:F:300:TYR:CD1	2.45	0.51
1:C:113:GLY:HA3	1:C:111:MET:SD	2.51	0.51
1:C:346:LEU:N	1:C:346:LEU:CD2	2.73	0.51
1:D:116:LEU:HD11	1:D:129:THR:HG23	1.93	0.51
1:E:351:ILE:CD1	1:E:351:ILE:N	2.73	0.51
1:F:37:HIS:CG	1:F:38:SER:H	2.26	0.51
1:B:139:ILE:HG13	1:B:141:VAL:HG23	1.92	0.51
1:E:225:LYS:O	1:E:228:THR:HG22	2.10	0.51
1:C:347:LYS:CD	1:C:347:LYS:N	2.73	0.51
1:D:161:SER:O	1:D:164:ARG:HG2	2.10	0.51
1:E:229:GLN:OE1	1:E:229:GLN:HA	2.11	0.51
1:F:269:TYR:CE1	1:F:385:PRO:HD2	2.46	0.51
1:B:274:THR:HG21	1:B:299:THR:HB	1.92	0.51
1:D:231:ASN:ND2	1:D:232:GLU:HG2	2.26	0.51
1:E:309:ASP:HB3	1:E:312:LEU:HD23	1.93	0.51
1:B:171:LYS:HA	1:B:176:GLU:HG3	1.92	0.51
1:D:27:GLN:HG3	1:D:33:TRP:CE2	2.46	0.51
1:E:3:TRP:CD1	1:E:85:PHE:HB2	2.46	0.51
1:F:393:ILE:HG23	1:F:413:VAL:HB	1.92	0.50
1:F:250:ASP:H	1:F:276:ILE:HG13	1.76	0.50
1:C:256:LEU:O	1:C:314:SER:HB2	2.11	0.50
1:B:243:ILE:HG21	1:B:389:TRP:CH2	2.47	0.50
1:E:17:HIS:ND1	1:E:128:GLN:HB2	2.26	0.50
1:B:279:ILE:HG21	1:B:289:ALA:HB2	1.92	0.50
1:D:401:ILE:HD13	1:D:406:ARG:HB2	1.93	0.50
1:A:287:LYS:HE2	1:E:353:ALA:HB3	1.92	0.50
1:F:328:ASN:HD21	1:F:381:GLU:CD	2.14	0.50
1:D:327:TRP:CE2	1:D:385:PRO:HG3	2.46	0.50
1:B:18:VAL:HG23	1:B:128:GLN:OE1	2.11	0.50
1:F:9:GLU:HG3	1:F:10:VAL:HG12	1.93	0.50
1:A:361:VAL:O	1:A:364:SER:OG	2.24	0.50
1:B:254:LYS:NZ	1:B:319:ALA:O	2.42	0.50
1:C:131:GLU:OE2	1:C:340:VAL:HA	2.12	0.50
1:D:146:ILE:HG13	1:D:178:VAL:HG11	1.94	0.50
1:A:59:CYS:CB	1:A:62:CYS:SG	3.00	0.50
1:D:170:THR:O	1:D:173:THR:OG1	2.21	0.50
1:E:213:PRO:HB2	1:E:247:PHE:CE2	2.46	0.50
1:E:64:LYS:HE3	1:E:68:TYR:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:PHE:CE1	1:F:253:ILE:HD11	2.47	0.50
1:B:46:THR:O	1:B:48:LYS:HG3	2.11	0.49
1:D:160:LEU:O	1:D:163:TYR:HB3	2.12	0.49
1:F:255:VAL:HG11	1:F:311:LEU:HD23	1.94	0.49
1:C:17:HIS:ND1	1:C:128:GLN:HB2	2.28	0.49
1:D:351:ILE:CD1	1:D:399:ARG:CZ	2.90	0.49
1:F:47:ILE:O	1:F:47:ILE:HD12	2.12	0.49
1:F:13:GLY:HA2	1:F:92:ILE:HG12	1.94	0.49
1:D:249:VAL:HG23	1:D:287:LYS:O	2.13	0.49
1:D:396:VAL:CG2	1:D:407:MET:HG2	2.43	0.49
1:C:246:LEU:HD11	1:C:288:GLU:HB2	1.94	0.49
1:E:48:LYS:NZ	1:E:309:ASP:OD2	2.41	0.49
1:F:9:GLU:O	1:F:207:ARG:NH1	2.43	0.49
1:F:268:SER:HA	1:F:327:TRP:CZ2	2.47	0.49
1:F:160:LEU:O	1:F:163:TYR:HB3	2.12	0.49
1:D:347:LYS:HZ2	1:D:348:VAL:N	2.08	0.49
1:A:187:HIS:CE1	1:C:367:LEU:HD13	2.48	0.49
1:A:58:VAL:CG2	1:A:86:LEU:HD11	2.42	0.49
1:D:264:GLN:HA	1:D:264:GLN:OE1	2.12	0.49
1:F:330:ARG:HD3	1:F:379:GLU:CG	2.43	0.49
1:D:179:PRO:C	1:D:180:ILE:HG22	2.33	0.49
1:D:242:ILE:HB	1:D:291:PRO:HA	1.93	0.49
1:D:309:ASP:O	1:D:312:LEU:HB2	2.13	0.49
1:E:338:ARG:HB3	1:E:345:MET:O	2.13	0.49
1:F:351:ILE:HG12	1:F:357:LEU:HD11	1.95	0.48
1:F:357:LEU:N	1:F:368:GLY:O	2.39	0.48
1:F:39:GLU:CD	1:F:40:GLU:H	2.16	0.48
1:A:225:LYS:HG3	1:A:226:PRO:HD3	1.94	0.48
1:C:372:SER:O	1:C:378:ILE:HG13	2.13	0.48
1:D:275:LYS:HD2	1:D:300:TYR:HE2	1.79	0.48
