



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 PM GMT

PDB ID : 4I63
Title : Crystal Structure of E-R ClpX Hexamer
Authors : Glynn, S.E.; Nager, A.R.; Stinson, B.S.; Schmitz, K.R.; Baker, T.A.; Sauer, R.T.
Deposited on : 2012-11-29
Resolution : 5.71 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

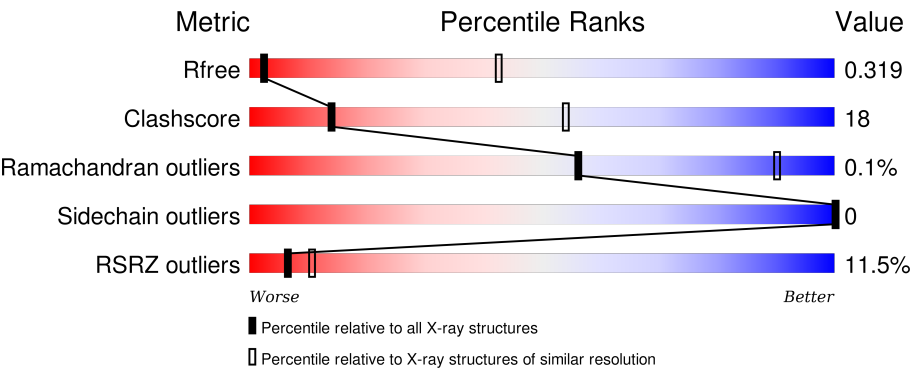
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.71 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	1006 (7.66-3.64)
Clashscore	102246	1037 (7.66-3.70)
Ramachandran outliers	100387	1011 (7.60-3.66)
Sidechain outliers	100360	1001 (7.60-3.64)
RSRZ outliers	91569	1005 (7.66-3.64)

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	363	<div><div>13%</div><div>53%</div><div>33%</div><div>14%</div></div>
1	B	363	<div><div>10%</div><div>52%</div><div>32%</div><div>15%</div></div>
1	C	363	<div><div>10%</div><div>53%</div><div>29%</div><div>18%</div></div>
1	D	363	<div><div>9%</div><div>56%</div><div>29%</div><div>15%</div></div>
1	E	363	<div><div>10%</div><div>54%</div><div>33%</div><div>13%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	363	

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
2	SO4	B	500	-	-	X	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13933 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 ATP-dependent Clp protease ATP-binding subunit ClpX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2332	1484	386	456	6			
1	B	307	Total	C	N	O	S	0	0	0
			2304	1467	379	452	6			
1	C	298	Total	C	N	O	S	0	0	0
			2273	1448	378	441	6			
1	D	310	Total	C	N	O	S	0	0	0
			2317	1472	385	454	6			
1	E	315	Total	C	N	O	S	0	0	0
			2356	1498	390	462	6			
1	F	305	Total	C	N	O	S	0	0	0
			2321	1477	389	449	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLU	LYS	CONFLICT	UNP P0A6H1
B	408	GLU	LYS	CONFLICT	UNP P0A6H1
C	408	GLU	LYS	CONFLICT	UNP P0A6H1
D	408	GLU	LYS	CONFLICT	UNP P0A6H1
E	408	GLU	LYS	CONFLICT	UNP P0A6H1
F	408	GLU	LYS	CONFLICT	UNP P0A6H1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

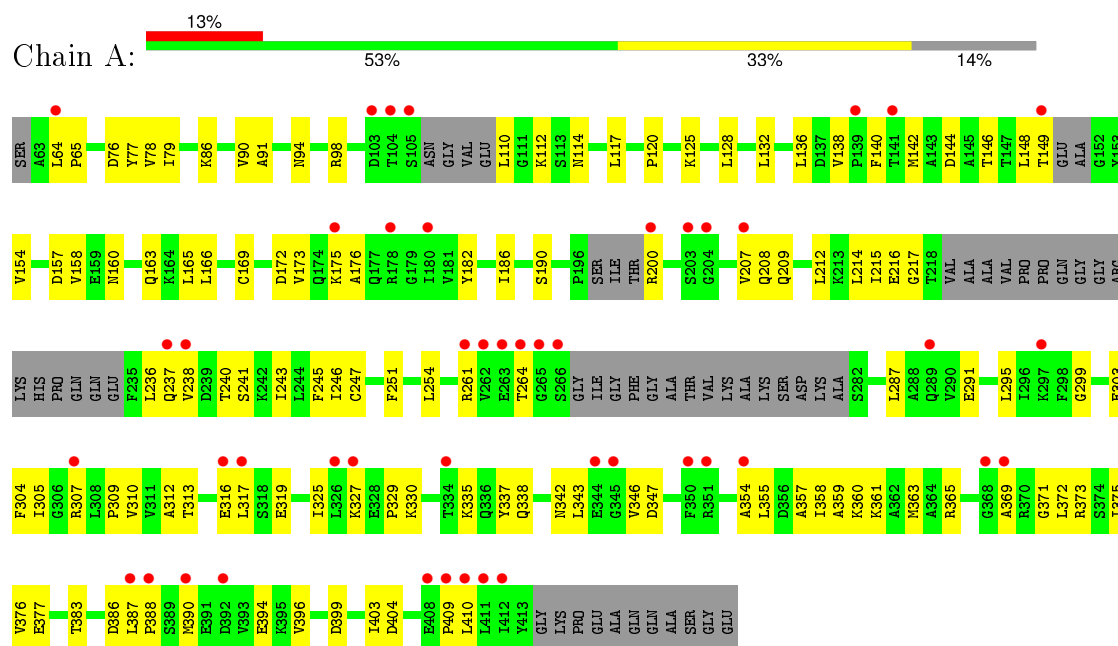


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

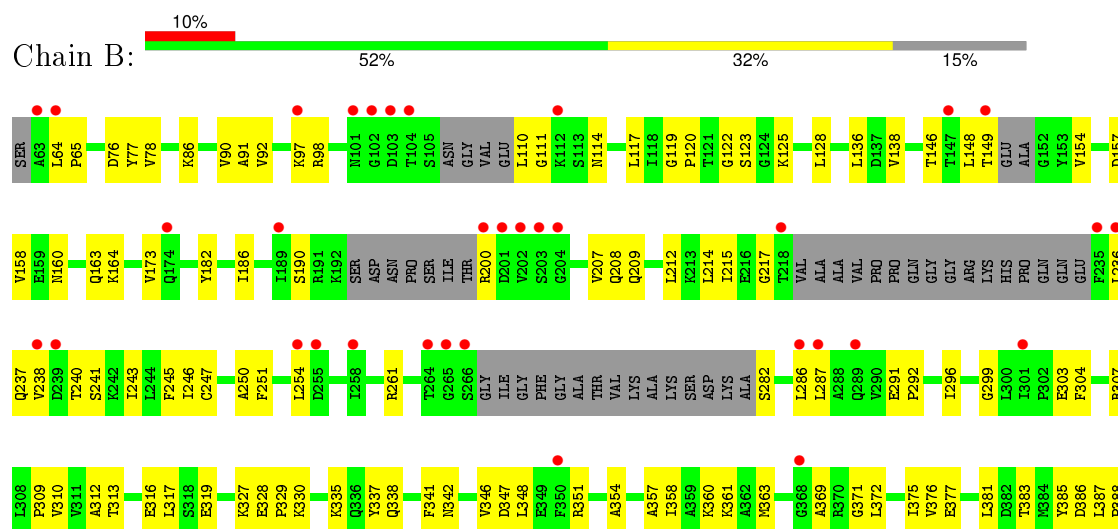
3 Residue-property plots

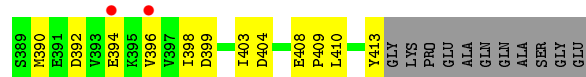
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

