Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 12:16 AM EDT

PDB ID	:	3VBB
Title	:	Crystal Structure of Seryl-tRNA Synthetase from Human at 2.9 angstroms
Authors	:	Xu, X.L.; Yang, X.-L.
Deposited on	:	2012-01-02
Resolution	:	2.89 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

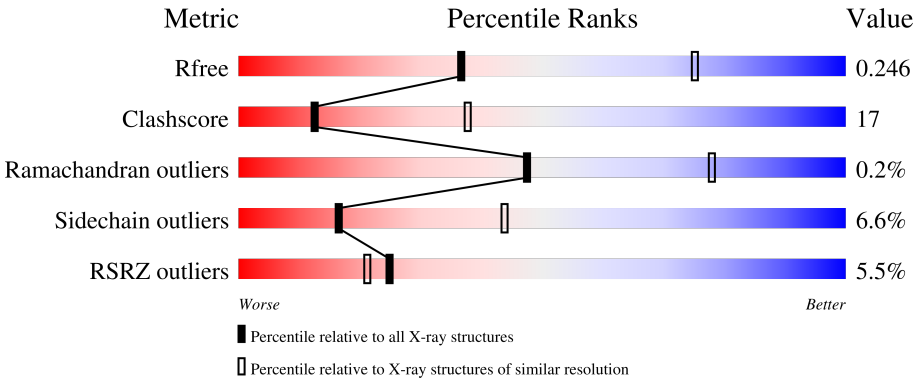
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	522	6% 57% 27% · 14%
1	B	522	4% 59% 25% · 13%
1	C	522	7% 55% 30% · 13%
1	D	522	4% 54% 29% · 14%
1	E	522	2% 59% 23% · 16%

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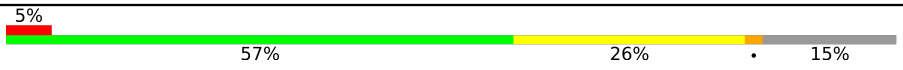
Mol	Chain	Length	Quality of chain
1	F	522	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21387 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 Seryl-tRNA synthetase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	5	1	0
			3606	2301	619	668	18			
1	B	454	Total	C	N	O	S	0	1	0
			3625	2311	623	671	20			
1	C	456	Total	C	N	O	S	3	1	0
			3588	2291	609	669	19			
1	D	450	Total	C	N	O	S	7	1	0
			3533	2264	602	649	18			
1	E	440	Total	C	N	O	S	1	1	0
			3469	2216	596	638	19			
1	F	443	Total	C	N	O	S	11	1	0
			3519	2247	604	650	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	515	LEU	-	expression tag	UNP P49591
A	516	GLU	-	expression tag	UNP P49591
A	517	HIS	-	expression tag	UNP P49591
A	518	HIS	-	expression tag	UNP P49591
A	519	HIS	-	expression tag	UNP P49591
A	520	HIS	-	expression tag	UNP P49591
A	521	HIS	-	expression tag	UNP P49591
A	522	HIS	-	expression tag	UNP P49591
B	515	LEU	-	expression tag	UNP P49591
B	516	GLU	-	expression tag	UNP P49591
B	517	HIS	-	expression tag	UNP P49591
B	518	HIS	-	expression tag	UNP P49591
B	519	HIS	-	expression tag	UNP P49591
B	520	HIS	-	expression tag	UNP P49591
B	521	HIS	-	expression tag	UNP P49591
B	522	HIS	-	expression tag	UNP P49591
C	515	LEU	-	expression tag	UNP P49591

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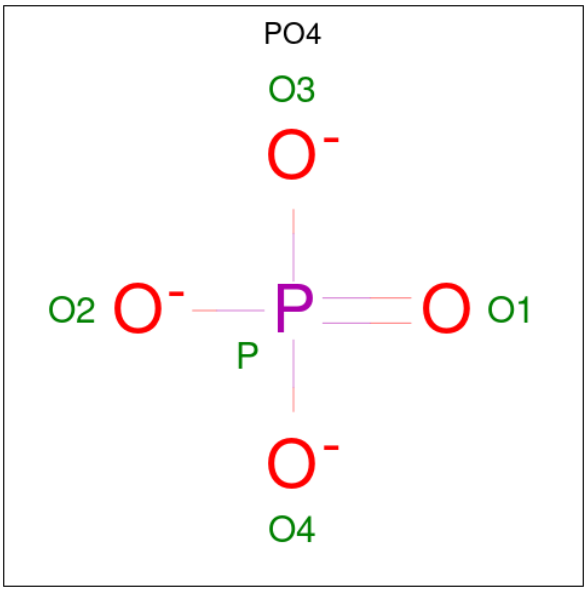
Chain	Residue	Modelled	Actual	Comment	Reference
C	516	GLU	-	expression tag	UNP P49591
C	517	HIS	-	expression tag	UNP P49591
C	518	HIS	-	expression tag	UNP P49591
C	519	HIS	-	expression tag	UNP P49591
C	520	HIS	-	expression tag	UNP P49591
C	521	HIS	-	expression tag	UNP P49591
C	522	HIS	-	expression tag	UNP P49591
D	515	LEU	-	expression tag	UNP P49591
D	516	GLU	-	expression tag	UNP P49591
D	517	HIS	-	expression tag	UNP P49591
D	518	HIS	-	expression tag	UNP P49591
D	519	HIS	-	expression tag	UNP P49591
D	520	HIS	-	expression tag	UNP P49591
D	521	HIS	-	expression tag	UNP P49591
D	522	HIS	-	expression tag	UNP P49591
E	515	LEU	-	expression tag	UNP P49591
E	516	GLU	-	expression tag	UNP P49591
E	517	HIS	-	expression tag	UNP P49591
E	518	HIS	-	expression tag	UNP P49591
E	519	HIS	-	expression tag	UNP P49591
E	520	HIS	-	expression tag	UNP P49591
E	521	HIS	-	expression tag	UNP P49591
E	522	HIS	-	expression tag	UNP P49591
F	515	LEU	-	expression tag	UNP P49591
F	516	GLU	-	expression tag	UNP P49591
F	517	HIS	-	expression tag	UNP P49591
F	518	HIS	-	expression tag	UNP P49591
F	519	HIS	-	expression tag	UNP P49591
F	520	HIS	-	expression tag	UNP P49591
F	521	HIS	-	expression tag	UNP P49591
F	522	HIS	-	expression tag	UNP P49591

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is water.

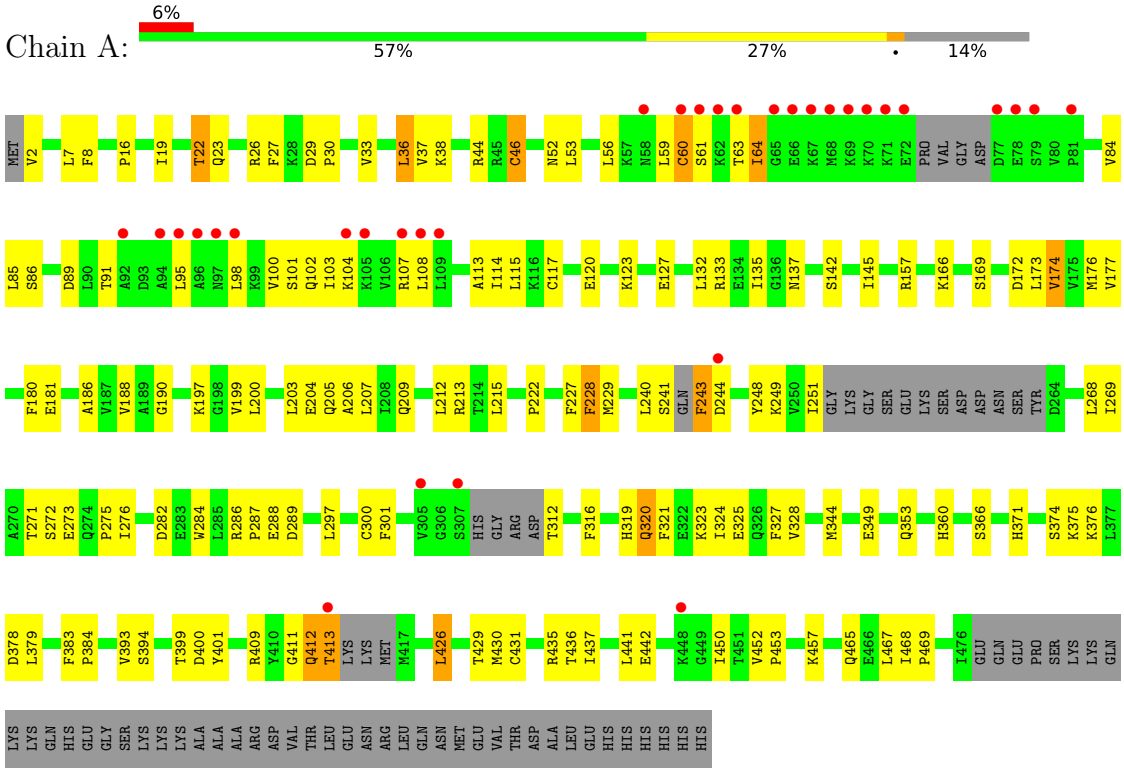
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	3	Total O 3 3	0	0
4	C	1	Total O 1 1	0	0
4	D	2	Total O 2 2	0	0
4	E	2	Total O 2 2	0	0
4	F	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

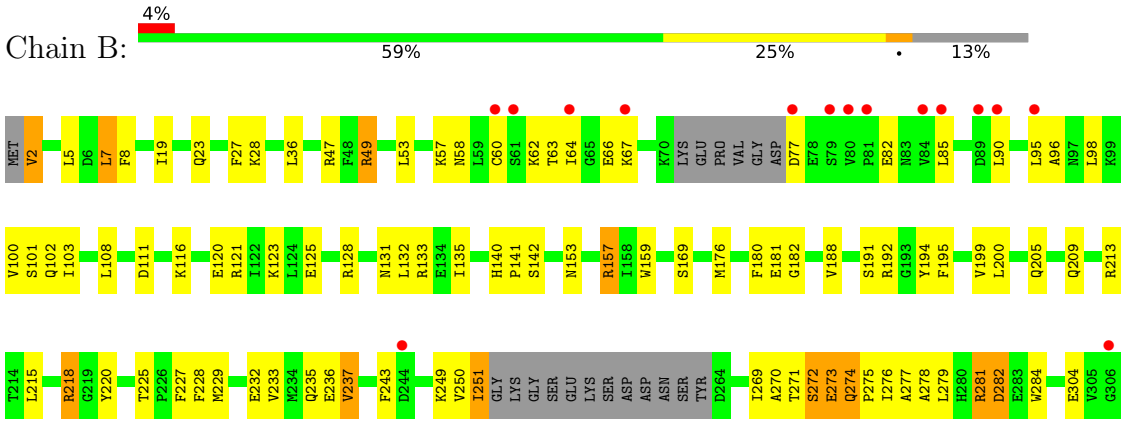
• Molecule 1: Seryl-tRNA synthetase, cytoplasmic

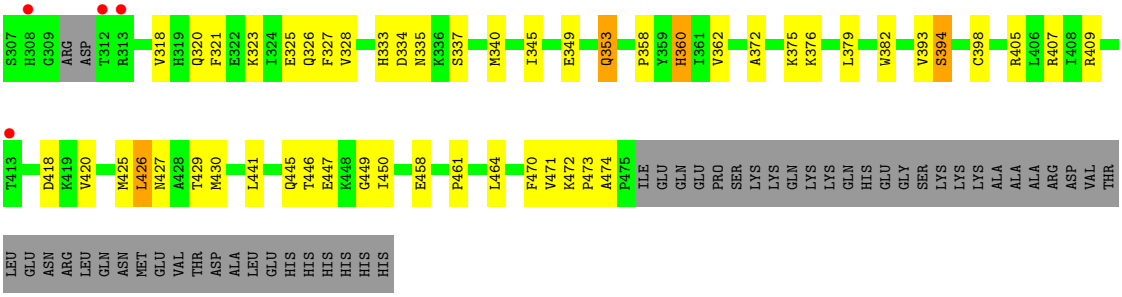
Chain A:



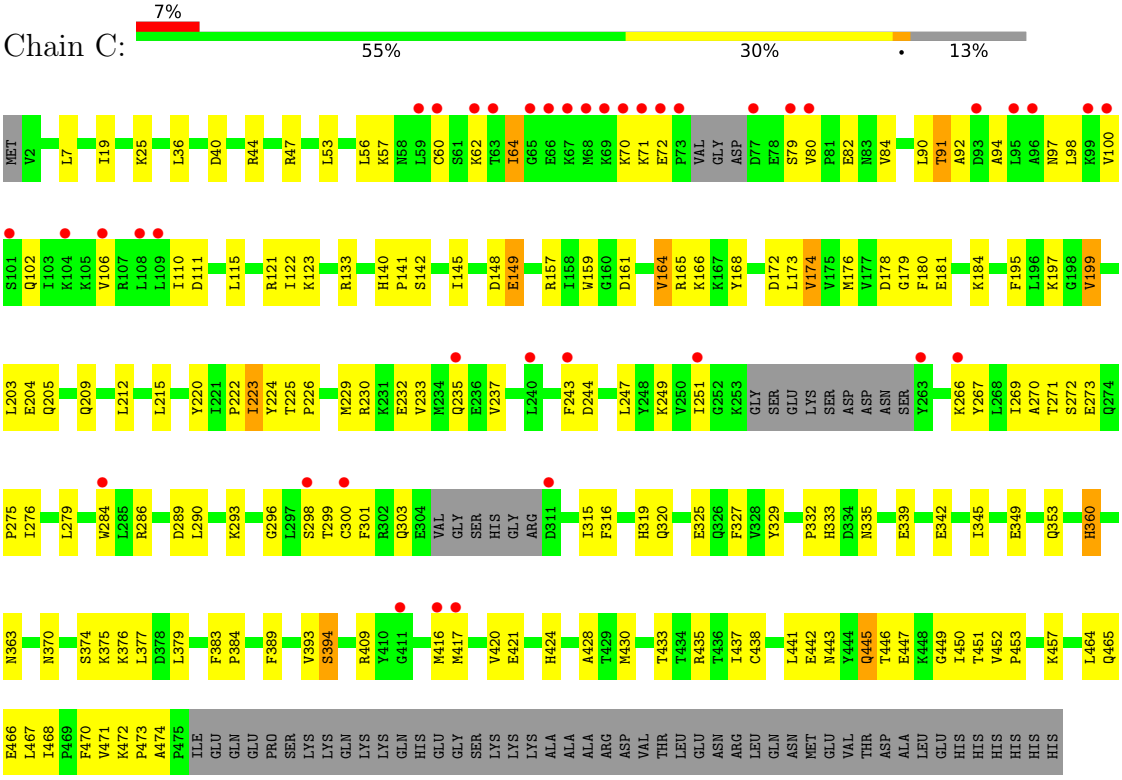
• Molecule 1: Seryl-tRNA synthetase, cytoplasmic

Chain B:

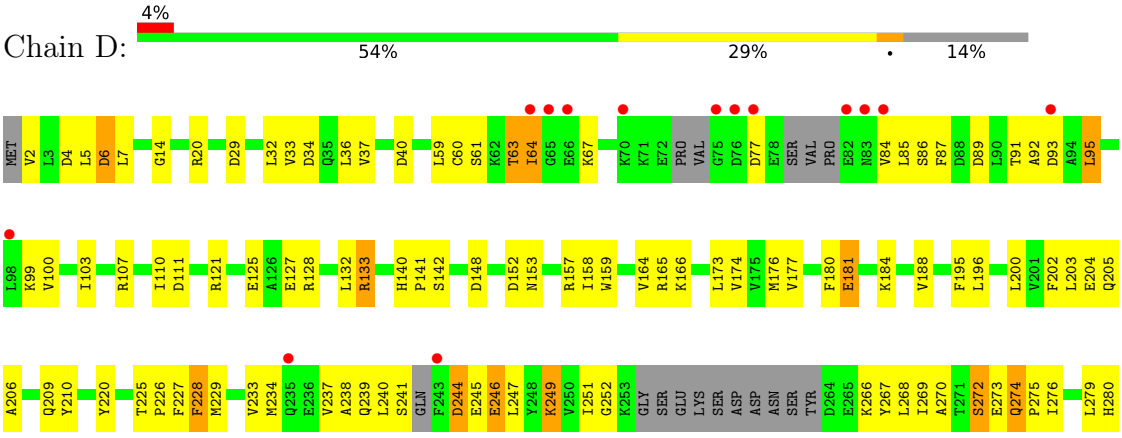


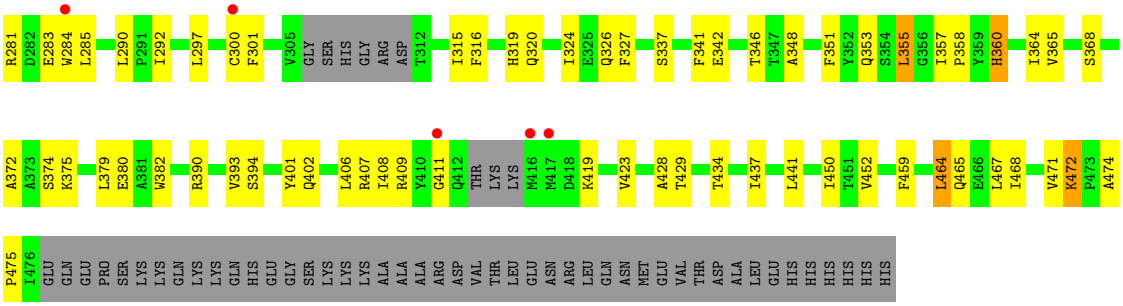


• Molecule 1: Seryl-tRNA synthetase, cytoplasmic



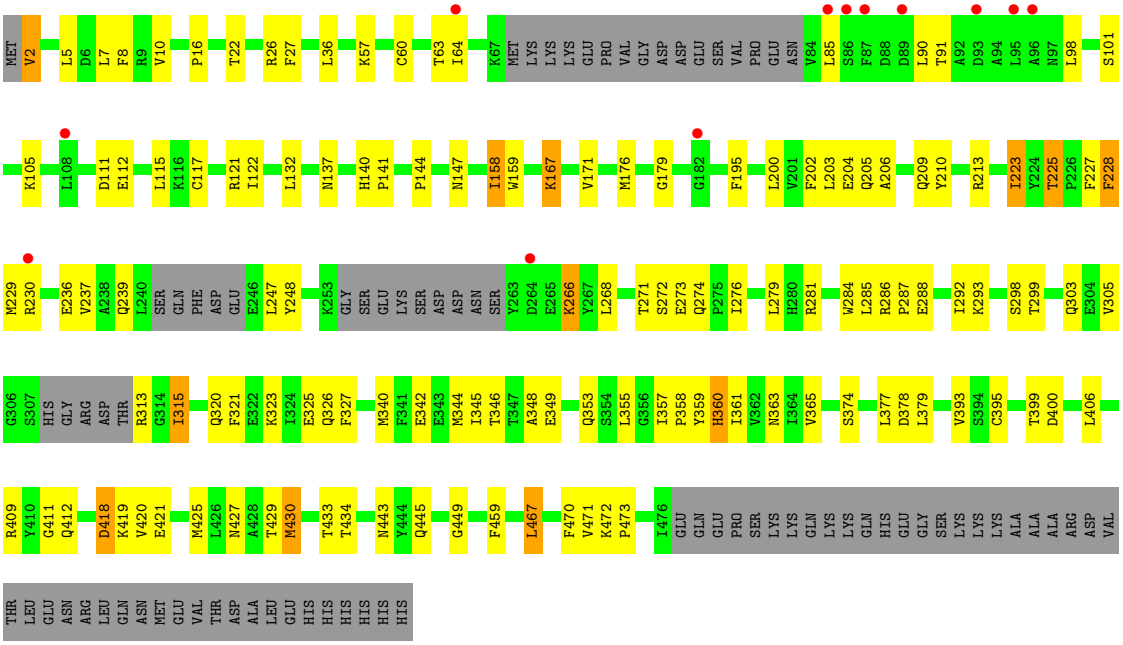
• Molecule 1: Seryl-tRNA synthetase, cytoplasmic





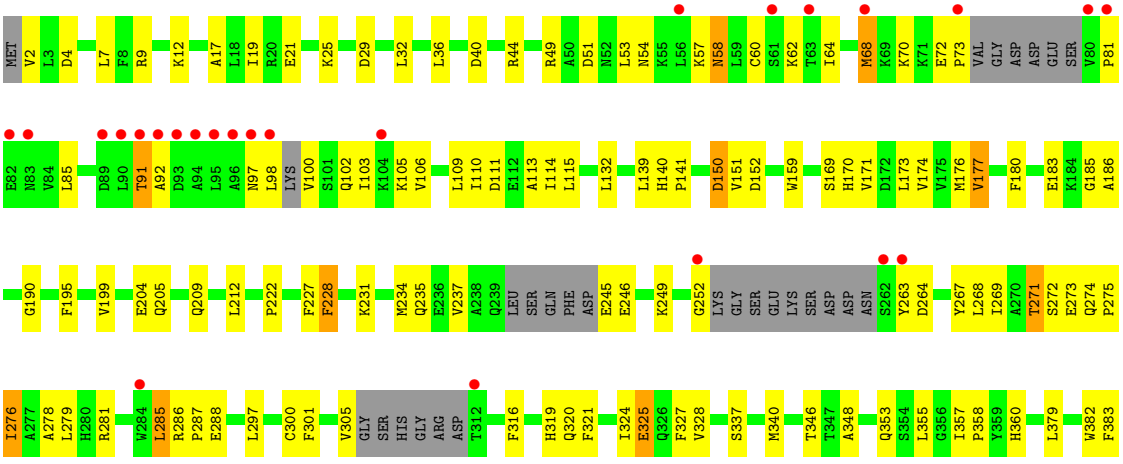
• Molecule 1: Seryl-tRNA synthetase, cytoplasmic

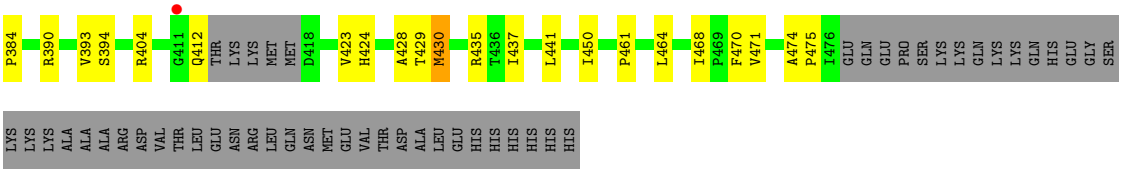
Chain E:



• Molecule 1: Seryl-tRNA synthetase, cytoplasmic

Chain F:




P384 R390 V393 S394 R404 G411 Q412 THR LYS LYS MET MET D418 V423 H424 A428 T429 M430 R435 T436 I437 L441 I450 P461 L464 I468 P469 F470 V471 A474 P475 I476 GLU GLN GLU PRO SER LYS LYS GLN LYS LYS GLN HIS GLU GLY SER
LYS LYS LYS ALA ALA ALA ARG ASP VAL THR LEU GLU ASN ARG LEU GLN ASN MET GLU VAL THR ASP ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.80Å 189.42Å 230.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.89 48.59 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.59-2.89) 98.8 (48.59-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.194 , 0.250 0.190 , 0.246	Depositor DCC
R_{free} test set	5677 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	72.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21387	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/3677	0.62	0/4957
1	B	0.49	0/3697	0.64	0/4982
1	C	0.44	0/3661	0.62	0/4949
1	D	0.48	0/3601	0.64	1/4858 (0.0%)
1	E	0.50	0/3539	0.64	0/4777
1	F	0.48	0/3589	0.64	0/4841
All	All	0.48	0/21764	0.63	1/29364 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	6	ASP	N-CA-C	-5.11	97.21	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3606	0	3584	123	0
1	B	3625	0	3600	127	0
1	C	3588	0	3506	144	0
1	D	3533	0	3483	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3469	0	3414	111	0
1	F	3519	0	3465	115	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
All	All	21387	0	21052	712	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 17.