1:F:302:ASP:OD1	1:F:303:PRO:HD2	2.13	0.48
1:A:28:ALA:HA	1:A:188:LYS:HE3	1.95	0.48
1:B:274:THR:CG2	1:B:275:LYS:N	2.77	0.48
1:D:47:ILE:HD11	1:D:218:ILE:HG23	1.95	0.48
1:C:215:MET:HB3	1:C:316:ILE:HB	1.95	0.48
1:D:231:ASN:HD22	1:D:231:ASN:N	2.11	0.48
1:D:281:PHE:HB2	1:D:286:PHE:CE2	2.48	0.48
1:B:248:LYS:H	1:B:251:GLN:CD	2.15	0.48
1:B:2:ALA:HA	1:B:82:GLU:OE2	2.14	0.48
1:E:213:PRO:HA	1:E:244:GLN:O	2.13	0.48
1:B:338:ARG:HH21	1:B:345:MET:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:VAL:HG12	1:B:385:PRO:HB2	1.94	0.48
1:D:301:LEU:HB3	1:D:305:LEU:HD11	1.95	0.48
1:D:374:LYS:HD2	1:D:377:GLU:HB3	1.94	0.48
1:D:338:ARG:HD3	1:D:345:MET:HA	1.95	0.48
1:F:119:ALA:O	1:F:162:GLN:NE2	2.42	0.48
1:A:229:GLN:CB	1:A:233:LEU:HD23	2.40	0.47
1:D:15:VAL:HG12	1:D:100:LEU:HD11	1.96	0.47
1:F:145:ILE:HD11	1:F:201:TYR:HB2	1.96	0.47
1:F:258:GLY:HA3	1:F:271:PRO:HA	1.96	0.47
1:C:249:VAL:HG12	1:C:250:ASP:OD1	2.15	0.47
1:F:208:ASP:HB3	1:F:211:GLN:NE2	2.27	0.47
1:A:303:PRO:O	1:A:307:LYS:HB3	2.14	0.47
1:B:170:THR:HB	1:B:175:ALA:O	2.15	0.47
1:C:155:SER:OG	1:C:158:GLU:HG3	2.13	0.47
1:A:236:GLY:O	1:A:299:THR:OG1	2.28	0.47
1:A:41:LEU:HD23	1:A:42:LYS:HG2	1.95	0.47
1:D:351:ILE:HD13	1:D:399:ARG:CZ	2.45	0.47
1:E:184:SER:O	1:E:188:LYS:N	2.48	0.47
1:E:27:GLN:HG3	1:E:33:TRP:CD1	2.50	0.47
1:A:110:LEU:HD21	1:A:243:ILE:HG12	1.96	0.47
1:A:157:GLU:O	1:A:160:LEU:HB3	2.15	0.47
1:D:57:GLY:HA2	1:D:86:LEU:HD13	1.96	0.47
1:E:246:LEU:HD13	1:E:290:LYS:HG3	1.97	0.47
1:E:213:PRO:HB2	1:E:247:PHE:CZ	2.50	0.47
1:A:64:LYS:NZ	1:A:68:TYR:OH	2.47	0.47
1:B:274:THR:CG2	1:B:275:LYS:H	2.28	0.47
1:C:229:GLN:HG3	1:C:232:GLU:CB	2.44	0.47
1:C:238:ILE:HD12	1:C:316:ILE:HD11	1.97	0.47
1:D:124:PHE:CE2	1:D:166:ILE:HA	2.50	0.47
1:A:155:SER:OG	1:A:158:GLU:HG3	2.15	0.47
1:C:153:VAL:HG23	1:D:405:TRP:CD1	2.50	0.46
1:D:231:ASN:ND2	1:D:231:ASN:N	2.61	0.46
1:D:331:ILE:HG12	1:D:413:VAL:HG22	1.96	0.46
1:F:135:ALA:O	1:F:139:ILE:HG13	2.15	0.46
1:A:48:LYS:HB3	1:A:95:PRO:HG2	1.98	0.46
1:B:330:ARG:HG3	1:B:379:GLU:HG2	1.96	0.46
1:E:27:GLN:HG3	1:E:33:TRP:CG	2.51	0.46
1:F:242:ILE:HD11	1:F:291:PRO:N	2.30	0.46
1:A:9:GLU:HG3	1:A:10:VAL:HG23	1.96	0.46
1:B:335:LEU:HD11	1:B:350:PRO:HA	1.96	0.46
1:A:59:CYS:O	1:A:67:ALA:HB1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LYS:HG2	2:B:501:GDP:C6	2.50	0.46
1:E:218:ILE:HG12	1:E:240:GLY:HA2	1.98	0.46
1:F:230:PHE:CD2	1:F:232:GLU:OE2	2.69	0.46
1:F:255:VAL:HG22	1:F:316:ILE:HD11	1.98	0.46
1:A:48:LYS:HE3	1:A:48:LYS:HB2	1.58	0.46
1:A:58:VAL:HG22	1:A:68:TYR:CE1	2.51	0.46
1:D:347:LYS:HZ3	1:D:347:LYS:CA	2.23	0.46
1:E:138:ILE:HG13	1:E:410:TRP:CZ2	2.51	0.46
1:F:260:ARG:HH22	1:F:383:ARG:NH2	2.14	0.46
1:B:274:THR:HG22	1:B:275:LYS:N	2.30	0.46
1:C:35:SER:HA	1:C:37:HIS:CE1	2.50	0.46
1:D:388:VAL:HG12	1:D:390:SER:O	2.16	0.46
1:D:396:VAL:HG21	1:D:407:MET:HG2	1.97	0.46
1:E:355:GLU:OE1	1:E:399:ARG:NE	2.46	0.46
1:B:212:LYS:HA	1:B:213:PRO:HD3	1.78	0.46