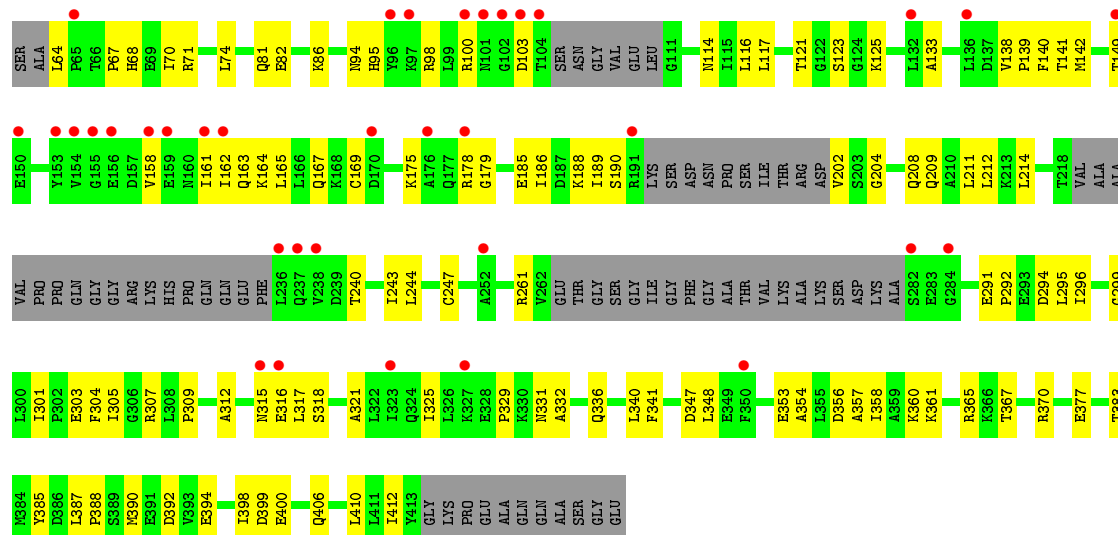


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

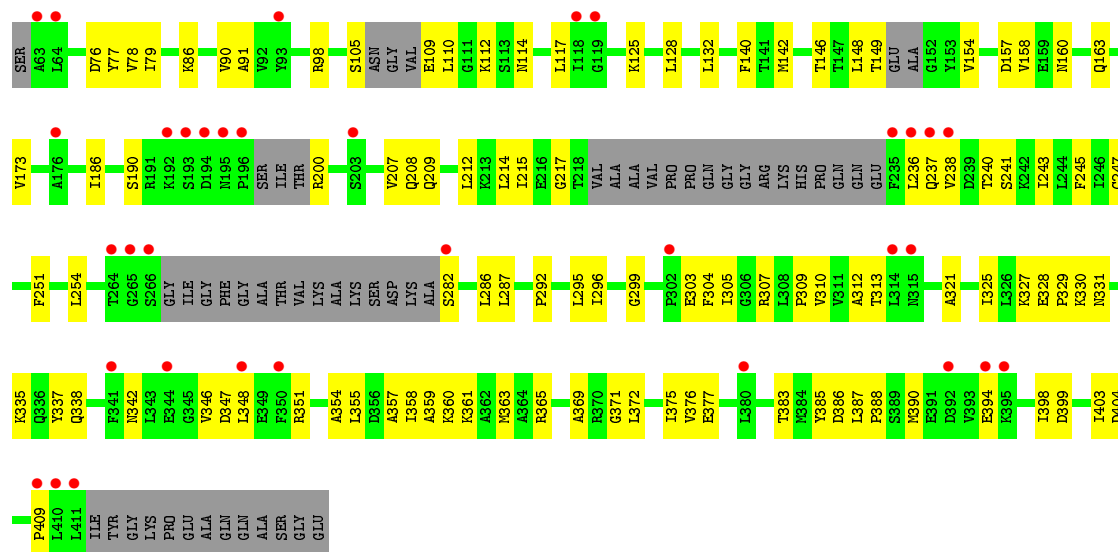




- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX

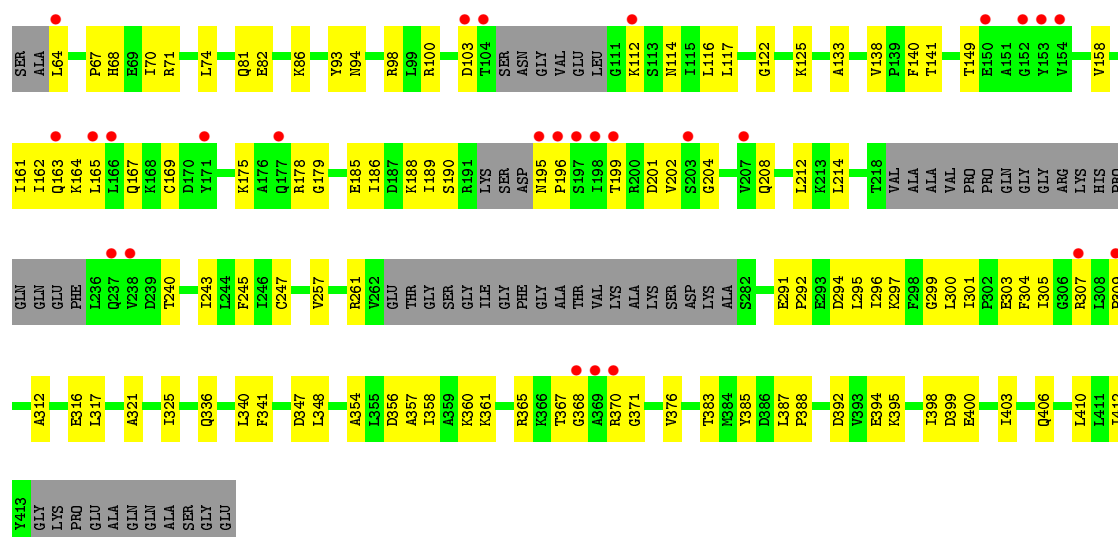


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX



- Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpX





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.22Å 201.17Å 222.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 5.71 49.06 – 5.71	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.06-5.71) 98.1 (49.06-5.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 5.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.307 , 0.315 0.290 , 0.319	Depositor DCC
R_{free} test set	348 reflections (4.58%)	DCC
Wilson B-factor (Å ²)	324.0	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 305.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 7607 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13933	wwPDB-VP
Average B, all atoms (Å ²)	322.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.21	0/2357	0.37	0/3191
1	B	0.21	0/2328	0.38	0/3151
1	C	0.20	0/2298	0.37	0/3108
1	D	0.21	0/2341	0.37	0/3169
1	E	0.21	0/2381	0.37	0/3224
1	F	0.21	0/2347	0.37	0/3176
All	All	0.21	0/14052	0.37	0/19019

There are no bond length outliers.

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	2332	0	2326	104	0
1	B	2304	0	2302	92	0
1	C	2273	0	2307	77	0
1	D	2317	0	2308	88	0
1	E	2356	0	2341	102	0
1	F	2321	0	2354	82	0
2	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	2	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
All	All	13933	0	13938	510	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 18.