All (712) 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:E:399:THR:HG22	1:E:400:ASP:H	0.97	1.08
1:B:157:ARG:HG3	1:B:157:ARG:HH11	1.20	1.05
1:B:276:ILE:HD12	1:B:327[B]:PHE:CD2	1.93	1.04
1:E:230:ARG:O	1:E:266:LYS:HA	1.58	1.03
1:B:218:ARG:HG3	1:B:218:ARG:HH11	1.27	0.98
1:B:472:LYS:HG3	1:B:473:PRO:HD2	1.44	0.97
1:E:399:THR:CG2	1:E:400:ASP:H	1.80	0.94
1:E:399:THR:HG22	1:E:400:ASP:N	1.79	0.94
1:D:7:LEU:HA	1:D:14:GLY:HA3	1.49	0.93
1:E:276:ILE:O	1:E:279:LEU:HB3	1.69	0.93
1:A:251:ILE:HD11	1:B:251:ILE:HD11	1.49	0.93
1:A:412:GLN:O	1:A:412:GLN:HG3	1.66	0.92
1:C:64:ILE:HG12	1:C:100:VAL:HG13	1.54	0.89
1:F:81:PRO:HB2	1:F:102:GLN:HE21	1.36	0.89
1:C:168:TYR:H	1:C:445:GLN:HE22	1.19	0.88
1:B:7:LEU:HD23	1:B:19:ILE:HD11	1.54	0.87
1:C:276:ILE:HD12	1:C:327[B]:PHE:CD2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:GLN:HE22	1:F:227:PHE:H	1.15	0.87
1:F:234:MET:HG2	1:F:267:TYR:HD2	1.38	0.87
1:B:63:THR:HG21	1:B:95:LEU:HD13	1.57	0.87
1:F:174:VAL:HG12	1:F:180:PHE:HB2	1.57	0.86
1:A:177:VAL:HG12	1:A:199:VAL:HG21	1.57	0.85
1:B:276:ILE:HD12	1:B:327[B]:PHE:HD2	1.37	0.85
1:A:177:VAL:CG1	1:A:199:VAL:HG21	2.08	0.84
1:F:231:LYS:HE2	1:F:235:GLN:NE2	1.90	0.84
1:D:159:TRP:CE2	1:D:353:GLN:HG2	2.13	0.83
1:E:321:PHE:HE2	1:E:323:LYS:HE3	1.44	0.83
1:F:36:LEU:HD11	1:F:132:LEU:HG	1.60	0.83
1:C:320:GLN:HE22	1:D:227:PHE:H	1.23	0.82
1:A:344:MET:HE1	1:A:426:LEU:HB2	1.60	0.82
1:A:284:TRP:HB2	1:A:413:THR:HG23	1.60	0.82
1:F:64:ILE:HG12	1:F:103:ILE:HG21	1.61	0.82
1:C:225:THR:HG22	1:C:226:PRO:O	1.79	0.81
1:B:272:SER:HB2	1:B:325:GLU:HG3	1.62	0.80
1:B:273:GLU:HB2	1:B:327[B]:PHE:CE1	2.17	0.80
1:F:441:LEU:HD22	1:F:450:ILE:HD13	1.63	0.80
1:A:60:CYS:HB3	1:A:107:ARG:HD3	1.64	0.79
1:C:416:MET:O	1:C:417:MET:HB3	1.81	0.79
1:D:6:ASP:O	1:D:7:LEU:HB3	1.83	0.79
1:A:344:MET:HE3	1:A:426:LEU:HD22	1.65	0.78
1:D:174:VAL:HG23	1:D:200:LEU:CD1	2.14	0.78
1:A:46:CYS:HB3	1:A:117:CYS:SG	2.24	0.77
1:E:159:TRP:CE2	1:E:353:GLN:HG2	2.20	0.77
1:A:174:VAL:HG13	1:A:180:PHE:HB2	1.65	0.77
1:D:441:LEU:HD22	1:D:450:ILE:HD13	1.66	0.77
1:D:471:VAL:HG12	1:D:472:LYS:HG2	1.67	0.76
1:B:218:ARG:HH11	1:B:218:ARG:CG	1.98	0.76
1:B:472:LYS:HG3	1:B:473:PRO:CD	2.14	0.76
1:E:225:THR:HG21	1:E:272:SER:HB2	1.68	0.76
1:A:227:PHE:H	1:B:320:GLN:HE22	1.33	0.76
1:F:278:ALA:HA	1:F:281:ARG:HG3	1.68	0.76
1:C:472:LYS:HB3	1:C:473:PRO:HD2	1.68	0.76
1:F:348:ALA:HA	1:F:430:MET:CE	2.16	0.75
1:A:60:CYS:O	1:A:64:ILE:HB	1.86	0.75
1:E:227:PHE:H	1:F:320:GLN:HE22	1.31	0.75
1:E:472:LYS:HB3	1:E:473:PRO:HD2	1.69	0.74
1:A:325:GLU:HG2	1:A:429:THR:HG22	1.68	0.74
1:B:276:ILE:HD12	1:B:327[B]:PHE:CE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:LEU:HD12	1:E:248:TYR:H	1.54	0.73
1:D:181:GLU:OE1	1:D:184:LYS:HB2	1.89	0.73
1:A:271:THR:HG22	1:A:323:LYS:NZ	2.04	0.72
1:C:56:LEU:HD22	1:C:90:LEU:HD22	1.70	0.72
1:C:225:THR:HG21	1:C:275:PRO:HG2	1.71	0.72
1:E:225:THR:HG21	1:E:272:SER:CB	2.19	0.72
1:A:229:MET:HE3	1:B:188:VAL:HG13	1.71	0.72
1:E:273:GLU:HB2	1:E:327[B]:PHE:CE1	2.25	0.71
1:C:251:ILE:HB	1:D:249:LYS:HB2	1.73	0.71
1:B:157:ARG:HH11	1:B:157:ARG:CG	2.00	0.71
1:F:174:VAL:CG1	1:F:180:PHE:HB2	2.20	0.70
1:B:205:GLN:O	1:B:209:GLN:HG2	1.91	0.70
1:F:170:HIS:O	1:F:174:VAL:HG23	1.91	0.70
1:B:194:TYR:CE1	1:B:318:VAL:HG21	2.26	0.70
1:B:447:GLU:HA	1:B:447:GLU:OE2	1.92	0.70
1:D:6:ASP:O	1:D:7:LEU:CB	2.39	0.70
1:E:57:LYS:HD2	1:E:111:ASP:OD2	1.91	0.70
1:D:7:LEU:HA	1:D:14:GLY:CA	2.22	0.70
1:E:247:LEU:HD12	1:E:248:TYR:N	2.07	0.69
1:B:176:MET:SD	1:B:474:ALA:HB2	2.31	0.69
1:F:234:MET:HG2	1:F:267:TYR:CD2	2.26	0.69
1:A:204:GLU:HB2	1:A:437:ILE:HD11	1.73	0.69
1:C:327[A]:PHE:HE2	1:C:329:TYR:CZ	2.10	0.69
1:C:299:THR:HG21	1:D:227:PHE:CE2	2.28	0.69
1:F:40:ASP:O	1:F:44:ARG:HG3	1.93	0.69
1:C:40:ASP:O	1:C:44:ARG:HG3	1.92	0.68
1:C:230:ARG:HG2	1:C:266:LYS:HG2	1.73	0.68
1:E:2:VAL:HG22	1:E:132:LEU:HG	1.75	0.68
1:E:228:PHE:HD1	1:E:228:PHE:O	1.76	0.68
1:A:241:SER:HA	1:A:244:ASP:HB2	1.76	0.68
1:E:117:CYS:O	1:E:121:ARG:HG3	1.93	0.68
1:B:133:ARG:NH1	1:B:405:ARG:HH12	1.91	0.68
1:F:325:GLU:HG3	1:F:429:THR:HA	1.74	0.68
1:D:174:VAL:HG22	1:D:180:PHE:HB2	1.75	0.68
1:C:276:ILE:HD12	1:C:327[B]:PHE:CE2	2.29	0.67
1:A:23:GLN:HE22	1:A:135:ILE:HA	1.59	0.67
1:D:174:VAL:HG23	1:D:200:LEU:HD11	1.76	0.67
1:F:159:TRP:CE2	1:F:353:GLN:HG2	2.28	0.67
1:D:315:ILE:HG22	1:D:434:THR:HB	1.75	0.67
1:D:4:ASP:OD2	1:D:419:LYS:HE3	1.94	0.67
1:F:174:VAL:HG12	1:F:180:PHE:CB	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:PRO:HB2	1:F:102:GLN:NE2	2.10	0.66
1:C:203:LEU:HD23	1:C:437:ILE:HD12	1.78	0.66
1:F:2:VAL:HG22	1:F:132:LEU:HD22	1.76	0.66
1:E:349:GLU:HG2	1:E:359:TYR:OH	1.96	0.66
1:D:320:GLN:O	1:D:320:GLN:HG3	1.96	0.65
1:A:441:LEU:HD22	1:A:450:ILE:HG13	1.76	0.65
1:C:57:LYS:HE2	1:C:111:ASP:HB2	1.78	0.65
1:D:342:GLU:O	1:D:346:THR:HG23	1.96	0.65
1:E:236:GLU:HG2	1:E:281:ARG:HH12	1.61	0.65
1:C:229:MET:O	1:C:266:LYS:HB3	1.95	0.65
1:D:205:GLN:O	1:D:209:GLN:HG2	1.97	0.65
1:C:273:GLU:HA	1:C:327[B]:PHE:CE1	2.31	0.65
1:D:159:TRP:CZ2	1:D:353:GLN:HG2	2.31	0.65
1:E:36:LEU:HD11	1:E:132:LEU:HD13	1.79	0.65
1:A:328:VAL:HB	1:A:344:MET:HE1	1.78	0.64
1:A:344:MET:CE	1:A:426:LEU:HB2	2.27	0.64
1:D:237:VAL:HG12	1:D:238:ALA:H	1.62	0.64
1:F:29:ASP:HB3	1:F:32:LEU:HD13	1.78	0.64
1:C:176:MET:HB3	1:C:470:PHE:HD1	1.61	0.64
1:E:276:ILE:HD12	1:E:327[B]:PHE:CD2	2.33	0.64
1:B:276:ILE:CD1	1:B:327[B]:PHE:HD2	2.08	0.64
1:F:68:MET:SD	1:F:100:VAL:HG13	2.38	0.64
1:B:140:HIS:CG	1:B:141:PRO:HD2	2.32	0.64
1:C:168:TYR:H	1:C:445:GLN:NE2	1.93	0.64
1:D:204:GLU:HB2	1:D:437:ILE:HD11	1.80	0.64
1:A:100:VAL:C	1:A:102:GLN:H	2.01	0.64
1:E:236:GLU:HB3	1:E:406:LEU:HD21	1.79	0.64
1:C:98:LEU:HA	1:C:102:GLN:HE21	1.63	0.64
1:B:142:SER:OG	1:B:375:LYS:HE3	1.98	0.63
1:E:287:PRO:HD3	1:E:411:GLY:O	1.98	0.63
1:A:286:ARG:HB3	1:A:288:GLU:HG2	1.80	0.63
1:C:199:VAL:HG12	1:C:464:LEU:HD11	1.79	0.63
1:F:57:LYS:CB	1:F:110:ILE:HG21	2.28	0.63
1:B:220:TYR:OH	1:B:326:GLN:NE2	2.30	0.63
1:D:467:LEU:HG	1:D:468:ILE:N	2.13	0.63
1:B:271:THR:HB	1:B:325:GLU:OE2	1.99	0.62
1:A:284:TRP:CB	1:A:413:THR:HG23	2.29	0.62
1:C:433:THR:O	1:C:437:ILE:HG12	1.99	0.62
1:D:63:THR:HG21	1:D:95:LEU:HD11	1.81	0.62
1:B:325:GLU:CB	1:B:327[B]:PHE:CZ	2.82	0.62
1:D:247:LEU:HD21	1:D:270:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLN:OE1	1:B:205:GLN:HB3	2.00	0.62
1:D:7:LEU:CA	1:D:14:GLY:HA3	2.27	0.62
1:B:157:ARG:HG3	1:B:157:ARG:NH1	2.01	0.61
1:B:194:TYR:CD1	1:B:318:VAL:HG21	2.35	0.61
1:C:316:PHE:CE1	1:C:435:ARG:HG2	2.34	0.61
1:B:2:VAL:HG22	1:B:132:LEU:HG	1.83	0.61
1:B:67:LYS:HE2	1:B:98:LEU:O	2.00	0.61
1:B:116:LYS:O	1:B:120:GLU:HG2	2.00	0.61
1:B:323:LYS:NZ	1:B:429:THR:HG21	2.15	0.61
1:A:272:SER:O	1:A:275:PRO:HD2	2.01	0.61
1:B:407:ARG:HG2	1:B:407:ARG:HH11	1.66	0.61
1:E:22:THR:O	1:E:26:ARG:HG3	2.00	0.61
1:A:286:ARG:HD3	1:A:288:GLU:OE2	2.00	0.60
1:F:186:ALA:HA	1:F:190:GLY:O	2.01	0.60
1:D:407:ARG:HD3	1:D:409:ARG:HH21	1.64	0.60
1:B:325:GLU:HB3	1:B:327[B]:PHE:CZ	2.35	0.60
1:E:247:LEU:HD11	1:E:268:LEU:O	2.02	0.60
1:E:315:ILE:O	1:E:434:THR:HB	2.01	0.60
1:F:204:GLU:HB2	1:F:437:ILE:HD11	1.84	0.60
1:C:56:LEU:O	1:C:60:CYS:HB2	2.02	0.60
1:F:228:PHE:HB3	1:F:268:LEU:HD23	1.83	0.60
1:A:64:ILE:HD11	1:A:100:VAL:HG13	1.83	0.60
1:A:157:ARG:NH1	1:A:349:GLU:OE1	2.35	0.60
1:A:174:VAL:HG13	1:A:180:PHE:CB	2.31	0.60
1:C:383:PHE:HB3	1:C:442:GLU:OE2	2.02	0.60
1:D:121:ARG:O	1:D:125:GLU:HG3	2.02	0.59
1:D:29:ASP:HB3	1:D:32:LEU:HD13	1.85	0.59
1:C:349:GLU:O	1:C:353:GLN:HB2	2.02	0.59
1:A:205:GLN:O	1:A:209:GLN:HG2	2.02	0.59
1:B:270:ALA:H	1:B:274:GLN:HE21	1.50	0.59
1:A:273:GLU:HB2	1:A:327[B]:PHE:CE1	2.38	0.59
1:C:223:ILE:HG22	1:C:296:GLY:HA2	1.84	0.59
1:D:241:SER:C	1:D:244:ASP:HB2	2.21	0.59
1:E:321:PHE:CE2	1:E:323:LYS:HE3	2.32	0.59
1:C:176:MET:CE	1:C:474:ALA:HB2	2.33	0.58
1:D:234:MET:HG2	1:D:267:TYR:HD2	1.67	0.58
1:B:181:GLU:HB3	1:B:195:PHE:HB2	1.85	0.58
1:B:379:LEU:HB3	1:B:393:VAL:HB	1.85	0.58
1:D:176:MET:SD	1:D:474:ALA:HB2	2.43	0.58
1:C:7:LEU:HG	1:C:19:ILE:HD11	1.85	0.58
1:A:284:TRP:CE2	1:A:409:ARG:HD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HD12	1:A:431:CYS:HB3	1.85	0.58
1:A:393:VAL:HG13	1:A:429:THR:O	2.03	0.58
1:B:276:ILE:O	1:B:279:LEU:HB3	2.04	0.58
1:F:54:ASN:O	1:F:58:ASN:HB2	2.04	0.58
1:A:379:LEU:HB3	1:A:393:VAL:HB	1.85	0.57
1:C:199:VAL:HG12	1:C:464:LEU:CD1	2.34	0.57
1:F:177:VAL:HG13	1:F:199:VAL:HG21	1.86	0.57
1:C:204:GLU:HG3	1:C:433:THR:HB	1.86	0.57
1:E:284:TRP:CE2	1:E:409:ARG:HD2	2.39	0.57
1:A:243:PHE:CD1	1:A:243:PHE:N	2.70	0.57
1:B:407:ARG:HG2	1:B:407:ARG:NH1	2.20	0.57
1:A:33:VAL:O	1:A:37:VAL:HG23	2.04	0.57
1:B:446:THR:OG1	1:B:447:GLU:N	2.35	0.57
1:F:316:PHE:CE1	1:F:435:ARG:HG2	2.40	0.57
1:A:8:PHE:O	1:A:16:PRO:HG3	2.05	0.56
1:C:161:ASP:OD1	1:C:164:VAL:HG13	2.05	0.56
1:D:226:PRO:O	1:D:269:ILE:HD13	2.05	0.56
1:A:272:SER:HB2	1:A:327[B]:PHE:HE2	1.70	0.56
1:C:379:LEU:HB3	1:C:393:VAL:HB	1.86	0.56
1:F:231:LYS:HE2	1:F:235:GLN:HE21	1.69	0.56
1:B:441:LEU:HD22	1:B:450:ILE:HG12	1.87	0.56
1:C:53:LEU:HD22	1:C:110:ILE:HG23	1.87	0.56
1:C:91:THR:HG23	1:C:94:ALA:HB3	1.87	0.56
1:C:394:SER:O	1:C:428:ALA:HA	2.06	0.56
1:E:303:GLN:OE1	1:F:252:GLY:HA2	2.05	0.56
1:A:376:LYS:HE2	1:A:394:SER:HB2	1.87	0.56
1:F:231:LYS:HE2	1:F:235:GLN:HE22	1.68	0.56
1:B:358:PRO:HG2	1:B:382:TRP:HB3	1.88	0.56
1:E:276:ILE:HD12	1:E:327[B]:PHE:CE2	2.40	0.56
1:C:71:LYS:O	1:C:72:GLU:HG2	2.04	0.56
1:F:383:PHE:CE2	1:F:390:ARG:HB2	2.42	0.55
1:D:225:THR:HG21	1:D:272:SER:HB3	1.88	0.55
1:A:132:LEU:HA	1:A:135:ILE:HD12	1.87	0.55
1:D:33:VAL:O	1:D:37:VAL:HG23	2.06	0.55
1:D:358:PRO:HG2	1:D:382:TRP:HB3	1.89	0.55
1:E:137:ASN:HD21	1:E:399:THR:HB	1.71	0.55
1:C:172:ASP:HB3	1:C:176:MET:CE	2.36	0.55
1:A:186:ALA:HA	1:A:190:GLY:O	2.06	0.55
1:D:379:LEU:HB3	1:D:393:VAL:HB	1.89	0.55
1:A:271:THR:HG22	1:A:323:LYS:HZ2	1.70	0.55
1:F:176:MET:SD	1:F:474:ALA:HB2	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:PHE:CZ	1:F:435:ARG:NH1	2.75	0.55
1:A:328:VAL:HG21	1:A:344:MET:HE2	1.89	0.55
1:D:393:VAL:HG13	1:D:429:THR:O	2.07	0.55
1:E:418:ASP:OD2	1:E:418:ASP:N	2.37	0.55
1:A:61:SER:O	1:A:64:ILE:HG22	2.07	0.54
1:C:441:LEU:HD22	1:C:450:ILE:HD13	1.88	0.54
1:E:271:THR:OG1	1:E:273:GLU:HB3	2.07	0.54
1:F:382:TRP:O	1:F:384:PRO:HD3	2.08	0.54
1:B:360:HIS:HD2	1:B:360:HIS:O	1.91	0.54
1:C:417:MET:HG2	1:C:417:MET:O	2.08	0.54
1:F:4:ASP:HB2	1:F:404:ARG:NH2	2.23	0.54
1:F:103:ILE:O	1:F:106:VAL:HG22	2.07	0.54
1:B:215:LEU:HG	1:B:430:MET:HE1	1.90	0.54
1:F:273:GLU:HB2	1:F:327[B]:PHE:HE1	1.71	0.54
1:A:177:VAL:HG12	1:A:199:VAL:CG2	2.33	0.54
1:B:273:GLU:N	1:B:327[B]:PHE:CZ	2.76	0.54
1:B:274:GLN:HB2	1:B:275:PRO:HD3	1.90	0.54
1:C:223:ILE:CD1	1:D:195:PHE:HD1	2.20	0.54
1:E:399:THR:CG2	1:E:400:ASP:N	2.49	0.54
1:F:245:GLU:HG2	1:F:246:GLU:H	1.72	0.54