1:E:213:PRO:HA	1:E:245:GLY:HA3	1.97	0.46
1:E:254:LYS:HD2	1:E:256:LEU:HD11	1.97	0.46
1:C:340:VAL:O	1:C:406:ARG:NH2	2.49	0.46
1:D:230:PHE:HA	1:D:233:LEU:CD2	2.46	0.46
1:E:12:ILE:HD12	1:E:202:ILE:HG21	1.97	0.46
1:E:94:ALA:HB3	1:E:100:LEU:HG	1.98	0.46
1:A:340:VAL:HG13	1:A:340:VAL:O	2.16	0.46
1:B:351:ILE:O	1:B:373:VAL:HG21	2.16	0.46
1:D:58:VAL:HG12	1:D:86:LEU:HD11	1.97	0.46
1:B:309:ASP:HB3	1:B:312:LEU:HD13	1.98	0.45
1:D:253:ILE:HD11	1:D:316:ILE:HG21	1.97	0.45
1:D:333:TYR:HE2	1:D:335:LEU:HD13	1.80	0.45
1:D:384:ARG:HA	1:D:385:PRO:HD3	1.85	0.45
1:A:366:THR:HB	1:A:384:ARG:HB3	1.97	0.45
1:B:415:ILE:HD12	1:B:415:ILE:HA	1.78	0.45
1:B:216:LEU:O	1:B:240:GLY:HA3	2.15	0.45
1:C:374:LYS:HD3	1:C:377:GLU:HG3	1.99	0.45
1:F:261:VAL:HG22	1:F:268:SER:O	2.17	0.45
1:F:331:ILE:O	1:F:377:GLU:HA	2.16	0.45
1:F:333:TYR:HE2	1:F:351:ILE:HD13	1.82	0.45
1:E:155:SER:OG	1:E:158:GLU:HG3	2.17	0.45
1:E:338:ARG:CD	1:E:345:MET:HA	2.37	0.45
1:A:51:TYR:CD2	1:A:294:LEU:HB2	2.52	0.45
1:F:80:ASP:OD1	1:F:80:ASP:N	2.49	0.45
1:C:371:THR:N	1:C:379:GLU:O	2.42	0.45
1:A:148:GLN:HB3	1:A:182:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:N	1:A:298:GLY:O	2.49	0.45
1:A:404:ARG:HD3	1:A:405:TRP:N	2.31	0.45
1:F:254:LYS:HG2	1:F:319:ALA:HA	1.99	0.45
1:A:178:VAL:HA	1:A:179:PRO:HD3	1.75	0.44
1:D:332:LYS:HB2	1:D:414:GLU:OE1	2.17	0.44
1:F:42:LYS:HE2	1:F:95:PRO:HB2	1.99	0.44
1:E:9:GLU:O	1:E:207:ARG:NH2	2.50	0.44
1:F:262:GLU:HG3	1:F:267:VAL:HA	1.99	0.44
1:B:27:GLN:HG3	1:B:33:TRP:CE2	2.52	0.44
1:B:59:CYS:SG	1:B:83:PRO:HB3	2.57	0.44
1:D:347:LYS:NZ	1:D:348:VAL:N	2.60	0.44
1:F:302:ASP:OD2	1:F:304:SER:OG	2.24	0.44
1:C:345:MET:HG2	1:C:345:MET:H	1.51	0.44
1:A:225:LYS:CG	1:A:226:PRO:CD	2.92	0.44
1:C:124:PHE:CE2	1:C:166:ILE:HA	2.53	0.44
1:F:344:GLU:HG3	1:F:347:LYS:NZ	2.32	0.44
1:B:63:LYS:HB2	5:B:663:HOH:O	2.18	0.44
1:A:373:VAL:HB	1:A:378:ILE:HG22	2.00	0.44
1:D:180:ILE:HG13	1:D:180:ILE:O	2.17	0.44
1:E:10:VAL:HG13	1:E:89:ILE:HG22	2.00	0.44
1:C:132:HIS:O	1:C:136:LEU:HB2	2.18	0.44
1:C:281:PHE:CE1	1:C:295:VAL:HB	2.52	0.44
1:F:36:LYS:HE3	1:F:36:LYS:HB2	1.62	0.44
1:B:373:VAL:HG23	1:B:378:ILE:CG2	2.29	0.43
1:C:229:GLN:HG2	1:C:232:GLU:CB	2.47	0.43
1:A:170:THR:O	1:A:173:THR:OG1	2.25	0.43
1:B:274:THR:CG2	1:B:299:THR:HB	2.48	0.43
1:D:339:VAL:HB	1:D:342:ALA:HB2	2.00	0.43
1:B:309:ASP:O	1:B:312:LEU:HB2	2.19	0.43
1:E:22:LYS:HE2	5:E:637:HOH:O	2.19	0.43
1:B:124:PHE:CE1	1:B:166:ILE:HA	2.54	0.43
1:B:353:ALA:O	1:B:370:VAL:HB	2.19	0.43
1:D:239:GLY:HA2	1:D:295:VAL:O	2.19	0.43
1:D:81:ASP:N	1:D:81:ASP:OD1	2.51	0.43
1:E:163:TYR:CE2	1:E:180:ILE:HB	2.54	0.43
1:B:152:ASP:O	1:E:400:GLN:NE2	2.52	0.43
1:F:146:ILE:HG13	1:F:178:VAL:HG11	2.00	0.43
1:D:264:GLN:HB3	1:D:265:GLY:H	1.61	0.43
1:E:236:GLY:HA3	1:E:306:THR:HG21	2.01	0.43
1:E:339:VAL:HB	1:E:342:ALA:HB2	2.00	0.43
1:E:389:TRP:CZ3	1:E:390:SER:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:OD1	1:A:193:SER:N	2.52	0.43