All (510) 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:186:ILE:HG13	1:C:247:CYS:HB3	1.46	0.97
1:F:186:ILE:HG13	1:F:247:CYS:HB3	1.50	0.94
1:B:186:ILE:HG13	1:B:247:CYS:HB3	1.51	0.93
1:E:357:ALA:HB1	1:E:403:ILE:HG13	1.52	0.91
1:D:186:ILE:HG13	1:D:247:CYS:HB3	1.54	0.90
1:E:186:ILE:HG13	1:E:247:CYS:HB3	1.53	0.89
1:D:215:ILE:HG21	1:D:307:ARG:HB3	1.56	0.88
1:A:215:ILE:HG21	1:A:307:ARG:HB3	1.55	0.87
1:A:186:ILE:HG13	1:A:247:CYS:HB3	1.55	0.87
1:D:76:ASP:HB3	1:D:330:LYS:HE3	1.56	0.85
1:E:173:VAL:HG13	1:E:238:VAL:HG22	1.59	0.85
1:E:215:ILE:HG21	1:E:307:ARG:HB3	1.56	0.84
1:B:76:ASP:HB3	1:B:330:LYS:HE3	1.59	0.83
1:D:105:SER:HA	1:D:109:GLU:N	1.93	0.82
1:B:120:PRO:HG2	1:B:316:GLU:HA	1.62	0.81
1:A:307:ARG:HH22	1:F:370:ARG:HD2	1.47	0.80
1:C:161:ILE:HA	1:C:164:LYS:HE2	1.62	0.80
1:F:175:LYS:HD3	1:F:178:ARG:HH12	1.48	0.79
1:B:123:SER:HA	1:B:317:LEU:HD21	1.66	0.77
1:E:112:LYS:HE3	1:E:307:ARG:HE	1.48	0.77
1:A:173:VAL:HG13	1:A:238:VAL:HG22	1.66	0.76
1:F:161:ILE:HA	1:F:164:LYS:HE2	1.67	0.76
1:B:319:GLU:HB3	1:B:363:MET:SD	2.25	0.76
1:D:386:ASP:HB3	1:E:68:HIS:NE2	2.01	0.76
1:D:112:LYS:HE3	1:D:307:ARG:HE	1.50	0.76
1:F:169:CYS:SG	1:F:175:LYS:HB2	2.26	0.75
1:C:175:LYS:HD3	1:C:178:ARG:HH12	1.51	0.75
1:A:169:CYS:SG	1:A:175:LYS:HB2	2.25	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:VAL:HG13	1:D:238:VAL:HG22	1.68	0.74
1:D:214:LEU:HD22	1:D:240:THR:HG21	1.69	0.74
1:B:173:VAL:HG13	1:B:238:VAL:HG22	1.69	0.74
1:F:81:GLN:HE22	1:F:316:GLU:H	1.35	0.74
1:E:387:LEU:HB3	1:E:388:PRO:HD3	1.70	0.74
1:F:190:SER:HB2	1:F:299:GLY:HA3	1.71	0.73
1:B:337:TYR:OH	1:B:377:GLU:HG2	1.89	0.72
1:A:337:TYR:OH	1:A:377:GLU:HG2	1.90	0.72
1:C:169:CYS:SG	1:C:175:LYS:HB2	2.30	0.71
1:A:357:ALA:HB1	1:A:403:ILE:HG23	1.72	0.71
1:C:121:THR:HG21	1:C:370:ARG:HE	1.55	0.71
1:A:214:LEU:HD22	1:A:240:THR:HG21	1.72	0.71
1:D:337:TYR:OH	1:D:377:GLU:HG2	1.91	0.71
1:B:214:LEU:HD22	1:B:240:THR:HG21	1.73	0.70
1:B:357:ALA:HB1	1:B:403:ILE:HG23	1.71	0.70
1:A:359:ALA:O	1:A:363:MET:HG3	1.92	0.70
1:E:214:LEU:HD22	1:E:240:THR:HG21	1.73	0.70
1:B:387:LEU:HB3	1:B:388:PRO:HD3	1.74	0.69
1:E:337:TYR:OH	1:E:377:GLU:HG2	1.93	0.69
1:D:357:ALA:HB1	1:D:403:ILE:HG23	1.73	0.69
1:A:112:LYS:HE3	1:A:307:ARG:HE	1.58	0.68
1:C:190:SER:HB2	1:C:299:GLY:HA3	1.75	0.68
1:F:257:VAL:HG13	1:F:297:LYS:HD3	1.76	0.67
1:B:114:ASN:ND2	1:B:215:ILE:HG23	2.10	0.67
1:A:114:ASN:ND2	1:A:215:ILE:HG23	2.10	0.67
1:D:114:ASN:ND2	1:D:215:ILE:HG23	2.09	0.67
1:D:77:TYR:CZ	1:D:330:LYS:HD2	2.30	0.67
1:B:385:TYR:OH	1:C:71:ARG:HD3	1.95	0.66
1:A:365:ARG:NH2	1:B:292:PRO:HG2	2.10	0.66
1:B:148:LEU:HA	1:B:154:VAL:HG21	1.78	0.66
1:E:148:LEU:HA	1:E:154:VAL:HG21	1.77	0.66
1:E:71:ARG:HH12	1:E:86:LYS:HE2	1.59	0.66
1:C:398:ILE:HD11	1:C:410:LEU:HD11	1.77	0.66
1:A:78:VAL:HG21	1:A:128:LEU:HD23	1.78	0.66
1:D:387:LEU:HB3	1:D:388:PRO:HD3	1.75	0.66
1:A:317:LEU:HD13	1:A:325:ILE:HD11	1.78	0.65
1:E:386:ASP:HB3	1:F:68:HIS:NE2	2.10	0.65
1:A:387:LEU:HB3	1:A:388:PRO:HD3	1.79	0.65
1:E:114:ASN:ND2	1:E:215:ILE:HG23	2.13	0.65
1:B:360:LYS:HA	1:B:363:MET:HE2	1.79	0.64
1:C:385:TYR:HD1	1:D:90:VAL:HG22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HD13	1:B:304:PHE:HA	1.80	0.64
1:B:399:ASP:O	1:B:403:ILE:HG12	1.98	0.64
1:D:359:ALA:O	1:D:363:MET:HG3	1.97	0.64
1:F:291:GLU:HG3	1:F:292:PRO:HD2	1.79	0.64
1:C:123:SER:HA	1:C:317:LEU:HD21	1.79	0.63
1:C:186:ILE:O	1:C:189:ILE:HG12	1.99	0.63
1:A:148:LEU:HA	1:A:154:VAL:HG21	1.80	0.63
1:D:148:LEU:HA	1:D:154:VAL:HG21	1.79	0.62
1:A:399:ASP:O	1:A:403:ILE:HG12	1.99	0.62
1:B:403:ILE:HG13	1:B:404:ASP:H	1.65	0.61
1:A:190:SER:HB2	1:A:299:GLY:HA3	1.83	0.60
1:F:175:LYS:HD3	1:F:178:ARG:NH1	2.15	0.60
1:A:120:PRO:HG2	1:A:316:GLU:HB2	1.83	0.60
1:E:78:VAL:HG21	1:E:128:LEU:HD23	1.84	0.60
1:C:175:LYS:HD3	1:C:178:ARG:NH1	2.16	0.60
1:A:307:ARG:HH22	1:F:370:ARG:CD	2.13	0.60
1:E:319:GLU:HG2	1:E:363:MET:SD	2.41	0.60
1:A:172:ASP:HB3	1:A:175:LYS:HG3	1.84	0.60
1:A:79:ILE:HD11	1:A:329:PRO:HD3	1.84	0.59
1:E:79:ILE:HD12	1:E:325:ILE:HG12	1.82	0.59
1:B:114:ASN:HD22	1:B:215:ILE:HG23	1.67	0.59
1:F:186:ILE:O	1:F:189:ILE:HG12	2.03	0.58
1:A:217:GLY:HA2	1:A:240:THR:OG1	2.03	0.58
1:D:383:THR:OG1	1:D:409:PRO:HG3	2.03	0.58
1:B:78:VAL:HG21	1:B:128:LEU:HD23	1.86	0.58
1:D:190:SER:HB2	1:D:299:GLY:HA3	1.86	0.58
1:A:212:LEU:HD13	1:A:304:PHE:HA	1.86	0.58
1:D:78:VAL:HG21	1:D:128:LEU:HD23	1.86	0.58
1:A:98:ARG:HD2	1:A:110:LEU:CB	2.34	0.58
1:B:261:ARG:NH2	1:B:291:GLU:HG3	2.19	0.58
1:A:125:LYS:HB2	2:A:500:SO4:O3	2.04	0.57
1:E:286:LEU:HD12	1:E:286:LEU:N	2.19	0.57
1:A:212:LEU:CD1	1:A:307:ARG:HG3	2.35	0.57