1:F:348:ALA:HA	1:F:430:MET:HE1	1.88	0.54
1:A:426:LEU:N	1:A:426:LEU:HD12	2.23	0.54
1:C:325:GLU:HB2	1:C:327[B]:PHE:CE2	2.42	0.54
1:B:449:GLY:HA2	1:B:470:PHE:CE2	2.43	0.54
1:A:228:PHE:HB3	1:A:268:LEU:HD23	1.88	0.54
1:C:222:PRO:HG3	1:D:202:PHE:CE2	2.43	0.54
1:C:71:LYS:C	1:C:72:GLU:HG2	2.28	0.54
1:F:471:VAL:O	1:F:471:VAL:HG12	2.07	0.54
1:C:276:ILE:O	1:C:279:LEU:CB	2.56	0.53
1:E:276:ILE:CD1	1:E:327[B]:PHE:CD2	2.90	0.53
1:A:204:GLU:HB2	1:A:437:ILE:CD1	2.38	0.53
1:A:215:LEU:HD11	1:A:430:MET:HE2	1.88	0.53
1:D:244:ASP:HB3	1:D:246:GLU:HG3	1.90	0.53
1:E:205:GLN:O	1:E:209:GLN:HG2	2.07	0.53
1:C:168:TYR:N	1:C:445:GLN:HE22	1.98	0.53
1:D:290:LEU:HD23	1:D:292:ILE:HG13	1.89	0.53
1:F:205:GLN:O	1:F:209:GLN:HG2	2.08	0.53
1:B:461:PRO:HG2	1:B:464:LEU:HB2	1.91	0.53
1:C:157:ARG:NH1	1:C:349:GLU:OE2	2.42	0.53
1:D:276:ILE:HD13	1:D:327[A]:PHE:CD2	2.44	0.53
1:B:227:PHE:O	1:B:269:ILE:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:GLU:HA	1:D:327[A]:PHE:CE1	2.44	0.53
1:E:325:GLU:HG2	1:E:429:THR:HA	1.91	0.53
1:F:91:THR:O	1:F:92:ALA:HB3	2.08	0.53
1:C:172:ASP:HB3	1:C:176:MET:HE2	1.90	0.53
1:B:95:LEU:HD12	1:B:96:ALA:N	2.24	0.53
1:B:327[A]:PHE:HZ	1:B:425:MET:HE3	1.74	0.53
1:C:376:LYS:HE2	1:C:394:SER:OG	2.09	0.53
1:F:54:ASN:OD1	1:F:114:ILE:HD13	2.08	0.53
1:A:271:THR:HG22	1:A:323:LYS:HZ1	1.73	0.53
1:C:205:GLN:O	1:C:209:GLN:HG2	2.10	0.52
1:C:251:ILE:HD11	1:D:251:ILE:CD1	2.39	0.52
1:E:393:VAL:HG13	1:E:429:THR:O	2.09	0.52
1:B:272:SER:HB3	1:B:327[B]:PHE:HE2	1.74	0.52
1:F:169:SER:O	1:F:173:LEU:HD12	2.10	0.52
1:C:233:VAL:O	1:C:237:VAL:HG23	2.08	0.52
1:C:303:GLN:OE1	1:D:252:GLY:HA2	2.10	0.52
1:E:8:PHE:O	1:E:16:PRO:HG3	2.08	0.52
1:B:159:TRP:CE2	1:B:353:GLN:HG3	2.44	0.52
1:D:285:LEU:HD12	1:D:423:VAL:HG11	1.92	0.52
1:B:159:TRP:CZ2	1:B:353:GLN:HG3	2.45	0.52
1:F:7:LEU:HG	1:F:19:ILE:HD11	1.92	0.52
1:A:2:VAL:CG2	1:A:132:LEU:HG	2.40	0.52
1:A:328:VAL:HB	1:A:344:MET:CE	2.40	0.52
1:D:77:ASP:CB	1:D:99:LYS:HD2	2.40	0.52
1:E:209:GLN:OE1	1:F:205:GLN:HB3	2.10	0.52
1:A:316:PHE:CE1	1:A:435:ARG:HG2	2.45	0.52
1:C:215:LEU:O	1:C:220:TYR:HB2	2.10	0.52
1:D:452:VAL:HB	1:D:465:GLN:O	2.10	0.52
1:F:98:LEU:HG	1:F:102:GLN:OE1	2.10	0.51
1:F:249:LYS:HD3	1:F:267:TYR:HE1	1.75	0.51
1:A:100:VAL:HG12	1:A:101:SER:N	2.26	0.51
1:F:285:LEU:HD23	1:F:423:VAL:HG11	1.91	0.51
1:A:272:SER:HB2	1:A:327[B]:PHE:CE2	2.45	0.51
1:B:218:ARG:CG	1:B:218:ARG:NH1	2.65	0.51
1:C:159:TRP:CE2	1:C:353:GLN:HG3	2.45	0.51
1:C:184:LYS:HD3	1:D:279:LEU:HD12	1.93	0.51
1:E:228:PHE:O	1:E:228:PHE:CD1	2.60	0.51
1:C:79:SER:O	1:C:102:GLN:OE1	2.28	0.51
1:C:179:GLY:HA2	1:C:197:LYS:O	2.10	0.51
1:C:333:HIS:HE2	1:C:421:GLU:CD	2.13	0.51
1:F:173:LEU:HD22	1:F:450:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.76	0.51
1:A:457:LYS:HG2	1:A:465:GLN:O	2.10	0.51
1:B:98:LEU:HD22	1:B:102:GLN:OE1	2.11	0.51
1:C:224:TYR:HB3	1:D:196:LEU:HB3	1.92	0.51
1:E:327[A]:PHE:HZ	1:E:425:MET:CE	2.23	0.51
1:A:177:VAL:HG12	1:A:177:VAL:O	2.10	0.51
1:A:301:PHE:HA	1:A:319:HIS:O	2.11	0.51
1:C:269:ILE:HG21	1:C:275:PRO:CG	2.41	0.51
1:A:269:ILE:O	1:A:269:ILE:HG13	2.11	0.51
1:A:301:PHE:HE2	1:A:320:GLN:HE21	1.58	0.51
1:C:249:LYS:HG2	1:C:267:TYR:CE1	2.45	0.51
1:C:270:ALA:O	1:C:300:CYS:HB3	2.11	0.51
1:C:327[A]:PHE:CE2	1:C:329:TYR:CE1	2.99	0.51
1:D:407:ARG:HD3	1:D:409:ARG:NH2	2.26	0.51
1:F:97:ASN:O	1:F:98:LEU:HD12	2.11	0.51
1:A:207:LEU:HD11	1:A:436:THR:CG2	2.42	0.51
1:C:70:LYS:HB3	1:C:72:GLU:OE1	2.11	0.51
1:D:210:TYR:CE2	1:D:355:LEU:HD21	2.46	0.51
1:B:272:SER:O	1:B:327[B]:PHE:CE2	2.63	0.50
1:C:466:GLU:O	1:C:467:LEU:HB2	2.12	0.50
1:C:203:LEU:CD2	1:C:437:ILE:HD12	2.42	0.50
1:B:445:GLN:O	1:B:445:GLN:HG3	2.11	0.50
1:C:272:SER:C	1:C:275:PRO:HD2	2.32	0.50
1:C:286:ARG:O	1:C:289:ASP:HB2	2.11	0.50
1:B:8:PHE:CE2	1:B:36:LEU:HD23	2.46	0.50
1:E:223:ILE:HD13	1:F:195:PHE:HD2	1.76	0.50
1:B:284:TRP:CE2	1:B:409:ARG:HD2	2.47	0.50
1:E:358:PRO:HD2	1:E:443:ASN:ND2	2.27	0.50
1:A:36:LEU:HD12	1:A:127:GLU:HB3	1.94	0.50
1:C:276:ILE:O	1:C:279:LEU:HB3	2.11	0.50
1:B:108:LEU:O	1:B:108:LEU:HG	2.10	0.50
1:D:59:LEU:HD21	1:D:95:LEU:HD13	1.93	0.50
1:D:181:GLU:O	1:D:181:GLU:HG3	2.12	0.50
1:E:27:PHE:CD1	1:E:147:ASN:HB2	2.47	0.50
1:E:236:GLU:HG2	1:E:281:ARG:NH1	2.27	0.50
1:F:159:TRP:CZ2	1:F:353:GLN:HG2	2.46	0.50
1:A:142:SER:OG	1:A:375:LYS:HE3	2.11	0.49
1:D:360:HIS:HE1	1:D:380:GLU:OE2	1.95	0.49
1:C:449:GLY:O	1:C:470:PHE:HE2	1.95	0.49
1:D:276:ILE:O	1:D:279:LEU:HB3	2.12	0.49
1:F:328:VAL:HG11	1:F:340:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:379:LEU:HD23	1:F:379:LEU:C	2.32	0.49
1:B:82:GLU:CB	1:B:102:GLN:NE2	2.74	0.49
1:E:101:SER:O	1:E:105:LYS:HB2	2.12	0.49
1:B:215:LEU:HD11	1:B:430:MET:HE2	1.94	0.49
1:D:407:ARG:O	1:D:409:ARG:HG3	2.12	0.49
1:A:46:CYS:SG	1:A:120:GLU:OE1	2.69	0.49
1:B:323:LYS:HZ1	1:B:429:THR:HG21	1.76	0.49
1:C:176:MET:HE1	1:C:474:ALA:HB2	1.94	0.49
1:C:449:GLY:HA2	1:C:470:PHE:CD2	2.47	0.49
1:E:293:LYS:HD3	1:E:340:MET:CE	2.43	0.49
1:E:327[A]:PHE:HZ	1:E:425:MET:HE2	1.78	0.49
1:C:215:LEU:HD21	1:C:430:MET:SD	2.53	0.49
1:C:225:THR:CG2	1:C:275:PRO:HG2	2.39	0.49
1:E:276:ILE:CD1	1:E:327[B]:PHE:HD2	2.26	0.49
1:A:273:GLU:HB2	1:A:327[B]:PHE:HE1	1.77	0.49
1:B:327[B]:PHE:CE1	1:B:427:ASN:HB2	2.47	0.49
1:D:140:HIS:CG	1:D:141:PRO:HD2	2.47	0.49
1:F:151:VAL:HG23	1:F:152:ASP:N	2.28	0.49
1:A:22:THR:HG22	1:A:23:GLN:N	2.28	0.49
1:A:325:GLU:CG	1:A:429:THR:HG22	2.39	0.49
1:C:47:ARG:NH1	1:C:47:ARG:HG3	2.28	0.49
1:C:91:THR:OG1	1:C:92:ALA:N	2.45	0.49
1:D:316:PHE:CE2	1:D:390:ARG:HD2	2.47	0.49
1:F:379:LEU:HB3	1:F:393:VAL:HB	1.95	0.48
1:A:300:CYS:SG	1:A:323:LYS:HE3	2.53	0.48
1:B:376:LYS:HE2	1:B:394:SER:HB2	1.95	0.48
1:B:64:ILE:HG13	1:B:103:ILE:CG2	2.43	0.48
1:C:140:HIS:CG	1:C:141:PRO:HD2	2.49	0.48
1:A:86:SER:HB3	1:A:89:ASP:HB2	1.95	0.48
1:A:98:LEU:O	1:A:102:GLN:HB2	2.13	0.48
1:F:276:ILE:HD12	1:F:327[B]:PHE:CD2	2.48	0.48
1:B:57:LYS:HD2	1:B:111:ASP:OD2	2.13	0.48
1:D:64:ILE:HD11	1:D:103:ILE:CG2	2.44	0.48
1:D:297:LEU:HD13	1:D:324:ILE:HD13	1.96	0.48
1:D:300:CYS:O	1:D:320:GLN:HA	2.13	0.48
1:D:228:PHE:HB3	1:D:268:LEU:HD23	1.95	0.48
1:B:236:GLU:OE2	1:B:281:ARG:NH1	2.47	0.48
1:D:233:VAL:HG23	1:D:281:ARG:NH1	2.28	0.48
1:D:406:LEU:HB2	1:D:408:ILE:HD12	1.96	0.48
1:E:140:HIS:CG	1:E:141:PRO:HD2	2.48	0.48
1:E:176:MET:HE1	1:E:470:PHE:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:GLU:C	1:F:185:GLY:H	2.17	0.48
1:E:276:ILE:O	1:E:279:LEU:CB	2.52	0.47
1:E:379:LEU:HB3	1:E:393:VAL:HB	1.96	0.47
1:C:327[A]:PHE:HE2	1:C:329:TYR:CE1	2.32	0.47
1:C:178:ASP:HB2	1:C:471:VAL:CG2	2.44	0.47
1:E:449:GLY:HA3	1:E:467:LEU:HD21	1.96	0.47
1:F:249:LYS:HD3	1:F:267:TYR:CE1	2.49	0.47
1:D:140:HIS:ND1	1:D:142:SER:OG	2.38	0.47
1:E:36:LEU:C	1:E:36:LEU:HD23	2.34	0.47
1:A:26:ARG:O	1:A:27:PHE:HB2	2.14	0.47
1:B:121:ARG:O	1:B:125:GLU:HG3	2.13	0.47
1:C:249:LYS:HG2	1:C:267:TYR:HE1	1.79	0.47
1:A:212:LEU:HD22	1:A:222:PRO:HB3	1.97	0.47
1:B:272:SER:C	1:B:327[B]:PHE:CE2	2.88	0.47
1:C:25:LYS:HB3	1:C:145:ILE:HD12	1.96	0.47
1:C:100:VAL:HG12	1:C:100:VAL:O	2.14	0.47
1:C:223:ILE:CD1	1:D:195:PHE:CD1	2.98	0.47
1:D:159:TRP:CE2	1:D:353:GLN:CG	2.91	0.47
1:E:419:LYS:HB2	1:E:419:LYS:HE3	1.69	0.47
1:A:300:CYS:HB2	1:A:321:PHE:CE2	2.50	0.47
1:B:213:ARG:HH11	1:B:213:ARG:HG3	1.80	0.47
1:C:335:ASN:O	1:C:339:GLU:HG3	2.14	0.47
1:E:90:LEU:HD23	1:E:91:THR:N	2.29	0.47
1:E:357:ILE:HG23	1:E:443:ASN:ND2	2.30	0.47
1:C:225:THR:HG23	1:C:275:PRO:HB2	1.96	0.47
1:D:164:VAL:HG22	1:D:165:ARG:N	2.30	0.47
1:A:321:PHE:HE2	1:A:323:LYS:HE2	1.80	0.47
1:B:36:LEU:CD1	1:B:128:ARG:HG3	2.45	0.47
1:C:47:ARG:HG3	1:C:47:ARG:HH11	1.79	0.47
1:C:271:THR:C	1:C:273:GLU:H	2.19	0.47
1:D:220:TYR:HE1	1:D:326:GLN:HB3	1.79	0.47
1:B:325:GLU:HB2	1:B:327[B]:PHE:CE2	2.50	0.47
1:C:301:PHE:HA	1:C:319:HIS:O	2.15	0.47
1:C:384:PRO:CG	1:C:443:ASN:OD1	2.64	0.47
1:B:176:MET:HB3	1:B:176:MET:HE2	1.70	0.46
1:D:234:MET:HG2	1:D:267:TYR:CD2	2.49	0.46
1:E:57:LYS:HA	1:E:60:CYS:HB2	1.97	0.46
1:A:133:ARG:HE	1:A:240:LEU:HD21	1.80	0.46
1:E:349:GLU:HG3	1:E:361:ILE:HD11	1.97	0.46
1:C:97:ASN:O	1:C:98:LEU:CB	2.63	0.46
1:D:63:THR:HG22	1:D:64:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:THR:OG1	1:D:95:LEU:HD11	2.15	0.46
1:E:2:VAL:CG2	1:E:132:LEU:HG	2.44	0.46
1:F:337:SER:HB3	1:F:424:HIS:HD2	1.81	0.46
1:B:64:ILE:HG13	1:B:103:ILE:HG21	1.97	0.46
1:C:269:ILE:HG21	1:C:275:PRO:HG3	1.97	0.46
1:E:63:THR:O	1:E:63:THR:HG22	2.14	0.46
1:E:210:TYR:HD2	1:E:355:LEU:HD21	1.81	0.46
1:F:81:PRO:O	1:F:102:GLN:HG2	2.15	0.46
1:F:269:ILE:HG21	1:F:275:PRO:HG3	1.97	0.46
1:D:315:ILE:HG22	1:D:315:ILE:O	2.16	0.46
1:A:100:VAL:C	1:A:102:GLN:N	2.68	0.46
1:B:123:LYS:O	1:B:123:LYS:HG2	2.15	0.46
1:B:215:LEU:HD21	1:B:430:MET:SD	2.56	0.46
1:B:27:PHE:O	1:B:28:LYS:HD3	2.16	0.46
1:C:164:VAL:O	1:C:165:ARG:HD2	2.16	0.46
1:C:232:GLU:O	1:C:235:GLN:HG2	2.15	0.46
1:E:363:ASN:HA	1:E:377:LEU:HD23	1.96	0.46
1:A:276:ILE:HD13	1:A:327[B]:PHE:CD2	2.51	0.46
1:C:64:ILE:CG1	1:C:100:VAL:HG13	2.37	0.46
1:C:91:THR:HG23	1:C:94:ALA:CB	2.45	0.46
1:C:332:PRO:HA	1:C:424:HIS:CE1	2.51	0.46
1:C:416:MET:O	1:C:417:MET:CB	2.59	0.46
1:C:471:VAL:HG23	1:C:472:LYS:HG3	1.98	0.46
1:F:273:GLU:HA	1:F:327[B]:PHE:CE1	2.51	0.46
1:A:23:GLN:NE2	1:A:135:ILE:HA	2.27	0.46
1:A:286:ARG:HB3	1:A:288:GLU:CG	2.46	0.45
1:B:153:ASN:HB3	1:B:362:VAL:CG1	2.46	0.45
1:C:251:ILE:HD11	1:D:251:ILE:HD11	1.98	0.45
1:D:92:ALA:O	1:D:95:LEU:HB3	2.16	0.45
1:D:276:ILE:O	1:D:279:LEU:CB	2.64	0.45
1:F:70:LYS:HG3	1:F:70:LYS:O	2.16	0.45
1:C:472:LYS:HB3	1:C:473:PRO:CD	2.43	0.45
1:D:284:TRP:HE3	1:D:411:GLY:O	1.99	0.45
1:E:159:TRP:CZ2	1:E:353:GLN:HG2	2.51	0.45
1:A:240:LEU:HD12	1:A:371:HIS:ND1	2.32	0.45
1:B:235:GLN:HA	1:B:243:PHE:HZ	1.80	0.45
1:D:274:GLN:HB2	1:D:275:PRO:HD3	1.98	0.45
1:F:140:HIS:CG	1:F:141:PRO:HD2	2.51	0.45
1:A:114:ILE:O	1:A:115:LEU:HD23	2.17	0.45
1:A:284:TRP:CD2	1:A:409:ARG:HD2	2.51	0.45
1:C:284:TRP:CE2	1:C:409:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ILE:HD12	1:D:357:ILE:N	2.30	0.45
1:E:286:ARG:NH1	1:E:288:GLU:OE2	2.47	0.45
1:B:345:ILE:O	1:B:349:GLU:HG3	2.17	0.45
1:C:273:GLU:CB	1:C:327[B]:PHE:HE1	2.29	0.45
1:F:57:LYS:HA	1:F:60:CYS:HB3	1.99	0.45
1:A:177:VAL:HG11	1:A:199:VAL:HG21	1.95	0.45
1:B:326:GLN:O	1:B:327[B]:PHE:CD1	2.70	0.45
1:C:452:VAL:HG12	1:C:457:LYS:HG3	1.98	0.45
1:D:40:ASP:OD1	1:D:128:ARG:NH1	2.49	0.45
1:F:29:ASP:HB3	1:F:32:LEU:CD1	2.44	0.45
1:A:248:TYR:HB2	1:A:268:LEU:HB2	1.99	0.45
1:B:49:ARG:HE	1:B:53:LEU:HD11	1.82	0.45
1:C:80:VAL:HG13	1:C:106:VAL:HG23	1.99	0.45
1:E:202:PHE:CE2	1:F:222:PRO:HG3	2.51	0.45
1:B:58:ASN:HB3	1:B:62:LYS:HE3	1.99	0.44
1:C:62:LYS:HB2	1:C:62:LYS:HE3	1.79	0.44
1:C:122:ILE:HG22	1:C:123:LYS:N	2.31	0.44
1:D:203:LEU:O	1:D:206:ALA:HB3	2.17	0.44
1:D:280:HIS:O	1:D:283:GLU:HG2	2.17	0.44