1:A:275:LYS:HB3	1:A:300:TYR:CD1	2.53	0.43
1:C:359:LEU:HD11	1:C:380:VAL:HG11	2.00	0.43
1:C:3:TRP:CD1	1:C:85:PHE:HB2	2.54	0.43
1:D:110:LEU:HD21	1:D:241:SER:HB3	2.01	0.43
1:E:303:PRO:HA	1:E:306:THR:HG22	2.01	0.43
1:F:124:PHE:HA	1:F:125:PRO:HA	1.77	0.43
1:A:287:LYS:HD3	1:A:287:LYS:N	2.34	0.43
1:B:214:VAL:O	1:B:243:ILE:N	2.51	0.43
1:B:280:ARG:HB2	1:B:296:ALA:HB3	1.99	0.43
1:C:136:LEU:HD21	1:C:144:LEU:HD13	2.01	0.43
1:C:66:GLU:HG3	1:D:262:GLU:O	2.18	0.43
1:F:262:GLU:HG3	1:F:267:VAL:CA	2.49	0.43
1:F:335:LEU:HD12	1:F:335:LEU:HA	1.73	0.43
1:F:81:ASP:HB2	1:F:82:GLU:H	1.51	0.43
1:F:178:VAL:HG13	1:F:179:PRO:HD2	2.01	0.43
1:A:404:ARG:HD3	1:A:405:TRP:H	1.84	0.42
1:F:247:PHE:HB2	1:F:289:ALA:HB3	2.01	0.42
1:C:27:GLN:HG3	1:C:33:TRP:CE2	2.53	0.42
1:D:279:ILE:HG21	1:D:289:ALA:HB2	2.01	0.42
1:D:324:PRO:HB2	1:D:326:LEU:CD1	2.49	0.42
1:D:51:TYR:HA	1:D:91:PHE:O	2.19	0.42
1:A:343:LYS:O	1:A:344:GLU:HB3	2.19	0.42
1:A:345:MET:HB3	1:A:346:LEU:HD12	2.02	0.42
1:B:360:SER:HB2	1:B:396:VAL:CG1	2.49	0.42
1:B:357:LEU:HD13	1:B:397:ILE:HG23	2.00	0.42
1:E:270:GLU:HA	1:E:271:PRO:HD3	1.87	0.42
1:E:346:LEU:HD22	1:E:346:LEU:HA	1.73	0.42
1:F:106:SER:OG	1:F:362:GLY:O	2.26	0.42
1:A:390:SER:OG	1:A:391:ASN:N	2.52	0.42
1:C:124:PHE:HA	1:C:125:PRO:HA	1.74	0.42
1:C:221:PHE:CD1	1:C:221:PHE:N	2.86	0.42
1:C:37:HIS:NE2	1:C:95:PRO:HB3	2.34	0.42
1:E:280:ARG:HG2	1:E:296:ALA:HB3	2.01	0.42
1:F:139:ILE:HG22	1:F:394:ARG:CZ	2.49	0.42
1:A:153:VAL:HG13	1:C:405:TRP:CD1	2.55	0.42
1:A:19:ASP:HA	2:A:501:GDP:H5'	2.00	0.42
1:C:221:PHE:HD1	1:C:221:PHE:N	2.18	0.42
1:C:229:GLN:NE2	1:C:232:GLU:HB2	2.34	0.42
1:F:332:LYS:NZ	1:F:414:GLU:HG3	2.34	0.42
1:D:369:ILE:HG22	1:D:381:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:MET:SD	1:F:297:ILE:HD13	2.59	0.42
1:D:253:ILE:HD11	1:D:316:ILE:CG2	2.49	0.42
1:B:186:LEU:HD12	1:B:187:HIS:CE1	2.55	0.42
1:D:261:VAL:O	1:D:267:VAL:HG13	2.20	0.42
1:E:12:ILE:HB	1:E:91:PHE:CD1	2.55	0.42
1:A:125:PRO:HG2	1:A:130:ARG:CZ	2.50	0.42
1:C:318:LEU:HA	1:C:318:LEU:HD23	1.86	0.42
1:D:56:ILE:HG13	1:D:89:ILE:HD12	2.00	0.42
1:E:27:GLN:HG3	1:E:33:TRP:CD2	2.55	0.42
1:F:186:LEU:HD23	1:F:187:HIS:CD2	2.55	0.42
1:F:304:SER:HA	1:F:307:LYS:HZ3	1.85	0.42
1:C:248:LYS:O	1:C:251:GLN:HB2	2.20	0.41
1:C:374:LYS:HD3	1:C:377:GLU:OE2	2.20	0.41
1:E:174:TRP:CZ3	1:E:175:ALA:HB2	2.54	0.41
1:E:254:LYS:HE3	1:E:273:PHE:CE1	2.55	0.41
1:F:280:ARG:HB3	1:F:296:ALA:HB3	2.01	0.41
1:F:330:ARG:HD3	1:F:379:GLU:HG2	2.02	0.41
1:A:254:LYS:HE3	1:A:256:LEU:HD21	2.01	0.41
1:D:164:ARG:HB2	1:D:168:GLN:HE22	1.86	0.41
1:D:255:VAL:HB	1:D:272:ILE:HB	2.01	0.41
1:A:262:GLU:HG2	1:D:66:GLU:HG2	2.02	0.41
1:D:8:PRO:HA	1:D:88:ARG:HB3	2.01	0.41
1:F:13:GLY:HA2	1:F:92:ILE:CG1	2.50	0.41
1:A:99:VAL:O	1:A:103:THR:HG23	2.19	0.41
1:A:345:MET:HB3	1:A:346:LEU:H	1.59	0.41
1:B:338:ARG:HH21	1:B:345:MET:CG	2.34	0.41
1:C:7:GLN:HE22	1:C:290:LYS:C	2.22	0.41
1:F:361:VAL:HG21	1:F:386:VAL:HG11	2.02	0.41