1:E:71:ARG:NH1	1:E:86:LYS:HE2	2.19	0.57
1:B:164:LYS:HE2	1:C:209:GLN:CB	2.33	0.57
1:A:373:ARG:CZ	1:B:111:GLY:HA2	2.33	0.57
1:A:403:ILE:HG13	1:A:404:ASP:H	1.69	0.57
1:A:360:LYS:HA	1:A:363:MET:HE2	1.86	0.57
1:D:212:LEU:HD13	1:D:304:PHE:HA	1.87	0.57
1:D:114:ASN:HD22	1:D:215:ILE:HG23	1.67	0.57
1:A:383:THR:OG1	1:A:409:PRO:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:THR:HG21	1:F:297:LYS:HE2	1.85	0.57
1:E:125:LYS:HB2	2:E:500:SO4:O3	2.04	0.57
1:D:125:LYS:HB2	2:D:500:SO4:O3	2.05	0.57
1:A:319:GLU:HB3	1:A:363:MET:SD	2.45	0.56
1:D:217:GLY:HA2	1:D:240:THR:OG1	2.05	0.56
1:F:82:GLU:OE2	1:F:86:LYS:HE3	2.06	0.56
1:B:383:THR:OG1	1:B:409:PRO:HG3	2.05	0.56
1:A:172:ASP:CG	1:A:175:LYS:HG3	2.26	0.56
1:C:162:ILE:HD11	1:C:214:LEU:HD11	1.88	0.56
1:E:338:GLN:O	1:E:342:ASN:HB2	2.06	0.56
1:A:117:LEU:HD23	1:A:312:ALA:HB3	1.88	0.56
1:A:287:LEU:O	1:A:313:THR:HG21	2.06	0.56
1:A:338:GLN:O	1:A:342:ASN:HB2	2.06	0.56
1:D:403:ILE:HG13	1:D:404:ASP:H	1.71	0.56
1:E:358:ILE:HD13	1:E:376:VAL:HG22	1.89	0.56
1:E:114:ASN:HD22	1:E:215:ILE:HG23	1.71	0.55
1:A:114:ASN:HD22	1:A:215:ILE:HG23	1.69	0.55
1:F:387:LEU:HB3	1:F:388:PRO:HD3	1.88	0.55
1:F:199:THR:HG22	1:F:201:ASP:H	1.71	0.55
1:D:287:LEU:O	1:D:313:THR:HG21	2.07	0.55
1:B:117:LEU:HD23	1:B:312:ALA:HB3	1.88	0.55
1:B:215:ILE:HG21	1:B:307:ARG:CB	2.37	0.55
1:B:217:GLY:HA3	1:B:241:SER:OG	2.07	0.55
1:D:117:LEU:HD23	1:D:312:ALA:HB3	1.89	0.55
1:A:144:ASP:OD2	1:A:146:THR:HB	2.06	0.55
1:E:287:LEU:O	1:E:313:THR:HG21	2.06	0.55
1:F:138:VAL:HG12	1:F:179:GLY:HA2	1.88	0.55
1:A:77:TYR:CE2	1:A:330:LYS:HD2	2.42	0.54
1:E:212:LEU:HD13	1:E:304:PHE:HA	1.88	0.54
1:E:190:SER:HB2	1:E:299:GLY:HA3	1.87	0.54
1:D:217:GLY:HA3	1:D:241:SER:OG	2.07	0.54
1:C:365:ARG:HB2	1:C:367:THR:HG23	1.90	0.54
1:B:190:SER:HB2	1:B:299:GLY:HA3	1.89	0.54
1:F:365:ARG:HB2	1:F:367:THR:HG23	1.90	0.54
1:B:358:ILE:HD13	1:B:376:VAL:HG22	1.89	0.54
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.89	0.54
1:D:360:LYS:HA	1:D:363:MET:HE2	1.89	0.54
1:A:261:ARG:NH2	1:A:291:GLU:HG3	2.23	0.54
1:D:208:GLN:O	1:D:212:LEU:HB2	2.08	0.54
1:F:162:ILE:HD11	1:F:214:LEU:HD11	1.90	0.54
1:E:217:GLY:HA2	1:E:240:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ASP:HB2	1:C:412:ILE:O	2.08	0.54
1:A:236:LEU:O	1:A:237:GLN:HG2	2.08	0.54
1:E:236:LEU:O	1:E:237:GLN:HG2	2.08	0.54
1:F:357:ALA:O	1:F:361:LYS:HG2	2.08	0.54
1:F:158:VAL:O	1:F:161:ILE:HG12	2.08	0.53
1:B:217:GLY:HA2	1:B:240:THR:OG1	2.08	0.53
1:C:332:ALA:O	1:C:336:GLN:HG3	2.09	0.53
1:F:81:GLN:NE2	1:F:316:GLU:H	2.05	0.53
1:C:163:GLN:O	1:C:167:GLN:HG3	2.08	0.53
1:B:86:LYS:O	1:B:90:VAL:HG23	2.09	0.53
1:D:351:ARG:HD2	1:D:398:ILE:HG22	1.91	0.53
1:D:154:VAL:O	1:D:158:VAL:HG23	2.09	0.53
1:D:236:LEU:O	1:D:237:GLN:HG2	2.09	0.53
1:F:398:ILE:HG22	1:F:399:ASP:N	2.24	0.53
1:A:208:GLN:O	1:A:212:LEU:HB2	2.09	0.53
1:B:77:TYR:CZ	1:B:330:LYS:HD2	2.44	0.53
1:D:399:ASP:O	1:D:403:ILE:HG12	2.09	0.53
1:D:354:ALA:O	1:D:358:ILE:HG13	2.08	0.53
1:D:91:ALA:HB2	1:D:310:VAL:HG11	1.89	0.53
1:C:212:LEU:HD21	1:C:303:GLU:HG2	1.91	0.53
1:F:212:LEU:HD11	1:F:307:ARG:HG3	1.90	0.53
1:F:212:LEU:HD21	1:F:303:GLU:HG2	1.91	0.53
1:E:217:GLY:HA3	1:E:241:SER:OG	2.08	0.53
1:A:148:LEU:O	1:A:154:VAL:HG21	2.09	0.53
1:E:146:THR:CG2	1:F:297:LYS:HE2	2.39	0.52
1:E:383:THR:OG1	1:E:409:PRO:HG3	2.09	0.52
1:E:208:GLN:O	1:E:212:LEU:HB2	2.09	0.52
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.91	0.52
1:E:361:LYS:HB2	1:E:375:ILE:HD13	1.91	0.52
1:A:307:ARG:NH2	1:F:370:ARG:HD2	2.20	0.52
1:A:217:GLY:HA3	1:A:241:SER:HG	1.74	0.52
1:A:172:ASP:CB	1:A:175:LYS:HG3	2.40	0.52
1:F:392:ASP:HB2	1:F:412:ILE:O	2.10	0.52
1:C:158:VAL:O	1:C:161:ILE:HG12	2.09	0.52
1:C:212:LEU:HD11	1:C:307:ARG:HG3	1.92	0.52
1:E:388:PRO:HG2	1:F:67:PRO:CD	2.40	0.52
1:E:261:ARG:NH2	1:E:291:GLU:HG3	2.24	0.52
1:C:295:LEU:HB2	1:C:305:ILE:HD13	1.92	0.52
1:B:236:LEU:O	1:B:237:GLN:HG2	2.10	0.52
1:C:292:PRO:O	1:C:296:ILE:HG13	2.10	0.51
1:D:388:PRO:HB2	1:E:66:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:GLN:O	1:D:342:ASN:HB2	2.09	0.51
1:B:154:VAL:O	1:B:158:VAL:HG23	2.09	0.51
1:B:386:ASP:HB3	1:C:68:HIS:NE2	2.24	0.51
1:A:251:PHE:HB3	1:A:254:LEU:HB2	1.92	0.51
1:D:86:LYS:O	1:D:90:VAL:HG23	2.11	0.51
1:F:400:GLU:HB2	1:F:406:GLN:HE21	1.75	0.51
1:C:387:LEU:HA	1:C:390:MET:HE2	1.92	0.51
1:D:307:ARG:C	1:D:309:PRO:HD3	2.30	0.51
1:C:64:LEU:HD22	1:C:100:ARG:HD2	1.93	0.51
1:B:77:TYR:CE1	1:B:330:LYS:HD2	2.46	0.50
1:C:261:ARG:HD3	1:C:294:ASP:OD1	2.11	0.50
1:B:338:GLN:O	1:B:342:ASN:HB2	2.10	0.50
1:A:358:ILE:HD13	1:A:376:VAL:HG22	1.93	0.50