1:F:17:ALA:O	1:F:21:GLU:HG3	2.17	0.44
1:B:180:PHE:CZ	1:B:182:GLY:HA3	2.52	0.44
1:B:360:HIS:O	1:B:360:HIS:CD2	2.70	0.44
1:E:210:TYR:CD2	1:E:355:LEU:HD21	2.53	0.44
1:E:227:PHE:HE1	1:E:298:SER:HA	1.83	0.44
1:E:342:GLU:HA	1:E:345:ILE:HG22	1.99	0.44
1:A:169:SER:O	1:A:173:LEU:HG	2.18	0.44
1:E:144:PRO:HG2	1:E:365:VAL:HA	1.99	0.44
1:F:91:THR:O	1:F:92:ALA:CB	2.65	0.44
1:A:100:VAL:CG1	1:A:101:SER:N	2.81	0.44
1:A:324:ILE:CD1	1:A:431:CYS:HB3	2.48	0.44
1:B:157:ARG:CG	1:B:157:ARG:NH1	2.70	0.44
1:C:166:LYS:HG3	1:C:384:PRO:HB3	1.99	0.44
1:E:272:SER:HB3	1:E:298:SER:HB3	1.99	0.44
1:B:328:VAL:HG11	1:B:340:MET:HG2	1.98	0.44
1:D:341:PHE:CE2	1:D:375:LYS:HD3	2.52	0.44
1:F:53:LEU:HD23	1:F:53:LEU:HA	1.85	0.44
1:F:464:LEU:HD23	1:F:464:LEU:HA	1.80	0.44
1:A:450:ILE:O	1:A:467:LEU:HD12	2.17	0.44
1:B:191:SER:O	1:B:192:ARG:HB2	2.17	0.44
1:B:199:VAL:HG23	1:B:200:LEU:N	2.32	0.44
1:B:272:SER:C	1:B:327[B]:PHE:CZ	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:HB2	1:B:327[B]:PHE:CZ	2.52	0.44
1:B:426:LEU:HD12	1:B:426:LEU:N	2.32	0.44
1:C:142:SER:OG	1:C:375:LYS:HE3	2.17	0.44
1:D:148:ASP:O	1:D:152:ASP:HB2	2.17	0.44
1:E:63:THR:O	1:E:63:THR:CG2	2.64	0.44
1:A:59:LEU:HD23	1:A:59:LEU:O	2.17	0.44
1:E:195:PHE:CE2	1:F:279:LEU:HD13	2.53	0.44
1:F:337:SER:CB	1:F:424:HIS:HD2	2.30	0.44
1:B:47:ARG:HB2	1:B:121:ARG:NH1	2.33	0.44
1:B:67:LYS:HB3	1:B:100:VAL:CG2	2.48	0.44
1:E:225:THR:HG21	1:E:272:SER:HB3	1.96	0.44
1:E:229:MET:SD	1:E:274:GLN:HB3	2.57	0.44
1:E:276:ILE:HD13	1:E:327[B]:PHE:HD2	1.82	0.44
1:A:452:VAL:HA	1:A:453:PRO:HD3	1.87	0.44
1:B:449:GLY:HA2	1:B:470:PHE:CZ	2.53	0.44
1:E:64:ILE:HG22	1:E:64:ILE:O	2.18	0.44
1:F:85:LEU:HD12	1:F:85:LEU:H	1.83	0.44
1:D:67:LYS:HE2	1:D:100:VAL:HG23	1.98	0.43
1:E:85:LEU:HD12	1:E:85:LEU:O	2.18	0.43
1:F:72:GLU:HG2	1:F:73:PRO:N	2.32	0.43
1:F:98:LEU:HD23	1:F:102:GLN:HB3	2.00	0.43
1:F:176:MET:HB3	1:F:176:MET:HE2	1.78	0.43
1:A:286:ARG:HB2	1:A:289:ASP:OD1	2.18	0.43
1:A:399:THR:OG1	1:A:400:ASP:N	2.50	0.43
1:E:472:LYS:HB3	1:E:473:PRO:CD	2.42	0.43
1:F:286:ARG:HA	1:F:287:PRO:HD3	1.78	0.43
1:C:181:GLU:HB3	1:C:195:PHE:HB2	2.01	0.43
1:A:38:LYS:HE2	1:A:38:LYS:HB3	1.77	0.43
1:A:166:LYS:HD2	1:A:384:PRO:CB	2.48	0.43
1:E:179:GLY:HA3	1:E:200:LEU:HD12	2.01	0.43
1:E:273:GLU:HB2	1:E:327[B]:PHE:CZ	2.54	0.43
1:B:36:LEU:HD12	1:B:128:ARG:HG3	2.01	0.43
1:B:372:ALA:O	1:B:398:CYS:HA	2.19	0.43
1:D:233:VAL:O	1:D:237:VAL:HG23	2.18	0.43
1:D:402:GLN:HE21	1:D:402:GLN:HB2	1.64	0.43
1:A:2:VAL:HG22	1:A:132:LEU:HG	1.99	0.43
1:D:229:MET:O	1:D:266:LYS:HB3	2.19	0.43
1:F:176:MET:HE1	1:F:470:PHE:CE2	2.54	0.43
1:B:237:VAL:HG11	1:B:277:ALA:HB3	2.01	0.43
1:C:229:MET:SD	1:D:188:VAL:HG13	2.59	0.43
1:C:467:LEU:HG	1:C:468:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ALA:O	1:D:351:PHE:HB3	2.18	0.43
1:E:112:GLU:O	1:E:112:GLU:HG2	2.18	0.43
1:F:252:GLY:C	1:F:263:TYR:HD1	2.21	0.43
1:D:36:LEU:HD11	1:D:132:LEU:CD1	2.49	0.43
1:D:274:GLN:CB	1:D:275:PRO:HD3	2.49	0.43
1:D:394:SER:O	1:D:428:ALA:HA	2.19	0.43
1:E:203:LEU:O	1:E:206:ALA:HB3	2.19	0.43
1:F:301:PHE:HA	1:F:319:HIS:O	2.19	0.43
1:A:7:LEU:HB3	1:A:19:ILE:HD11	2.00	0.43
1:A:383:PHE:HB3	1:A:442:GLU:OE1	2.18	0.43
1:B:131:ASN:O	1:B:135:ILE:HG13	2.19	0.43
1:F:9:ARG:HB2	1:F:12:LYS:HB2	2.01	0.43
1:C:56:LEU:HD13	1:C:90:LEU:HD13	2.01	0.42
1:C:98:LEU:CA	1:C:102:GLN:HE21	2.32	0.42
1:A:137:ASN:HB2	1:A:401:TYR:CD1	2.54	0.42
1:C:173:LEU:HD13	1:C:441:LEU:HB3	2.01	0.42
1:C:451:THR:O	1:C:453:PRO:HD3	2.19	0.42
1:F:70:LYS:HB2	1:F:70:LYS:HE2	1.70	0.42
1:F:474:ALA:HA	1:F:475:PRO:HD3	1.94	0.42
1:C:174:VAL:HG13	1:C:180:PHE:CB	2.49	0.42
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.51	0.42
1:B:67:LYS:NZ	1:B:96:ALA:HA	2.35	0.42
1:B:220:TYR:CZ	1:B:326:GLN:NE2	2.87	0.42
1:B:233:VAL:O	1:B:237:VAL:HG23	2.20	0.42
1:D:406:LEU:O	1:D:407:ARG:HB2	2.19	0.42
1:F:150:ASP:HB2	1:F:151:VAL:H	1.59	0.42
1:B:276:ILE:CD1	1:B:327[B]:PHE:CD2	2.81	0.42
1:C:315:ILE:HG13	1:C:438:CYS:SG	2.60	0.42
1:D:372:ALA:HA	1:D:401:TYR:CD2	2.55	0.42
1:E:36:LEU:HD11	1:E:132:LEU:CD1	2.46	0.42
1:F:355:LEU:HB2	1:F:357:ILE:CD1	2.49	0.42
1:A:145:ILE:HA	1:A:366:SER:OG	2.19	0.42
1:B:321:PHE:HE2	1:B:323:LYS:HD2	1.85	0.42
1:C:220:TYR:CD1	1:C:293:LYS:HB3	2.54	0.42
1:E:248:TYR:CE2	1:E:303:GLN:HA	2.55	0.42
1:E:299:THR:HG21	1:F:227:PHE:CE2	2.55	0.42
1:F:271:THR:HA	1:F:300:CYS:SG	2.60	0.42
1:F:394:SER:O	1:F:428:ALA:HA	2.19	0.42
1:A:412:GLN:O	1:A:412:GLN:CG	2.49	0.42
1:C:449:GLY:O	1:C:470:PHE:CE2	2.72	0.42
1:D:210:TYR:CD2	1:D:355:LEU:HD21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:GLU:CA	1:E:327[B]:PHE:CZ	3.03	0.42
1:C:98:LEU:HA	1:C:102:GLN:NE2	2.34	0.42
1:D:464:LEU:HD22	1:D:468:ILE:HG12	2.01	0.42
1:A:95:LEU:O	1:A:103:ILE:HD11	2.19	0.42
1:B:333:HIS:O	1:B:334:ASP:HB2	2.19	0.42
1:B:379:LEU:C	1:B:379:LEU:HD23	2.39	0.42
1:D:153:ASN:OD1	1:D:365:VAL:HG13	2.19	0.42
1:D:173:LEU:O	1:D:177:VAL:HG22	2.20	0.42
1:D:301:PHE:HA	1:D:319:HIS:O	2.19	0.42
1:F:110:ILE:O	1:F:113:ALA:HB3	2.20	0.42
1:A:172:ASP:O	1:A:176:MET:HG3	2.20	0.42
1:A:207:LEU:HD11	1:A:436:THR:HG22	2.01	0.42
1:C:7:LEU:CG	1:C:19:ILE:HD11	2.48	0.42
1:C:272:SER:HB3	1:C:298:SER:OG	2.20	0.42
1:D:85:LEU:HB2	1:D:89:ASP:OD1	2.20	0.42
1:D:87:PHE:HE1	1:D:110:ILE:HG13	1.85	0.42
1:E:286:ARG:HA	1:E:287:PRO:HD3	1.85	0.42
1:F:169:SER:HB3	1:F:171:VAL:HG22	2.02	0.42
1:F:337:SER:HB3	1:F:424:HIS:CD2	2.54	0.42
1:A:53:LEU:HD21	1:A:113:ALA:HB3	2.02	0.41
1:A:101:SER:HA	1:A:104:LYS:HB2	2.01	0.41
1:B:273:GLU:CA	1:B:327[B]:PHE:CZ	3.03	0.41
1:C:370:ASN:ND2	1:C:370:ASN:H	2.17	0.41
1:C:441:LEU:HD22	1:C:450:ILE:CD1	2.50	0.41
1:D:180:PHE:HD2	1:D:315:ILE:HD11	1.85	0.41
1:D:184:LYS:HD2	1:D:184:LYS:HA	1.84	0.41
1:B:325:GLU:OE1	1:B:429:THR:HG22	2.19	0.41
1:B:472:LYS:HG3	1:B:473:PRO:N	2.34	0.41
1:C:47:ARG:HD2	1:C:47:ARG:HA	1.88	0.41
1:E:158:ILE:HD13	1:E:360:HIS:HB3	2.02	0.41
1:E:357:ILE:HG23	1:E:443:ASN:HD22	1.84	0.41
1:F:68:MET:HE1	1:F:100:VAL:HG13	2.02	0.41
1:F:288:GLU:OE1	1:F:288:GLU:N	2.45	0.41
1:C:342:GLU:HA	1:C:345:ILE:HG22	2.01	0.41
1:C:363:ASN:HA	1:C:377:LEU:HD23	2.02	0.41
1:D:60:CYS:O	1:D:64:ILE:HG13	2.20	0.41
1:E:213:ARG:NE	1:F:461:PRO:HB3	2.34	0.41
1:E:326:GLN:NE2	1:E:430:MET:HE3	2.35	0.41
1:E:344:MET:HE2	1:E:395:CYS:SG	2.60	0.41
1:A:203:LEU:O	1:A:206:ALA:HB3	2.20	0.41
1:D:133:ARG:NH2	1:D:240:LEU:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ASN:OD1	1:D:364:ILE:HA	2.20	0.41
1:D:237:VAL:HG12	1:D:238:ALA:N	2.31	0.41
1:E:98:LEU:HD12	1:E:98:LEU:HA	1.78	0.41
1:E:171:VAL:HG13	1:E:313:ARG:HA	2.02	0.41
1:E:285:LEU:HD13	1:E:292:ILE:HD12	2.02	0.41
1:B:233:VAL:HG11	1:B:278:ALA:HB1	2.01	0.41
1:B:471:VAL:HG12	1:B:471:VAL:O	2.21	0.41
1:C:84:VAL:O	1:C:90:LEU:HB2	2.21	0.41
1:D:132:LEU:O	1:D:132:LEU:HG	2.21	0.41
1:F:272:SER:O	1:F:276:ILE:HG13	2.21	0.41
1:F:300:CYS:HB2	1:F:321:PHE:CE2	2.55	0.41
1:A:46:CYS:SG	1:A:120:GLU:HG2	2.60	0.41
1:A:212:LEU:HD11	1:A:297:LEU:HD22	2.01	0.41
1:C:166:LYS:HG3	1:C:384:PRO:CB	2.50	0.41
1:E:204:GLU:HG3	1:E:433:THR:HB	2.03	0.41
1:E:236:GLU:HB3	1:E:406:LEU:CD2	2.48	0.41
1:A:227:PHE:H	1:B:320:GLN:NE2	2.10	0.41
1:B:327[B]:PHE:HE1	1:B:427:ASN:HB2	1.85	0.41
1:C:102:GLN:H	1:C:102:GLN:HG2	1.77	0.41
1:D:64:ILE:HD11	1:D:103:ILE:HG21	2.02	0.41
1:F:269:ILE:HG21	1:F:275:PRO:CG	2.51	0.41
1:F:471:VAL:O	1:F:471:VAL:CG1	2.68	0.41
1:A:188:VAL:CG1	1:B:229:MET:HG2	2.50	0.41
1:A:249:LYS:O	1:B:250:VAL:HA	2.21	0.41
1:A:468:ILE:HA	1:A:469:PRO:HD3	1.86	0.41
1:B:272:SER:HB3	1:B:327[B]:PHE:CE2	2.55	0.41
1:B:393:VAL:HG13	1:B:429:THR:O	2.20	0.41
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.85	0.41
1:C:273:GLU:CG	1:C:327[B]:PHE:HE1	2.33	0.41
1:F:348:ALA:HA	1:F:430:MET:HE2	2.01	0.41
1:A:188:VAL:HG13	1:B:229:MET:HG2	2.01	0.41
1:A:213:ARG:HG3	1:A:213:ARG:NH1	2.35	0.41
1:B:90:LEU:HD21	1:B:95:LEU:HD23	2.03	0.41
1:C:203:LEU:HD23	1:C:437:ILE:HG23	2.02	0.41
1:C:247:LEU:HD22	1:C:270:ALA:HB2	2.03	0.41
1:C:360:HIS:CD2	1:C:389:PHE:CE2	3.08	0.41
1:D:20:ARG:NH1	1:D:34:ASP:OD1	2.54	0.41
1:D:91:THR:C	1:D:93:ASP:N	2.73	0.41
1:D:107:ARG:O	1:D:107:ARG:HG2	2.20	0.41
1:E:7:LEU:HD12	1:E:7:LEU:HA	1.74	0.41
1:E:348:ALA:HA	1:E:430:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:VAL:O	1:E:471:VAL:HG12	2.21	0.41
1:F:212:LEU:HD11	1:F:297:LEU:HD22	2.03	0.41
1:F:297:LEU:HD13	1:F:324:ILE:CD1	2.51	0.41
1:F:357:ILE:HA	1:F:358:PRO:HD2	1.89	0.41
1:A:29:ASP:HA	1:A:30:PRO:HD2	1.90	0.41
1:A:272:SER:C	1:A:275:PRO:HD2	2.41	0.41
1:A:287:PRO:HD3	1:A:411:GLY:HA2	2.02	0.41
1:D:315:ILE:CG2	1:D:434:THR:HB	2.47	0.41
1:E:327[B]:PHE:CD1	1:E:427:ASN:HB2	2.55	0.41
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.81	0.40
1:B:282:ASP:OD2	1:B:407:ARG:HD2	2.21	0.40
1:C:148:ASP:O	1:C:149:GLU:HG2	2.21	0.40
1:C:299:THR:HG21	1:D:227:PHE:CD2	2.56	0.40
1:D:157:ARG:O	1:D:360:HIS:HB2	2.21	0.40
1:F:58:ASN:O	1:F:62:LYS:HB2	2.21	0.40
1:F:237:VAL:HG12	1:F:237:VAL:O	2.19	0.40
1:B:472:LYS:HB2	1:B:472:LYS:HE2	1.88	0.40
1:C:140:HIS:HA	1:C:141:PRO:HD3	1.98	0.40
1:D:63:THR:CG2	1:D:95:LEU:HD11	2.47	0.40
1:E:379:LEU:C	1:E:379:LEU:HD23	2.42	0.40
1:F:106:VAL:O	1:F:109:LEU:HB2	2.21	0.40
1:F:173:LEU:HD23	1:F:470:PHE:HE2	1.85	0.40
1:D:5:LEU:C	1:D:6:ASP:O	2.54	0.40
1:E:60:CYS:O	1:E:64:ILE:HG12	2.20	0.40
1:E:122:ILE:HD13	1:E:122:ILE:HA	1.85	0.40
1:E:167:LYS:H	1:E:167:LYS:HD3	1.86	0.40
1:F:325:GLU:HB3	1:F:327[B]:PHE:CZ	2.57	0.40
1:A:52:ASN:O	1:A:56:LEU:HG	2.22	0.40
1:B:23:GLN:OE1	1:B:23:GLN:HA	2.21	0.40
1:B:249:LYS:HE3	1:B:249:LYS:HB2	1.89	0.40
1:D:165:ARG:O	1:D:166:LYS:HG2	2.22	0.40
1:E:425:MET:HE2	1:E:425:MET:HB3	1.79	0.40
1:F:25:LYS:HD2	1:F:139:LEU:HD12	2.03	0.40
1:F:60:CYS:O	1:F:64:ILE:HB	2.21	0.40
1:F:177:VAL:HG22	1:F:468:ILE:HG22	2.03	0.40
1:A:84:VAL:HG23	1:A:85:LEU:HD23	2.03	0.40
1:C:290:LEU:H	1:C:290:LEU:HG	1.69	0.40
1:C:465:GLN:HE21	1:C:465:GLN:HB2	1.66	0.40
1:D:474:ALA:HB1	1:D:475:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/522 (84%)	420 (96%)	20 (4%)	0	100 100
1	B	447/522 (86%)	433 (97%)	14 (3%)	0	100 100
1	C	449/522 (86%)	421 (94%)	27 (6%)	1 (0%)	47 78
1	D	437/522 (84%)	420 (96%)	16 (4%)	1 (0%)	47 78
1	E	431/522 (83%)	422 (98%)	7 (2%)	2 (0%)	29 61
1	F	430/522 (82%)	410 (95%)	20 (5%)	0	100 100
All	All	2634/3132 (84%)	2526 (96%)	104 (4%)	4 (0%)	47 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	VAL
1	E	315	ILE
1	E	305	VAL
1	C	420	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	388/461 (84%)	363 (94%)	25 (6%)	17 45
1	B	388/461 (84%)	356 (92%)	32 (8%)	11 32
1	C	379/461 (82%)	359 (95%)	20 (5%)	22 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	370/461 (80%)	343 (93%)	27 (7%)	14 38
1	E	365/461 (79%)	341 (93%)	24 (7%)	16 44
1	F	373/461 (81%)	351 (94%)	22 (6%)	19 49
All	All	2263/2766 (82%)	2113 (93%)	150 (7%)	16 44