1:F:146:ILE:N	5:F:622:HOH:O	2.52	0.41
1:A:373:VAL:HG22	1:A:373:VAL:O	2.21	0.41
1:D:231:ASN:H	1:D:231:ASN:ND2	2.18	0.41
1:E:301:LEU:HD22	1:E:305:LEU:HD11	2.03	0.41
1:F:404:ARG:HA	1:F:404:ARG:HD2	1.85	0.41
1:F:46:THR:C	1:F:47:ILE:HG13	2.41	0.41
1:F:155:SER:OG	1:F:158:GLU:HG3	2.21	0.41
1:A:36:LYS:O	1:A:37:HIS:C	2.59	0.41
1:C:154:VAL:CG1	1:C:158:GLU:HB2	2.49	0.41
1:C:212:LYS:HA	1:C:213:PRO:HD3	1.92	0.41
1:D:134:VAL:O	1:D:138:ILE:HG13	2.21	0.41
1:E:360:SER:HA	1:E:364:SER:O	2.21	0.41
1:F:259:LEU:O	1:F:269:TYR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PRO:C	1:A:183:VAL:HG13	2.41	0.41
1:C:81:ASP:OD1	1:C:81:ASP:N	2.54	0.41
1:D:139:ILE:HG13	1:D:141:VAL:HG23	2.02	0.41
1:E:253:ILE:HD13	1:E:276:ILE:HG12	2.03	0.41
1:F:333:TYR:CE2	1:F:351:ILE:HD13	2.56	0.41
1:F:37:HIS:CE1	1:F:39:GLU:H	2.39	0.41
1:A:37:HIS:O	1:A:38:SER:C	2.59	0.41
1:C:263:LYS:HD2	1:C:266:LYS:CE	2.49	0.41
1:C:27:GLN:HG3	1:C:33:TRP:CD1	2.56	0.41
1:D:162:GLN:O	1:D:166:ILE:HG13	2.21	0.41
1:F:344:GLU:H	1:F:344:GLU:HG2	1.60	0.41
1:A:175:ALA:O	1:A:178:VAL:HG22	2.20	0.41
1:B:281:PHE:HB2	1:B:286:PHE:CE1	2.56	0.41
1:C:108:ALA:HA	1:C:216:LEU:HD21	2.03	0.41
1:A:279:ILE:HG21	1:A:289:ALA:HB2	2.03	0.40
1:D:168:GLN:HA	1:D:171:LYS:HD2	2.01	0.40
1:A:224:ASN:ND2	1:A:233:LEU:HD22	2.36	0.40
1:B:353:ALA:O	1:B:355:GLU:N	2.45	0.40
1:D:179:PRO:HG3	1:D:201:TYR:CE1	2.56	0.40
1:E:279:ILE:HG12	1:E:297:ILE:HD13	2.03	0.40
1:F:270:GLU:HA	1:F:271:PRO:HD3	1.95	0.40
1:F:92:ILE:HG13	1:F:92:ILE:O	2.21	0.40
1:B:305:LEU:O	1:B:311:LEU:HD13	2.22	0.40
1:C:253:ILE:HD12	1:C:316:ILE:HG21	2.03	0.40
1:D:124:PHE:HA	1:D:125:PRO:HA	1.72	0.40
1:D:178:VAL:HA	1:D:179:PRO:HD3	1.81	0.40
1:F:47:ILE:HG12	1:F:312:LEU:HD11	2.03	0.40
1:C:348:VAL:HG22	1:C:349:ASP:N	2.37	0.40
1:E:222:ASP:CG	1:E:303:PRO:HB3	2.42	0.40
1:F:184:SER:O	1:F:188:LYS:N	2.54	0.40
1:F:209:LEU:HD11	1:F:246:LEU:HB2	2.04	0.40
1:A:208:ASP:OD2	1:A:211:GLN:HG3	2.21	0.40
1:A:230:PHE:O	1:A:231:ASN:CB	2.70	0.40
1:F:181:ILE:HA	1:F:182:PRO:HD3	1.96	0.40
1:F:183:VAL:HB	1:F:191:ILE:HD13	2.02	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	408/415 (98%)	378 (93%)	24 (6%)	6 (2%)	12	24
1	B	390/415 (94%)	355 (91%)	27 (7%)	8 (2%)	8	15
1	C	402/415 (97%)	383 (95%)	16 (4%)	3 (1%)	25	49
1	D	401/415 (97%)	371 (92%)	25 (6%)	5 (1%)	15	32
1	E	401/415 (97%)	367 (92%)	29 (7%)	5 (1%)	15	32
1	F	412/415 (99%)	371 (90%)	29 (7%)	12 (3%)	5	8
All	All	2414/2490 (97%)	2225 (92%)	150 (6%)	39 (2%)	11	23

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	GLU
1	A	346	LEU
1	B	46	THR
1	B	353	ALA
1	C	353	ALA
1	D	307	LYS
1	D	391	ASN
1	F	81	ASP
1	F	307	LYS
1	F	354	LYS
1	A	353	ALA
1	A	391	ASN
1	B	392	ASN
1	D	370	VAL
1	E	375	LYS
1	F	41	LEU
1	F	180	ILE
1	F	347	LYS
1	F	353	ALA
1	A	374	LYS

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Mol	Chain	Res	Type
1	B	354	LYS
1	B	391	ASN
1	E	391	ASN
1	F	80	ASP
1	F	348	VAL