1:E:117:LEU:HD23	1:E:312:ALA:HB3	1.92	0.50
1:D:76:ASP:CB	1:D:330:LYS:HE3	2.34	0.50
1:B:361:LYS:HB2	1:B:375:ILE:HD13	1.92	0.50
1:E:91:ALA:HB2	1:E:310:VAL:HG11	1.92	0.50
1:E:146:THR:O	1:E:149:THR:HG22	2.12	0.50
1:C:125:LYS:HB2	2:C:500:SO4:O3	2.10	0.50
1:B:212:LEU:HD21	1:B:303:GLU:HG3	1.94	0.50
1:E:346:VAL:HG13	1:E:394:GLU:HA	1.93	0.50
1:E:385:TYR:OH	1:F:71:ARG:HD3	2.11	0.50
1:C:158:VAL:HG11	1:C:214:LEU:HB2	1.93	0.50
1:E:154:VAL:O	1:E:158:VAL:HG23	2.11	0.50
1:F:398:ILE:HB	1:F:400:GLU:HG2	1.93	0.50
1:F:321:ALA:O	1:F:325:ILE:HG13	2.11	0.50
1:F:383:THR:O	1:F:387:LEU:HB2	2.11	0.49
1:B:396:VAL:HB	1:B:410:LEU:HB3	1.92	0.49
1:C:117:LEU:HD23	1:C:312:ALA:HB3	1.93	0.49
1:A:209:GLN:O	1:A:212:LEU:HB3	2.12	0.49
1:A:154:VAL:O	1:A:158:VAL:HG23	2.12	0.49
1:C:377:GLU:OE2	1:D:310:VAL:HG22	2.11	0.49
1:C:81:GLN:HE22	1:C:316:GLU:H	1.59	0.49
1:E:212:LEU:CD1	1:E:307:ARG:HG3	2.42	0.49
1:F:158:VAL:HG11	1:F:214:LEU:HB2	1.94	0.49
1:F:295:LEU:HB2	1:F:305:ILE:HD13	1.94	0.49
1:F:189:ILE:HD12	1:F:208:GLN:HG2	1.94	0.49
1:A:360:LYS:HA	1:A:363:MET:CE	2.42	0.49
1:A:146:THR:O	1:A:149:THR:HG22	2.13	0.49
1:C:400:GLU:HB2	1:C:406:GLN:HE21	1.76	0.49
1:A:361:LYS:HB2	1:A:375:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:O	1:B:154:VAL:HG21	2.11	0.49
1:B:307:ARG:O	1:B:309:PRO:HD3	2.12	0.49
1:A:369:ALA:HA	1:A:372:LEU:HG	1.94	0.49
1:D:282:SER:O	1:D:286:LEU:HD13	2.12	0.49
1:B:346:VAL:HG13	1:B:394:GLU:HA	1.95	0.49
1:A:91:ALA:HB2	1:A:310:VAL:HG11	1.94	0.49
1:C:240:THR:O	1:C:243:ILE:HG12	2.12	0.49
1:C:354:ALA:O	1:C:358:ILE:HG13	2.12	0.49
1:E:243:ILE:HD11	1:E:245:PHE:CZ	2.48	0.49
1:F:94:ASN:O	1:F:98:ARG:HG3	2.13	0.49
1:A:377:GLU:OE1	1:B:309:PRO:HB2	2.12	0.49
1:B:125:LYS:HB2	2:B:500:SO4:O3	2.11	0.49
1:E:357:ALA:HB1	1:E:403:ILE:CG1	2.35	0.49
1:D:148:LEU:O	1:D:154:VAL:HG21	2.11	0.49
1:B:338:GLN:HG2	1:B:348:LEU:HB3	1.95	0.49
1:F:163:GLN:O	1:F:167:GLN:HG3	2.12	0.49
1:F:292:PRO:O	1:F:296:ILE:HG13	2.13	0.48
1:A:217:GLY:HA3	1:A:241:SER:OG	2.12	0.48
1:C:94:ASN:O	1:C:98:ARG:HG3	2.12	0.48
1:C:189:ILE:O	1:C:204:GLY:HA3	2.13	0.48
1:F:117:LEU:HD23	1:F:312:ALA:HB3	1.94	0.48
1:D:209:GLN:O	1:D:212:LEU:HB3	2.13	0.48
1:C:383:THR:O	1:C:387:LEU:HB2	2.13	0.48
1:D:331:ASN:CG	1:E:109:GLU:HG3	2.34	0.48
1:F:240:THR:O	1:F:243:ILE:HG12	2.13	0.48
1:C:385:TYR:CD1	1:D:90:VAL:HG22	2.45	0.48
1:F:358:ILE:HD13	1:F:376:VAL:HG22	1.96	0.48
1:B:251:PHE:HB3	1:B:254:LEU:HB2	1.94	0.48
1:E:105:SER:HA	1:E:109:GLU:N	2.28	0.48
1:C:321:ALA:O	1:C:325:ILE:HG13	2.13	0.48
1:A:212:LEU:HD11	1:A:307:ARG:HG3	1.94	0.48
1:A:307:ARG:C	1:A:309:PRO:HD3	2.33	0.48
1:E:307:ARG:C	1:E:309:PRO:HD3	2.34	0.48
1:F:354:ALA:O	1:F:358:ILE:HG13	2.14	0.48
1:B:351:ARG:HD2	1:B:398:ILE:HG22	1.94	0.48
1:C:357:ALA:O	1:C:361:LYS:HG2	2.14	0.48
1:D:76:ASP:O	1:D:329:PRO:HA	2.14	0.47
1:B:122:GLY:HA2	2:B:500:SO4:O4	2.14	0.47
1:F:125:LYS:HB2	2:F:500:SO4:O3	2.13	0.47
1:E:251:PHE:HB3	1:E:254:LEU:HB2	1.96	0.47
1:E:182:TYR:HA	1:E:246:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:NH1	1:A:375:ILE:HG12	2.30	0.47
1:E:148:LEU:O	1:E:154:VAL:HG21	2.14	0.47
1:D:388:PRO:HG2	1:E:67:PRO:HD3	1.96	0.47
1:B:146:THR:O	1:B:149:THR:HG22	2.14	0.47
1:E:190:SER:HA	1:E:208:GLN:NE2	2.30	0.47
1:A:354:ALA:O	1:A:358:ILE:HG13	2.14	0.47
1:B:287:LEU:O	1:B:313:THR:HG21	2.13	0.47
1:F:116:LEU:HD12	1:F:247:CYS:O	2.14	0.47
1:D:212:LEU:CD1	1:D:307:ARG:HG3	2.45	0.47
1:F:291:GLU:CG	1:F:292:PRO:HD2	2.45	0.47
1:A:157:ASP:O	1:A:160:ASN:HB3	2.15	0.47
1:E:319:GLU:O	1:E:323:ILE:HG13	2.14	0.47
1:E:354:ALA:O	1:E:358:ILE:HG13	2.13	0.47
1:E:321:ALA:O	1:E:325:ILE:HG13	2.15	0.47
1:B:91:ALA:HB2	1:B:310:VAL:HG11	1.97	0.47
1:F:356:ASP:O	1:F:360:LYS:HG3	2.15	0.47
1:B:307:ARG:C	1:B:309:PRO:HD3	2.35	0.47
1:E:286:LEU:CD1	1:E:286:LEU:N	2.78	0.47
1:E:396:VAL:HB	1:E:410:LEU:HB3	1.97	0.47
1:B:328:GLU:HB2	1:B:329:PRO:HD3	1.97	0.47
1:B:282:SER:O	1:B:286:LEU:HD13	2.16	0.46
1:B:98:ARG:HD2	1:B:110:LEU:CB	2.46	0.46
1:E:209:GLN:O	1:E:212:LEU:HB3	2.15	0.46
1:C:336:GLN:O	1:C:340:LEU:HD13	2.15	0.46
1:C:356:ASP:O	1:C:360:LYS:HG3	2.16	0.46
1:C:185:GLU:HB3	1:C:188:LYS:HG3	1.98	0.46
1:C:70:ILE:O	1:C:74:LEU:HG	2.16	0.46
1:A:373:ARG:HG2	1:B:309:PRO:HB3	1.97	0.46
1:B:371:GLY:O	1:B:375:ILE:HG13	2.15	0.46
1:E:154:VAL:HA	1:E:157:ASP:HB3	1.97	0.46
1:B:212:LEU:HD21	1:B:303:GLU:CG	2.46	0.46
1:A:149:THR:HA	1:A:207:VAL:HG21	1.98	0.46
1:C:138:VAL:HG12	1:C:179:GLY:HA2	1.98	0.46
1:D:146:THR:O	1:D:149:THR:HG22	2.15	0.46
1:B:200:ARG:N	1:B:200:ARG:HD2	2.31	0.46
1:F:336:GLN:O	1:F:340:LEU:HD13	2.14	0.46
1:D:307:ARG:O	1:D:309:PRO:HD3	2.16	0.46