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	36	LEU
1	A	44	ARG
1	A	46	CYS
1	A	60	CYS
1	A	63	THR
1	A	64	ILE
1	A	91	THR
1	A	108	LEU
1	A	123	LYS
1	A	174	VAL
1	A	181	GLU
1	A	197	LYS
1	A	228	PHE
1	A	243	PHE
1	A	282	ASP
1	A	312	THR
1	A	320	GLN
1	A	353	GLN
1	A	360	HIS
1	A	374	SER
1	A	378	ASP
1	A	412	GLN
1	A	413	THR
1	A	426	LEU
1	B	2	VAL
1	B	5	LEU
1	B	7	LEU
1	B	49	ARG
1	B	60	CYS
1	B	66	GLU
1	B	77	ASP
1	B	85	LEU

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Mol	Chain	Res	Type
1	B	101	SER
1	B	157	ARG
1	B	169	SER
1	B	218	ARG
1	B	225	THR
1	B	228	PHE
1	B	232	GLU
1	B	237	VAL
1	B	251	ILE
1	B	272	SER
1	B	273	GLU
1	B	274	GLN
1	B	281	ARG
1	B	282	ASP
1	B	304	GLU
1	B	335	ASN
1	B	337	SER
1	B	353	GLN
1	B	360	HIS
1	B	394	SER
1	B	418	ASP
1	B	420	VAL
1	B	426	LEU
1	B	458	GLU
1	C	36	LEU
1	C	64	ILE
1	C	82	GLU
1	C	91	THR
1	C	115	LEU
1	C	121	ARG
1	C	133	ARG
1	C	149	GLU
1	C	164	VAL
1	C	174	VAL
1	C	199	VAL
1	C	223	ILE
1	C	243	PHE
1	C	244	ASP
1	C	360	HIS
1	C	374	SER
1	C	394	SER
1	C	445	GLN