1	A	40	GLU
1	C	180	ILE
1	E	306	THR
1	F	346	LEU
1	B	51	TYR
1	C	340	VAL
1	D	182	PRO
1	E	307	LYS
1	B	347	LYS
1	F	47	ILE
1	E	282	GLY
1	F	226	PRO
1	B	47	ILE
1	D	350	PRO

### 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	355/357 (99%)	327 (92%)	28 (8%)	14	28
1	B	340/357 (95%)	319 (94%)	21 (6%)	21	42
1	C	349/357 (98%)	321 (92%)	28 (8%)	14	27
1	D	348/357 (98%)	316 (91%)	32 (9%)	11	20
1	E	348/357 (98%)	321 (92%)	27 (8%)	15	29
1	F	356/357 (100%)	328 (92%)	28 (8%)	14	28
All	All	2096/2142 (98%)	1932 (92%)	164 (8%)	15	29

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	36	LYS
1	A	46	THR
1	A	47	ILE
1	A	66	GLU
1	A	75	LYS
1	A	77	CYS
1	A	100	LEU
1	A	105	LEU
1	A	110	LEU
1	A	129	THR
1	A	141	VAL
1	A	153	VAL
1	A	154	VAL
1	A	162	GLN
1	A	168	GLN
1	A	210	SER
1	A	225	LYS
1	A	228	THR
1	A	241	SER
1	A	285	GLU
1	A	287	LYS
1	A	301	LEU
1	A	307	LYS
1	A	310	ASN
1	A	366	THR
1	A	372	SER
1	A	373	VAL
1	B	5	LYS
1	B	19	ASP
1	B	46	THR
1	B	62	CYS
1	B	74	CYS
1	B	76	SER
1	B	116	LEU
1	B	153	VAL
1	B	157	GLU
1	B	160	LEU
1	B	173	THR
1	B	192	ASP
1	B	221	PHE
1	B	246	LEU
1	B	259	LEU

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Mol	Chain	Res	Type
1	B	306	THR
1	B	314	SER
1	B	337	GLU
1	B	346	LEU
1	B	348	VAL
1	B	373	VAL
1	C	19	ASP
1	C	34	THR
1	C	37	HIS
1	C	63	LYS
1	C	98	GLU
1	C	153	VAL
1	C	167	LYS
1	C	221	PHE
1	C	223	VAL
1	C	231	ASN
1	C	232	GLU
1	C	259	LEU
1	C	262	GLU
1	C	268	SER
1	C	307	LYS
1	C	343	LYS
1	C	344	GLU
1	C	345	MET
1	C	346	LEU
1	C	347	LYS
1	C	349	ASP
1	C	361	VAL
1	C	366	THR
1	C	369	ILE
1	C	371	THR
1	C	374	LYS
1	C	376	ASP
1	C	415	ILE
1	D	46	THR
1	D	47	ILE
1	D	75	LYS
1	D	79	SER
1	D	81	ASP
1	D	98	GLU
1	D	100	LEU
1	D	103	THR

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Mol	Chain	Res	Type
1	D	136	LEU
1	D	151	VAL
1	D	168	GLN
1	D	198	ILE
1	D	221	PHE
1	D	231	ASN
1	D	233	LEU
1	D	241	SER
1	D	250	ASP
1	D	264	GLN
1	D	305	LEU
1	D	312	LEU
1	D	323	VAL
1	D	335	LEU
1	D	345	MET
1	D	346	LEU
1	D	347	LYS
1	D	357	LEU
1	D	369	ILE
1	D	370	VAL
1	D	382	LEU
1	D	390	SER
1	D	395	THR
1	D	399	ARG
1	E	46	THR
1	E	48	LYS
1	E	59	CYS
1	E	77	CYS
1	E	82	GLU
1	E	100	LEU
1	E	138	ILE
1	E	192	ASP
1	E	215	MET
1	E	216	LEU
1	E	223	VAL
1	E	228	THR
1	E	229	GLN
1	E	254	LYS
1	E	259	LEU
1	E	305	LEU
1	E	312	LEU
1	E	338	ARG

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Mol	Chain	Res	Type
1	E	343	LYS
1	E	344	GLU
1	E	346	LEU
1	E	349	ASP
1	E	364	SER
1	E	370	VAL
1	E	379	GLU
1	E	390	SER
1	E	406	ARG
1	F	10	VAL
1	F	33	TRP
1	F	41	LEU
1	F	43	ARG
1	F	58	VAL
1	F	61	SER
1	F	66	GLU
1	F	81	ASP
1	F	98	GLU
1	F	106	SER
1	F	224	ASN
1	F	225	LYS
1	F	230	PHE
1	F	253	ILE
1	F	267	VAL
1	F	274	THR
1	F	275	LYS
1	F	276	ILE
1	F	287	LYS
1	F	318	LEU
1	F	330	ARG
1	F	333	TYR
1	F	335	LEU
1	F	352	ARG
1	F	361	VAL
1	F	367	LEU
1	F	388	VAL
1	F	406	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS

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Mol	Chain	Res	Type