1:D:365:ARG:NH1	1:D:375:ILE:HG12	2.31	0.46
1:C:398:ILE:HG22	1:C:399:ASP:N	2.30	0.46
1:F:261:ARG:HD3	1:F:294:ASP:OD1	2.16	0.46
1:D:149:THR:HA	1:D:207:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:THR:O	1:C:202:VAL:HB	2.15	0.46
1:C:301:ILE:HG13	1:C:304:PHE:H	1.80	0.46
1:E:64:LEU:HA	1:E:65:PRO:HD3	1.78	0.46
1:D:371:GLY:O	1:D:375:ILE:HG13	2.15	0.46
1:C:82:GLU:OE2	1:C:86:LYS:HE3	2.15	0.46
1:A:396:VAL:HB	1:A:410:LEU:HB3	1.98	0.45
1:D:251:PHE:HB3	1:D:254:LEU:HB2	1.97	0.45
1:D:346:VAL:HG13	1:D:394:GLU:HA	1.99	0.45
1:A:112:LYS:CE	1:A:307:ARG:HE	2.29	0.45
1:D:361:LYS:HB2	1:D:375:ILE:HD13	1.98	0.45
1:B:381:LEU:HD11	1:C:86:LYS:HB3	1.98	0.45
1:C:341:PHE:CD1	1:C:348:LEU:HD22	2.51	0.45
1:A:243:ILE:HD11	1:A:245:PHE:CZ	2.51	0.45
1:C:140:PHE:CE2	1:C:142:MET:HG3	2.51	0.45
1:A:346:VAL:HG13	1:A:394:GLU:HA	1.98	0.45
1:E:307:ARG:O	1:E:309:PRO:HD3	2.16	0.45
1:B:371:GLY:HA2	1:C:291:GLU:OE1	2.17	0.45
1:A:200:ARG:N	1:A:200:ARG:HD2	2.31	0.45
1:D:369:ALA:HA	1:D:372:LEU:HG	1.98	0.45
1:B:392:ASP:HB3	1:B:413:TYR:CD2	2.52	0.45
1:B:403:ILE:HG13	1:B:404:ASP:N	2.30	0.45
1:D:154:VAL:HA	1:D:157:ASP:HB3	1.98	0.45
1:A:291:GLU:CD	1:F:365:ARG:HH12	2.20	0.45
1:F:122:GLY:HA2	1:F:325:ILE:HD11	1.98	0.45
1:C:81:GLN:HE22	1:C:315:ASN:H	1.64	0.45
1:F:301:ILE:HG13	1:F:304:PHE:H	1.82	0.45
1:E:327:LYS:HD2	1:E:355:LEU:HD13	1.98	0.45
1:F:317:LEU:HD13	1:F:368:GLY:HA2	1.99	0.45
1:D:200:ARG:N	1:D:200:ARG:HD2	2.31	0.45
1:D:190:SER:HA	1:D:208:GLN:NE2	2.31	0.45
1:E:387:LEU:CB	1:E:388:PRO:HD3	2.43	0.45
1:A:251:PHE:HB3	1:A:254:LEU:CB	2.47	0.45
1:B:92:VAL:CG1	1:B:136:LEU:HD11	2.47	0.45
1:D:212:LEU:HD21	1:D:303:GLU:CG	2.47	0.45
1:A:357:ALA:O	1:A:361:LYS:HG2	2.16	0.45
1:F:64:LEU:HD22	1:F:100:ARG:HD2	1.98	0.45
1:E:295:LEU:HB2	1:E:305:ILE:HD13	1.99	0.45
1:E:369:ALA:HA	1:E:372:LEU:HG	1.99	0.45
1:B:385:TYR:O	1:C:67:PRO:HB2	2.17	0.44
1:D:327:LYS:O	1:D:335:LYS:HE3	2.17	0.44
1:F:341:PHE:CD1	1:F:348:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:GLY:O	1:E:375:ILE:HG13	2.18	0.44
1:A:212:LEU:HD21	1:A:303:GLU:HG3	1.98	0.44
1:E:303:GLU:HA	1:E:303:GLU:OE1	2.17	0.44
1:A:330:LYS:HB3	1:A:330:LYS:HE2	1.80	0.44
1:E:200:ARG:N	1:E:200:ARG:HD2	2.32	0.44
1:E:317:LEU:HD13	1:E:325:ILE:CD1	2.48	0.44
1:A:264:THR:O	1:A:264:THR:HG23	2.16	0.44
1:E:212:LEU:HD21	1:E:303:GLU:HG3	1.99	0.44
1:E:217:GLY:HA3	1:E:241:SER:HG	1.82	0.44
1:D:357:ALA:O	1:D:361:LYS:HG2	2.18	0.44
1:F:243:ILE:HD11	1:F:245:PHE:CZ	2.53	0.44
1:E:174:GLN:HG3	1:E:175:LYS:N	2.32	0.44
1:D:331:ASN:OD1	1:E:109:GLU:HG3	2.17	0.44
1:A:76:ASP:HB3	1:A:330:LYS:HE3	1.99	0.44
1:F:189:ILE:O	1:F:204:GLY:HA3	2.17	0.44
1:E:388:PRO:HB3	1:F:93:TYR:CZ	2.52	0.44
1:E:282:SER:O	1:E:286:LEU:HD13	2.17	0.44
1:E:328:GLU:HB2	1:E:329:PRO:HD3	2.00	0.44
1:A:136:LEU:O	1:A:138:VAL:HG23	2.18	0.44
1:F:208:GLN:O	1:F:212:LEU:HB2	2.18	0.44
1:A:212:LEU:HD21	1:A:303:GLU:CG	2.47	0.44
1:B:160:ASN:HA	1:B:163:GLN:HG2	1.99	0.44
1:E:280:LYS:CB	1:E:286:LEU:HD11	2.48	0.44
1:F:307:ARG:C	1:F:309:PRO:HD3	2.38	0.44
1:B:157:ASP:O	1:B:160:ASN:HB3	2.17	0.44
1:C:347:ASP:O	1:C:394:GLU:HB2	2.18	0.44
1:C:291:GLU:CG	1:C:292:PRO:HD2	2.47	0.43
1:D:388:PRO:HG2	1:E:67:PRO:CD	2.48	0.43
1:E:136:LEU:O	1:E:138:VAL:HG23	2.18	0.43
1:D:212:LEU:HD21	1:D:303:GLU:HG3	1.99	0.43
1:D:338:GLN:HG2	1:D:348:LEU:HB3	1.99	0.43
1:A:343:LEU:HD13	1:B:97:LYS:HE3	2.00	0.43
1:E:212:LEU:HD21	1:E:303:GLU:CG	2.48	0.43
1:B:136:LEU:O	1:B:138:VAL:HG23	2.18	0.43
1:B:119:GLY:O	1:B:250:ALA:HA	2.18	0.43
1:E:357:ALA:O	1:E:361:LYS:HG2	2.18	0.43
1:C:318:SER:H	1:C:321:ALA:HB3	1.82	0.43
1:D:328:GLU:HB2	1:D:329:PRO:HD3	2.00	0.43
1:A:403:ILE:HG13	1:A:404:ASP:N	2.31	0.43
1:E:157:ASP:O	1:E:160:ASN:HB3	2.18	0.43
1:B:208:GLN:O	1:B:212:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:SER:OG	1:E:286:LEU:HD23	2.19	0.43
1:B:243:ILE:HD11	1:B:245:PHE:CZ	2.53	0.43
1:A:371:GLY:O	1:A:375:ILE:HG13	2.18	0.43
1:B:154:VAL:HA	1:B:157:ASP:HB3	2.01	0.43
1:F:70:ILE:O	1:F:74:LEU:HG	2.18	0.43
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.19	0.43
1:A:307:ARG:O	1:A:309:PRO:HD3	2.19	0.43
1:E:160:ASN:HA	1:E:163:GLN:HG2	2.01	0.43
1:B:303:GLU:OE1	1:B:303:GLU:HA	2.19	0.43
1:E:133:ALA:CB	1:E:140:PHE:HB2	2.48	0.43
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.78	0.43
1:A:327:LYS:HD2	1:A:355:LEU:HD13	2.00	0.43
1:C:116:LEU:HD12	1:C:247:CYS:O	2.19	0.43
1:C:353:GLU:OE2	1:C:398:ILE:HG23	2.19	0.43
1:E:347:ASP:O	1:E:394:GLU:HB2	2.19	0.43
1:F:317:LEU:CD1	1:F:368:GLY:HA2	2.49	0.43
1:D:327:LYS:HD2	1:D:355:LEU:HD13	2.01	0.43
1:D:140:PHE:CE2	1:D:142:MET:HG3	2.53	0.43