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Mol	Chain	Res	Type
1	C	446	THR
1	C	447	GLU
1	D	2	VAL
1	D	61	SER
1	D	63	THR
1	D	64	ILE
1	D	86	SER
1	D	95	LEU
1	D	111	ASP
1	D	127	GLU
1	D	133	ARG
1	D	158	ILE
1	D	181	GLU
1	D	228	PHE
1	D	239	GLN
1	D	244	ASP
1	D	245	GLU
1	D	246	GLU
1	D	249	LYS
1	D	272	SER
1	D	274	GLN
1	D	337	SER
1	D	355	LEU
1	D	360	HIS
1	D	368	SER
1	D	374	SER
1	D	459	PHE
1	D	464	LEU
1	D	472	LYS
1	E	2	VAL
1	E	5	LEU
1	E	10	VAL
1	E	115	LEU
1	E	158	ILE
1	E	167	LYS
1	E	223	ILE
1	E	225	THR
1	E	228	PHE
1	E	237	VAL
1	E	239	GLN
1	E	266	LYS
1	E	346	THR

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Mol	Chain	Res	Type
1	E	360	HIS
1	E	374	SER
1	E	378	ASP
1	E	412	GLN
1	E	418	ASP
1	E	420	VAL
1	E	421	GLU
1	E	430	MET
1	E	445	GLN
1	E	459	PHE
1	E	467	LEU
1	F	49	ARG
1	F	51	ASP
1	F	58	ASN
1	F	68	MET
1	F	91	THR
1	F	105	LYS
1	F	111	ASP
1	F	115	LEU
1	F	150	ASP
1	F	177	VAL
1	F	228	PHE
1	F	264	ASP
1	F	271	THR
1	F	274	GLN
1	F	276	ILE
1	F	285	LEU
1	F	305	VAL
1	F	325	GLU
1	F	346	THR
1	F	360	HIS
1	F	412	GLN
1	F	430	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	131	ASN
1	A	320	GLN
1	B	170	HIS
1	B	274	GLN