1	B	55	ASN
1	B	391	ASN
1	B	392	ASN
1	C	229	GLN
1	D	231	ASN
1	E	148	GLN
1	E	162	GLN
1	F	7	GLN
1	F	244	GLN
1	F	264	GLN

### 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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\# Z  > 2$
2	GDP	A	501	3	25,30,30	1.09	2 (8%)	26,47,47	2.00	6 (23%)
2	GDP	B	501	3	25,30,30	1.08	2 (8%)	26,47,47	1.99	6 (23%)
2	GDP	C	501	3	25,30,30	1.14	2 (8%)	26,47,47	2.01	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GDP	D	501	3	25,30,30	1.09	2 (8%)	26,47,47	2.05	6 (23%)
2	GDP	E	501	3	25,30,30	1.11	2 (8%)	26,47,47	2.08	6 (23%)
4	PO4	E	503	-	4,4,4	0.78	0	6,6,6	0.43	0
2	GDP	F	501	3	25,30,30	1.11	2 (8%)	26,47,47	1.97	6 (23%)

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
2	GDP	A	501	3	-	0/12/32/32	0/3/3/3
2	GDP	B	501	3	-	0/12/32/32	0/3/3/3
2	GDP	C	501	3	-	0/12/32/32	0/3/3/3
2	GDP	D	501	3	-	0/12/32/32	0/3/3/3
2	GDP	E	501	3	-	0/12/32/32	0/3/3/3
4	PO4	E	503	-	-	0/0/0/0	0/0/0/0
2	GDP	F	501	3	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	GDP	C5-C4	2.69	1.46	1.40
2	E	501	GDP	C5-C4	2.79	1.46	1.40
2	B	501	GDP	C5-C4	2.80	1.46	1.40
2	F	501	GDP	C5-C4	2.85	1.46	1.40
2	A	501	GDP	C5-C4	2.89	1.47	1.40
2	C	501	GDP	C5-C4	2.91	1.47	1.40
2	A	501	GDP	C6-C5	3.42	1.47	1.41
2	B	501	GDP	C6-C5	3.44	1.47	1.41
2	D	501	GDP	C6-C5	3.45	1.47	1.41
2	F	501	GDP	C6-C5	3.63	1.48	1.41
2	E	501	GDP	C6-C5	3.68	1.48	1.41
2	C	501	GDP	C6-C5	3.69	1.48	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	GDP	C5-C6-N1	-4.08	117.67	123.48
2	D	501	GDP	C6-C5-C4	-4.02	116.84	120.84
2	A	501	GDP	C5-C6-N1	-3.91	117.91	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	GDP	C5-C6-N1	-3.89	117.94	123.48
2	B	501	GDP	C5-C6-N1	-3.86	117.98	123.48
2	C	501	GDP	C5-C6-N1	-3.83	118.03	123.48
2	B	501	GDP	C6-C5-C4	-3.82	117.05	120.84
2	E	501	GDP	C6-C5-C4	-3.78	117.09	120.84
2	F	501	GDP	C5-C6-N1	-3.75	118.14	123.48
2	C	501	GDP	C6-C5-C4	-3.74	117.13	120.84
2	F	501	GDP	C6-C5-C4	-3.51	117.35	120.84
2	A	501	GDP	C6-C5-C4	-3.38	117.48	120.84
2	E	501	GDP	C4-C5-N7	-3.29	106.23	109.41
2	C	501	GDP	C4-C5-N7	-3.13	106.38	109.41
2	D	501	GDP	N3-C2-N1	-3.07	122.97	127.46
2	E	501	GDP	N3-C2-N1	-3.07	122.98	127.46
2	F	501	GDP	N3-C2-N1	-3.03	123.04	127.46
2	B	501	GDP	N3-C2-N1	-2.98	123.11	127.46
2	C	501	GDP	N3-C2-N1	-2.97	123.13	127.46
2	D	501	GDP	C4-C5-N7	-2.94	106.57	109.41
2	B	501	GDP	C4-C5-N7	-2.92	106.59	109.41
2	F	501	GDP	C4-C5-N7	-2.90	106.61	109.41
2	A	501	GDP	N3-C2-N1	-2.89	123.24	127.46
2	A	501	GDP	C4-C5-N7	-2.75	106.75	109.41
2	F	501	GDP	C6-N1-C2	4.19	122.09	116.06
2	A	501	GDP	C6-N1-C2	4.21	122.12	116.06
2	C	501	GDP	C6-N1-C2	4.24	122.16	116.06
2	B	501	GDP	C6-N1-C2	4.30	122.24	116.06
2	D	501	GDP	C6-N1-C2	4.38	122.37	116.06
2	E	501	GDP	C6-N1-C2	4.44	122.45	116.06
2	D	501	GDP	C2-N3-C4	4.71	120.66	115.16
2	B	501	GDP	C2-N3-C4	4.72	120.67	115.16
2	A	501	GDP	C2-N3-C4	4.82	120.79	115.16