1:E:212:LEU:HD11	1:E:307:ARG:HG3	2.00	0.43
1:E:392:ASP:HB3	1:E:413:TYR:CD1	2.53	0.43
1:E:216:GLU:OE1	1:E:307:ARG:HD2	2.19	0.42
1:C:361:LYS:O	1:C:365:ARG:HG3	2.19	0.42
1:B:251:PHE:HB3	1:B:254:LEU:CB	2.49	0.42
1:F:114:ASN:HB2	1:F:307:ARG:O	2.19	0.42
1:D:212:LEU:HD11	1:D:307:ARG:HG3	2.01	0.42
1:A:165:LEU:O	1:A:169:CYS:HB2	2.18	0.42
1:D:160:ASN:HA	1:D:163:GLN:HG2	2.01	0.42
1:C:361:LYS:HE3	1:C:365:ARG:HH21	1.84	0.42
1:A:90:VAL:HG12	1:A:94:ASN:ND2	2.33	0.42
1:F:296:ILE:HA	1:F:300:LEU:O	2.20	0.42
1:C:133:ALA:CB	1:C:140:PHE:HB2	2.49	0.42
1:A:347:ASP:O	1:A:394:GLU:HB2	2.19	0.42
1:A:166:LEU:HA	1:A:169:CYS:HB3	2.01	0.42
1:B:64:LEU:HA	1:B:65:PRO:HD3	1.79	0.42
1:D:295:LEU:HB2	1:D:305:ILE:HD13	2.01	0.42
1:A:327:LYS:O	1:A:335:LYS:HE3	2.20	0.42
1:C:189:ILE:HD12	1:C:208:GLN:HG2	2.02	0.42
1:C:329:PRO:C	1:C:331:ASN:H	2.22	0.42
1:F:149:THR:O	1:F:202:VAL:HB	2.19	0.42
1:A:295:LEU:HB2	1:A:305:ILE:HD13	2.01	0.42
1:A:160:ASN:HA	1:A:163:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PHE:CD1	1:B:348:LEU:HD22	2.54	0.42
1:B:209:GLN:O	1:B:212:LEU:HB3	2.19	0.42
1:D:358:ILE:HD13	1:D:376:VAL:HG22	2.02	0.42
1:D:98:ARG:HD2	1:D:110:LEU:CB	2.50	0.42
1:A:386:ASP:O	1:A:390:MET:HG3	2.19	0.42
1:E:388:PRO:HG2	1:F:67:PRO:HD3	2.01	0.42
1:A:363:MET:HB2	1:A:363:MET:HE2	1.86	0.42
1:B:149:THR:HA	1:B:207:VAL:HG21	2.02	0.42
1:D:347:ASP:O	1:D:394:GLU:HB2	2.19	0.42
1:A:128:LEU:O	1:A:132:LEU:HG	2.19	0.42
1:D:292:PRO:O	1:D:296:ILE:HG12	2.19	0.42
1:C:114:ASN:HB2	1:C:307:ARG:O	2.19	0.41
1:E:386:ASP:O	1:E:390:MET:HG3	2.20	0.41
1:D:321:ALA:O	1:D:325:ILE:HG13	2.20	0.41
1:A:216:GLU:OE1	1:A:307:ARG:HD2	2.20	0.41
1:A:78:VAL:HG21	1:A:128:LEU:CD2	2.48	0.41
1:E:338:GLN:HG2	1:E:348:LEU:HB3	2.02	0.41
1:E:331:ASN:HB3	1:E:336:GLN:HE21	1.84	0.41
1:A:190:SER:HA	1:A:208:GLN:NE2	2.35	0.41
1:C:208:GLN:O	1:C:212:LEU:HB2	2.20	0.41
1:F:161:ILE:HD11	1:F:214:LEU:CD2	2.51	0.41
1:E:149:THR:HA	1:E:207:VAL:HG21	2.01	0.41
1:A:154:VAL:HA	1:A:157:ASP:HB3	2.02	0.41
1:B:327:LYS:O	1:B:335:LYS:HE3	2.20	0.41
1:C:141:THR:HG22	1:C:165:LEU:HD13	2.02	0.41
1:F:133:ALA:CB	1:F:140:PHE:HB2	2.51	0.41
1:B:388:PRO:HG2	1:C:67:PRO:CD	2.51	0.41
1:C:95:HIS:CD2	1:C:244:LEU:HD13	2.56	0.41
1:D:403:ILE:HG13	1:D:404:ASP:N	2.34	0.41
1:B:354:ALA:O	1:B:358:ILE:HG13	2.21	0.41
1:B:386:ASP:O	1:B:390:MET:HG3	2.20	0.41
1:F:347:ASP:O	1:F:394:GLU:HB2	2.21	0.41
1:F:395:LYS:HA	1:F:410:LEU:O	2.21	0.41
1:A:140:PHE:CE2	1:A:142:MET:HG3	2.56	0.41
1:C:307:ARG:C	1:C:309:PRO:HD3	2.41	0.41
1:F:112:LYS:O	1:F:309:PRO:HG2	2.21	0.41
1:D:79:ILE:HD11	1:D:329:PRO:HD3	2.02	0.41
1:C:211:LEU:O	1:C:214:LEU:HB3	2.21	0.41
1:E:344:GLU:OE2	1:F:93:TYR:HE2	2.04	0.41
1:D:385:TYR:OH	1:E:71:ARG:HD3	2.21	0.41
1:D:157:ASP:O	1:D:160:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:GLU:HB3	1:B:409:PRO:HD2	2.03	0.41
1:F:399:ASP:O	1:F:403:ILE:HG22	2.21	0.41
1:B:347:ASP:O	1:B:394:GLU:HB2	2.21	0.41
1:D:251:PHE:HB3	1:D:254:LEU:CB	2.51	0.41
1:A:176:ALA:O	1:A:243:ILE:HG22	2.20	0.41
1:A:182:TYR:HA	1:A:246:ILE:O	2.20	0.41
1:D:303:GLU:OE1	1:D:303:GLU:HA	2.20	0.41
1:D:386:ASP:O	1:D:390:MET:HG3	2.20	0.41
1:B:292:PRO:O	1:B:296:ILE:HG12	2.21	0.41
1:E:251:PHE:HB3	1:E:254:LEU:CB	2.51	0.41
1:E:292:PRO:O	1:E:296:ILE:HG12	2.21	0.41
1:F:185:GLU:HB3	1:F:188:LYS:HG3	2.02	0.41
1:B:369:ALA:HA	1:B:372:LEU:HG	2.03	0.41
1:C:138:VAL:HG13	1:C:139:PRO:HD2	2.03	0.40
1:A:86:LYS:O	1:A:90:VAL:HG23	2.21	0.40
1:F:141:THR:HG22	1:F:165:LEU:HD13	2.04	0.40
1:E:119:GLY:O	1:E:250:ALA:HA	2.21	0.40
1:D:243:ILE:HD11	1:D:245:PHE:CZ	2.56	0.40
1:F:190:SER:HB3	1:F:300:LEU:HD12	2.03	0.40
1:D:128:LEU:O	1:D:132:LEU:HG	2.21	0.40
1:B:92:VAL:HG11	1:B:136:LEU:HD11	2.02	0.40
1:A:86:LYS:HG3	1:F:385:TYR:CZ	2.55	0.40
1:F:367:THR:HB	1:F:371:GLY:HA3	2.04	0.40
1:B:392:ASP:HB3	1:B:413:TYR:CE2	2.55	0.40
1:C:329:PRO:C	1:C:331:ASN:N	2.73	0.40
1:B:357:ALA:O	1:B:361:LYS:HG2	2.21	0.40
1:E:327:LYS:O	1:E:335:LYS:HE3	2.21	0.40
1:B:182:TYR:HA	1:B:246:ILE:O	2.22	0.40
1:F:199:THR:HG22	1:F:201:ASP:N	2.36	0.40
1:E:296:ILE:CD1	1:E:305:ILE:HD12	2.52	0.40
1:F:195:ASN:HA	1:F:196:PRO:HD2	1.93	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	299/363 (82%)	286 (96%)	13 (4%)	0	100	100
1	B	295/363 (81%)	281 (95%)	14 (5%)	0	100	100
1	C	288/363 (79%)	274 (95%)	13 (4%)	1 (0%)	46	83
1	D	298/363 (82%)	285 (96%)	13 (4%)	0	100	100
1	E	303/363 (84%)	291 (96%)	12 (4%)	0	100	100
1	F	295/363 (81%)	281 (95%)	13 (4%)	1 (0%)	46	83
All	All	1778/2178 (82%)	1698 (96%)	78 (4%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	103	ASP
1	C	103	ASP