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	326	GLN
1	B	360	HIS
1	B	402	GLN
1	C	54	ASN
1	C	131	ASN
1	C	320	GLN
1	C	402	GLN
1	C	445	GLN
1	C	465	GLN
1	D	274	GLN
1	D	326	GLN
1	D	353	GLN
1	D	402	GLN
1	D	412	GLN
1	D	465	GLN
1	E	35	GLN
1	E	235	GLN
1	E	320	GLN
1	F	102	GLN
1	F	235	GLN
1	F	274	GLN
1	F	319	HIS
1	F	320	GLN
1	F	353	GLN
1	F	412	GLN
1	F	424	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	PO4	F	601	-	4,4,4	0.74	0	6,6,6	0.56	0
3	PO4	E	601	-	4,4,4	0.76	0	6,6,6	0.41	0
3	PO4	A	602	-	4,4,4	0.85	0	6,6,6	0.39	0
3	PO4	B	602	-	4,4,4	0.82	0	6,6,6	0.49	0
3	PO4	C	601	-	4,4,4	0.84	0	6,6,6	0.33	0
3	PO4	D	601	-	4,4,4	0.71	0	6,6,6	0.58	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.

No monomer is involved in short contacts.

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^{th} 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	451/522 (86%)	0.20	33 (7%)	15	11	47, 74, 146, 167	1 (0%)
1	B	454/522 (86%)	0.15	19 (4%)	36	32	47, 70, 126, 153	0
1	C	456/522 (87%)	0.31	39 (8%)	10	8	52, 78, 147, 165	1 (0%)
1	D	450/522 (86%)	0.13	19 (4%)	36	32	46, 72, 140, 156	3 (0%)
1	E	440/522 (84%)	0.05	12 (2%)	54	50	43, 72, 133, 149	1 (0%)
1	F	443/522 (84%)	0.16	26 (5%)	22	18	50, 71, 152, 176	3 (0%)
All	All	2694/3132 (86%)	0.17	148 (5%)	25	21	43, 73, 142, 176	9 (0%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	VAL	5.9
1	F	252	GLY	5.0
1	C	240	LEU	5.0
1	C	311	ASP	5.0
1	A	105	LYS	4.9
1	D	417	MET	4.7
1	F	91	THR	4.4
1	C	69	LYS	4.3
1	F	63	THR	4.3
1	B	89	ASP	4.2
1	F	80	VAL	4.2
1	C	104	LYS	4.1
1	D	84	VAL	4.0
1	A	69	LYS	4.0
1	F	284	TRP	4.0
1	A	72	GLU	3.9
1	A	62	LYS	3.9
1	A	68	MET	3.9
1	E	264	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	99	LYS	3.8
1	F	93	ASP	3.8
1	A	79	SER	3.7
1	C	251	ILE	3.7
1	D	98	LEU	3.7
1	F	263	TYR	3.6
1	E	64	ILE	3.6
1	D	416	MET	3.5
1	E	85	LEU	3.5
1	B	413	THR	3.5
1	D	93	ASP	3.5
1	F	81	PRO	3.4
1	C	263	TYR	3.4
1	A	71	LYS	3.4
1	F	95	LEU	3.4
1	B	90	LEU	3.3
1	C	66	GLU	3.3
1	A	96	ALA	3.2
1	D	65	GLY	3.2
1	A	95	LEU	3.2
1	B	64	ILE	3.2
1	F	90	LEU	3.2
1	B	77	ASP	3.1
1	F	82	GLU	3.1
1	E	87	PHE	3.1
1	F	56	LEU	3.1
1	A	67	LYS	3.1
1	D	83	ASN	3.1
1	C	67	LYS	3.0
1	F	89	ASP	3.0
1	A	107	ARG	3.0
1	F	96	ALA	3.0
1	A	77	ASP	3.0
1	B	95	LEU	3.0
1	F	68	MET	3.0
1	C	109	LEU	3.0
1	D	75	GLY	3.0
1	E	93	ASP	3.0
1	C	70	LYS	2.9
1	B	313	ARG	2.9
1	C	68	MET	2.9
1	C	79	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	413	THR	2.9
1	D	411	GLY	2.9
1	C	65	GLY	2.8
1	C	417	MET	2.8
1	B	85	LEU	2.8
1	F	98	LEU	2.8
1	A	60	CYS	2.8
1	E	86	SER	2.8
1	A	78	GLU	2.8
1	A	109	LEU	2.8
1	B	312	THR	2.7
1	C	411	GLY	2.7
1	F	83	ASN	2.7
1	B	79	SER	2.7
1	A	81	PRO	2.7
1	D	70	LYS	2.7
1	A	61	SER	2.6
1	C	243	PHE	2.6
1	C	106	VAL	2.6
1	C	73	PRO	2.6
1	F	92	ALA	2.6
1	A	97	ASN	2.6
1	E	182	GLY	2.6
1	A	307	SER	2.6
1	C	266	LYS	2.6
1	A	65	GLY	2.6
1	B	60	CYS	2.6
1	D	64	ILE	2.5
1	C	63	THR	2.5
1	C	59	LEU	2.5
1	C	95	LEU	2.5
1	A	63	THR	2.5
1	A	92	ALA	2.5
1	D	66	GLU	2.5
1	C	108	LEU	2.5
1	E	230	ARG	2.5
1	C	416	MET	2.5
1	B	81	PRO	2.4
1	F	104	LYS	2.4
1	D	284	TRP	2.4
1	A	58	ASN	2.4
1	C	60	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	262	SER	2.4
1	C	300	CYS	2.4
1	B	84	VAL	2.3
1	B	306	GLY	2.3
1	C	80	VAL	2.3
1	A	104	LYS	2.3
1	C	96	ALA	2.3
1	A	70	LYS	2.3
1	A	108	LEU	2.3
1	E	108	LEU	2.3
1	F	312	THR	2.3
1	D	77	ASP	2.3
1	E	89	ASP	2.3
1	E	96	ALA	2.3
1	C	101	SER	2.3
1	C	298	SER	2.3
1	D	76	ASP	2.2
1	A	94	ALA	2.2
1	A	98	LEU	2.2
1	C	62	LYS	2.2
1	F	61	SER	2.2
1	D	82	GLU	2.2
1	A	244	ASP	2.1
1	F	411	GLY	2.1
1	D	243	PHE	2.1
1	B	308	HIS	2.1
1	B	80	VAL	2.1
1	C	77	ASP	2.1
1	F	94	ALA	2.1
1	A	305	VAL	2.1
1	E	95	LEU	2.1
1	D	300	CYS	2.1
1	A	66	GLU	2.1
1	B	67	LYS	2.1
1	C	235	GLN	2.1
1	C	93	ASP	2.0
1	A	448	LYS	2.0
1	B	61	SER	2.0
1	C	284	TRP	2.0
1	C	72	GLU	2.0
1	F	73	PRO	2.0
1	D	235	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	244	ASP	2.0
1	C	71	LYS	2.0
1	F	97	ASN	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	PO4	C	601	5/5	0.68	0.28	126,131,151,163	0
3	PO4	D	601	5/5	0.68	0.23	117,134,150,164	0
3	PO4	A	602	5/5	0.73	0.19	115,118,145,154	0
3	PO4	E	601	5/5	0.74	0.22	125,128,143,154	0
3	PO4	B	602	5/5	0.79	0.19	134,146,154,159	0
2	MG	A	601	1/1	0.83	0.40	86,86,86,86	0
2	MG	B	601	1/1	0.85	0.58	90,90,90,90	0
3	PO4	F	601	5/5	0.85	0.25	121,124,146,155	0

6.5 Other polymers (i)

There are no such residues in this entry.