2	E	501	GDP	C2-N3-C4	4.84	120.81	115.16
2	C	501	GDP	C2-N3-C4	4.89	120.86	115.16
2	F	501	GDP	C2-N3-C4	4.97	120.97	115.16

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
2	A	501	GDP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	GDP	1	0
2	C	501	GDP	1	0
2	E	501	GDP	2	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	412/415 (99%)	-0.21	11 (2%) 55 48	30, 43, 77, 130	366 (88%)
1	B	396/415 (95%)	-0.28	4 (1%) 82 79	29, 47, 71, 84	323 (81%)
1	C	406/415 (97%)	-0.13	15 (3%) 42 34	26, 42, 88, 127	332 (81%)
1	D	405/415 (97%)	-0.07	12 (2%) 51 43	29, 50, 75, 133	341 (84%)
1	E	405/415 (97%)	-0.07	11 (2%) 55 48	26, 58, 82, 129	298 (73%)
1	F	414/415 (99%)	0.18	17 (4%) 38 30	44, 68, 110, 151	291 (70%)
All	All	2438/2490 (97%)	-0.10	70 (2%) 52 45	26, 52, 84, 151	1951 (80%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	37	HIS	7.6
1	F	40	GLU	6.4
1	E	47	ILE	6.3
1	F	228	THR	6.0
1	D	227	GLY	5.2
1	C	346	LEU	4.9
1	E	46	THR	4.8
1	C	230	PHE	4.6
1	A	228	THR	4.5
1	D	265	GLY	4.3
1	D	345	MET	4.3
1	C	232	GLU	4.3
1	C	265	GLY	4.2
1	F	344	GLU	4.1
1	F	346	LEU	4.1
1	E	228	THR	4.0
1	E	227	GLY	3.9
1	A	347	LYS	3.4
1	B	345	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	347	LYS	3.4
1	C	345	MET	3.4
1	C	37	HIS	3.3
1	F	206	TYR	3.2
1	F	392	ASN	3.2
1	F	341	GLY	3.1
1	C	343	LYS	3.1
1	A	227	GLY	3.1
1	D	172	GLY	3.1
1	A	345	MET	3.1
1	F	2	ALA	3.0
1	E	230	PHE	3.0
1	D	348	VAL	2.9
1	A	230	PHE	2.9
1	A	341	GLY	2.9
1	F	415	ILE	2.9
1	E	226	PRO	2.8
1	A	346	LEU	2.8
1	D	346	LEU	2.8
1	C	348	VAL	2.8
1	F	226	PRO	2.7
1	C	377	GLU	2.7
1	D	375	LYS	2.7
1	F	42	LYS	2.7
1	B	34	THR	2.7
1	E	78	GLY	2.6
1	C	415	ILE	2.6
1	A	41	LEU	2.6
1	F	41	LEU	2.5
1	F	411	GLY	2.5
1	E	36	LYS	2.5
1	A	77	CYS	2.5
1	E	117	VAL	2.4
1	F	264	GLN	2.4
1	D	2	ALA	2.4
1	C	226	PRO	2.4
1	C	225	LYS	2.3
1	D	226	PRO	2.3
1	F	78	GLY	2.3
1	C	263	LYS	2.2
1	D	158	GLU	2.2
1	A	40	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	231	ASN	2.2
1	F	47	ILE	2.1
1	C	36	LYS	2.1
1	A	38	SER	2.1
1	D	46	THR	2.1
1	C	344	GLU	2.1
1	E	266	LYS	2.0
1	E	58	VAL	2.0
1	B	45	MET	2.0

## 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(Å <sup>2</sup> )	Q<0.9
4	PO4	E	503	5/5	0.97	0.18	0.61	36,42,45,45	5
2	GDP	F	501	28/28	0.96	0.13	-0.58	35,43,48,48	28
2	GDP	C	501	28/28	0.97	0.12	-0.59	18,35,39,40	28
2	GDP	D	501	28/28	0.97	0.11	-0.81	24,30,36,46	28
2	GDP	A	501	28/28	0.96	0.12	-0.92	26,37,41,44	28
2	GDP	E	501	28/28	0.95	0.14	-0.99	41,55,62,72	28
2	GDP	B	501	28/28	0.97	0.11	-1.17	28,32,38,40	28
3	MG	C	503	1/1	0.95	0.07	-2.31	30,30,30,30	0
3	MG	E	502	1/1	0.86	0.06	-	46,46,46,46	1
3	MG	A	502	1/1	0.95	0.06	-	24,24,24,24	1
3	MG	F	502	1/1	0.71	0.11	-	58,58,58,58	0
3	MG	D	502	1/1	0.97	0.09	-	33,33,33,33	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	502	1/1	0.97	0.10	-	25,25,25,25	1
3	MG	C	502	1/1	0.95	0.11	-	25,25,25,25	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.