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	243/299 (81%)	243 (100%)	0	100	100
1	B	241/299 (81%)	241 (100%)	0	100	100
1	C	242/299 (81%)	242 (100%)	0	100	100
1	D	241/299 (81%)	241 (100%)	0	100	100
1	E	244/299 (82%)	244 (100%)	0	100	100
1	F	247/299 (83%)	247 (100%)	0	100	100
All	All	1458/1794 (81%)	1458 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	B	83	GLN
1	C	81	GLN
1	C	101	ASN
1	C	406	GLN
1	E	83	GLN
1	F	81	GLN
1	F	101	ASN
1	F	406	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](#)

6 ligands are modelled in this entry.

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	SO4	A	500	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	500	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	C	500	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	D	500	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	E	500	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	F	500	-	4,4,4	0.25	0	6,6,6	0.07	0

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	SO4	A	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	500	-	-	0/0/0/0	0/0/0/0
2	SO4	C	500	-	-	0/0/0/0	0/0/0/0
2	SO4	D	500	-	-	0/0/0/0	0/0/0/0
2	SO4	E	500	-	-	0/0/0/0	0/0/0/0
2	SO4	F	500	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	SO4	1	0
2	B	500	SO4	2	0
2	C	500	SO4	1	0
2	D	500	SO4	1	0
2	E	500	SO4	1	0
2	F	500	SO4	1	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, 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	311/363 (85%)	0.98	46 (14%) 3 8	221, 311, 448, 562	0
1	B	307/363 (84%)	0.78	36 (11%) 6 10	188, 302, 448, 502	0
1	C	298/363 (82%)	0.96	35 (11%) 6 10	205, 303, 437, 529	0
1	D	310/363 (85%)	0.64	34 (10%) 7 11	217, 309, 429, 492	0
1	E	315/363 (86%)	0.73	35 (11%) 7 11	254, 330, 398, 461	0
1	F	305/363 (84%)	0.61	27 (8%) 12 15	201, 298, 486, 605	0
All	All	1846/2178 (84%)	0.78	213 (11%) 6 11	188, 310, 444, 605	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	13.6
1	B	200	ARG	9.7
1	A	266	SER	8.7
1	F	195	ASN	8.5
1	A	264	THR	8.1
1	F	197	SER	7.7
1	C	103	ASP	7.3
1	A	263	GLU	7.1
1	B	266	SER	6.8
1	D	266	SER	6.5
1	A	149	THR	6.3
1	B	203	SER	6.2
1	C	101	ASN	6.1
1	B	63	ALA	5.8
1	C	191	ARG	5.6
1	D	195	ASN	5.5
1	A	203	SER	5.5
1	C	102	GLY	5.5
1	F	153	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	100	ARG	5.1
1	B	235	PHE	5.1
1	B	149	THR	4.9
1	C	162	ILE	4.9
1	E	203	SER	4.8
1	A	344	GLU	4.8
1	C	154	VAL	4.8
1	D	196	PRO	4.7
1	C	104	THR	4.7
1	D	392	ASP	4.6
1	C	150	GLU	4.6
1	B	265	GLY	4.5
1	F	196	PRO	4.5
1	D	315	ASN	4.5
1	A	104	THR	4.4
1	C	153	TYR	4.4
1	E	317	LEU	4.4
1	D	264	THR	4.4
1	D	193	SER	4.4
1	E	149	THR	4.4
1	B	218	THR	4.4
1	E	350	PHE	4.3
1	A	105	SER	4.3
1	A	390	MET	4.3
1	A	392	ASP	4.2
1	E	79	ILE	4.2
1	C	282	SER	4.2
1	C	149	THR	4.2
1	D	237	GLN	4.1
1	B	204	GLY	4.1
1	B	201	ASP	3.9
1	C	161	ILE	3.9
1	E	265	GLY	3.9
1	A	200	ARG	3.8
1	A	351	ARG	3.8
1	E	264	THR	3.8
1	C	158	VAL	3.8
1	A	238	VAL	3.8
1	D	64	LEU	3.7
1	A	317	LEU	3.6
1	D	236	LEU	3.6
1	E	64	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	388	PRO	3.6
1	E	266	SER	3.6
1	C	159	GLU	3.6
1	E	237	GLN	3.6
1	E	200	ARG	3.6
1	C	237	GLN	3.5
1	B	254	LEU	3.5
1	D	238	VAL	3.4
1	B	102	GLY	3.4
1	C	236	LEU	3.4
1	F	368	GLY	3.4
1	D	394	GLU	3.4
1	E	349	GLU	3.4
1	F	198	ILE	3.4
1	C	350	PHE	3.3
1	F	103	ASP	3.3
1	B	202	VAL	3.3
1	A	411	LEU	3.3
1	D	411	LEU	3.2
1	B	103	ASP	3.2
1	F	369	ALA	3.2
1	E	78	VAL	3.2
1	E	238	VAL	3.2
1	C	96	TYR	3.2
1	E	394	GLU	3.1
1	A	410	LEU	3.1
1	D	235	PHE	3.1
1	E	80	GLY	3.1
1	F	154	VAL	3.1
1	A	261	ARG	3.1
1	D	282	SER	3.1
1	F	207	VAL	3.1
1	F	171	TYR	3.1
1	A	64	LEU	3.0
1	A	204	GLY	3.0
1	A	207	VAL	3.0
1	D	265	GLY	3.0
1	D	119	GLY	3.0
1	D	194	ASP	3.0
1	B	104	THR	2.9
1	B	264	THR	2.9
1	B	396	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	350	PHE	2.9
1	A	103	ASP	2.9
1	E	251	PHE	2.9
1	C	252	ALA	2.9
1	D	63	ALA	2.9
1	A	178	ARG	2.9
1	E	65	PRO	2.9
1	D	344	GLU	2.8
1	E	279	ASP	2.8
1	E	334	THR	2.8
1	C	136	LEU	2.8
1	B	258	ILE	2.8
1	A	387	LEU	2.8
1	C	238	VAL	2.7
1	E	153	TYR	2.7
1	B	97	LYS	2.7
1	B	64	LEU	2.7
1	E	152	GLY	2.7
1	A	237	GLN	2.7
1	B	101	ASN	2.6
1	A	289	GLN	2.6
1	A	316	GLU	2.6
1	F	203	SER	2.6
1	C	284	GLY	2.6
1	A	139	PRO	2.6
1	A	345	GLY	2.6
1	B	289	GLN	2.5
1	F	152	GLY	2.5
1	D	348	LEU	2.5
1	B	239	ASP	2.5
1	C	170	ASP	2.5
1	E	173	VAL	2.5
1	E	207	VAL	2.5
1	D	176	ALA	2.5
1	B	350	PHE	2.5
1	A	409	PRO	2.5
1	B	255	ASP	2.5
1	E	254	LEU	2.5
1	D	350	PHE	2.5
1	E	100	ARG	2.5
1	E	236	LEU	2.4
1	C	155	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	287	LEU	2.4
1	B	112	LYS	2.4
1	D	395	LYS	2.4
1	B	147	THR	2.4
1	C	327	LYS	2.4
1	A	408	GLU	2.4
1	F	163	GLN	2.4
1	E	187	ASP	2.4
1	D	192	LYS	2.3
1	A	327	LYS	2.3
1	F	370	ARG	2.3
1	F	64	LEU	2.3
1	D	410	LEU	2.3
1	E	356	ASP	2.3
1	D	93	TYR	2.3
1	D	203	SER	2.3
1	C	315	ASN	2.3
1	A	326	LEU	2.3
1	F	112	LYS	2.3
1	B	286	LEU	2.3
1	B	368	GLY	2.2
1	E	235	PHE	2.2
1	A	141	THR	2.2
1	B	236	LEU	2.2
1	E	96	TYR	2.2
1	A	180	ILE	2.2
1	C	65	PRO	2.2
1	B	189	ILE	2.2
1	F	309	PRO	2.2
1	C	316	GLU	2.2
1	F	165	LEU	2.2
1	F	237	GLN	2.2
1	F	307	ARG	2.2
1	A	307	ARG	2.2
1	A	368	GLY	2.2
1	B	301	ILE	2.2
1	D	118	ILE	2.2
1	F	238	VAL	2.2
1	C	132	LEU	2.1
1	B	394	GLU	2.1
1	D	409	PRO	2.1
1	A	175	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	97	LYS	2.1
1	F	166	LEU	2.1
1	F	177	GLN	2.1
1	B	238	VAL	2.1
1	E	392	ASP	2.1
1	C	156	GLU	2.1
1	A	297	LYS	2.1
1	F	150	GLU	2.1
1	C	323	ILE	2.1
1	A	334	THR	2.1
1	C	176	ALA	2.1
1	E	323	ILE	2.1
1	D	380	LEU	2.0
1	A	262	VAL	2.0
1	D	341	PHE	2.0
1	F	104	THR	2.0
1	B	174	GLN	2.0
1	E	189	ILE	2.0
1	F	199	THR	2.0
1	C	178	ARG	2.0
1	A	412	ILE	2.0
1	A	354	ALA	2.0
1	E	145	ALA	2.0
1	D	314	LEU	2.0
1	A	369	ALA	2.0
1	D	302	PRO	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, 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
2	SO4	B	500	5/5	0.83	0.44	2.78	202,202,210,220	0
2	SO4	D	500	5/5	0.95	0.37	0.55	191,193,199,205	0
2	SO4	A	500	5/5	0.95	0.27	-0.67	190,191,201,210	0
2	SO4	C	500	5/5	0.91	0.28	-0.82	200,203,210,217	0
2	SO4	E	500	5/5	0.89	0.25	-0.88	203,204,209,215	0
2	SO4	F	500	5/5	0.95	0.22	-1.54	200,202,208,215	0

6.5 Other polymers [i](#)

There are no such residues in this entry.