



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:29 PM UTC

PDB ID : 3VBB / pdb_00003vbb
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

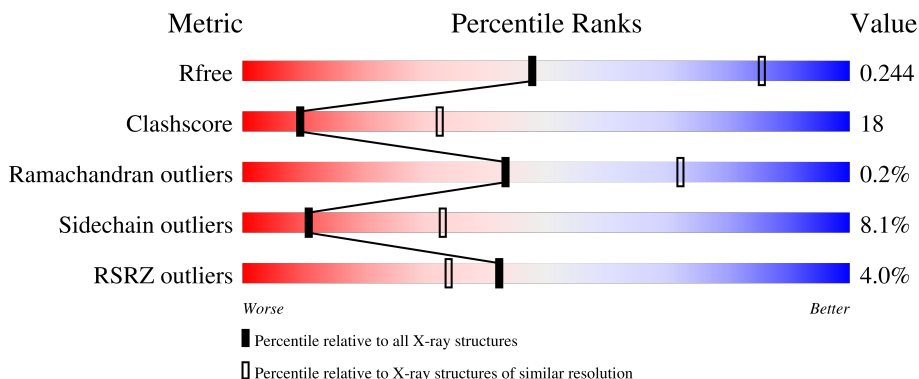
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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.



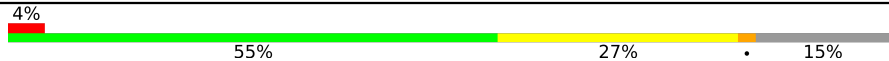
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	522	 2% 54% 30% 14%
1	B	522	 2% 56% 27% 13%
1	C	522	 4% 53% 30% 13%
1	D	522	 4% 51% 30% 5% 14%
1	E	522	 4% 57% 24% 16%

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Mol	Chain	Length	Quality of chain
1	F	522	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (4%), a large green segment (55%), a medium yellow segment (27%), and a small grey segment (15%).</p>

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

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 (CCD ID: 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

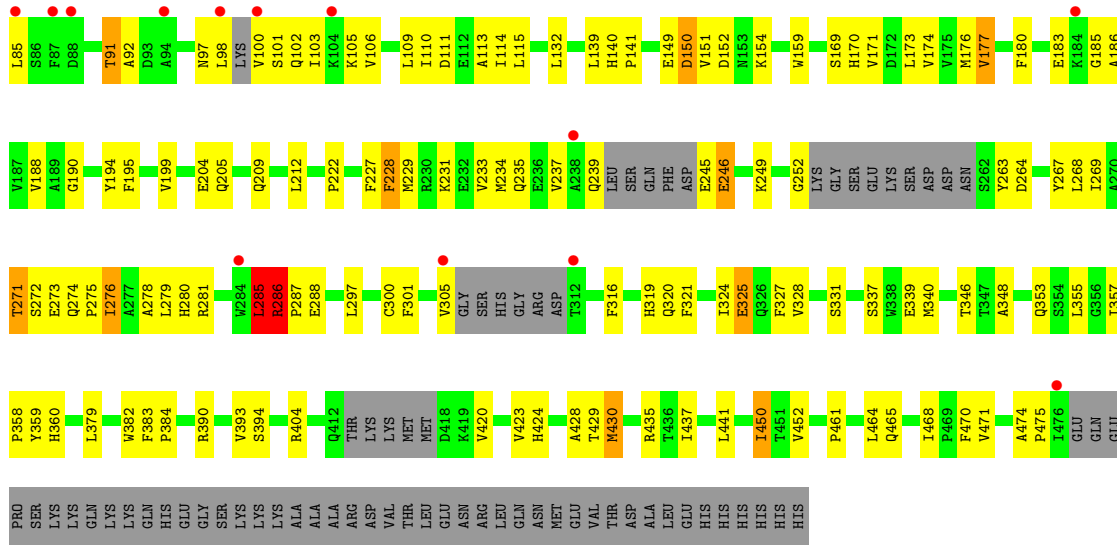
- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is water.

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



4 Data and refinement statistics

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) 98.7 (48.59-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.194 , 0.250 0.191 , 0.244	Depositor DCC
R_{free} test set	5680 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtrriage
Anisotropy	0.373	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.59	0/3677	0.98	10/4957 (0.2%)
1	B	0.61	0/3697	0.99	12/4982 (0.2%)
1	C	0.56	0/3661	1.01	14/4949 (0.3%)
1	D	0.60	0/3601	1.02	16/4858 (0.3%)
1	E	0.62	0/3539	0.97	7/4777 (0.1%)
1	F	0.60	0/3589	0.99	14/4841 (0.3%)
All	All	0.60	0/21764	0.99	73/29364 (0.2%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	6	ASP	N-CA-C	-10.09	97.21	110.43
1	C	242	GLN	N-CA-C	-8.68	102.39	113.16
1	B	26	ARG	N-CA-C	-8.38	99.47	110.53
1	F	331	SER	CA-C-N	7.97	127.61	119.56
1	F	331	SER	C-N-CA	7.97	127.61	119.56
1	C	237	VAL	N-CA-C	7.91	119.63	111.00
1	B	331	SER	CA-C-N	7.90	128.08	119.87
1	B	331	SER	C-N-CA	7.90	128.08	119.87
1	A	84	VAL	N-CA-C	7.78	120.54	112.83
1	A	131	ASN	N-CA-C	7.51	120.93	111.69
1	C	131	ASN	N-CA-C	7.29	121.41	112.23
1	A	99	LYS	CB-CA-C	-7.22	108.25	116.63
1	B	156	GLU	N-CA-C	7.16	120.49	111.69
1	C	188	VAL	N-CA-C	6.80	116.92	110.53
1	E	414	LYS	N-CA-C	6.72	119.96	111.69
1	B	26	ARG	CA-C-N	-6.70	113.22	123.14
1	B	26	ARG	C-N-CA	-6.70	113.22	123.14
1	D	474	ALA	CA-C-N	6.60	126.99	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	474	ALA	C-N-CA	6.60	126.99	119.92
1	E	188	VAL	N-CA-C	6.60	117.22	110.82
1	F	285	LEU	N-CA-C	6.47	118.48	110.91
1	C	152	ASP	N-CA-C	6.39	121.07	113.28
1	F	188	VAL	N-CA-C	6.37	116.41	110.42
1	A	152	ASP	N-CA-C	6.31	121.12	113.17
1	A	339	GLU	N-CA-C	-6.26	104.00	111.69
1	B	452	VAL	CA-C-N	6.24	126.60	119.93
1	B	452	VAL	C-N-CA	6.24	126.60	119.93
1	F	452	VAL	CA-C-N	6.16	126.10	119.76
1	F	452	VAL	C-N-CA	6.16	126.10	119.76
1	B	152	ASP	N-CA-C	6.03	120.79	113.38
1	C	85	LEU	N-CA-C	6.02	120.62	113.16
1	A	306	GLY	N-CA-C	5.98	121.81	114.69
1	F	149	GLU	N-CA-C	-5.96	100.48	109.60
1	C	225	THR	CA-C-N	-5.95	113.65	119.78
1	C	225	THR	C-N-CA	-5.95	113.65	119.78
1	D	383	PHE	CA-C-N	5.93	126.08	119.32
1	D	383	PHE	C-N-CA	5.93	126.08	119.32
1	D	339	GLU	N-CA-C	-5.89	104.77	111.07
1	D	144	PRO	CA-C-N	-5.83	115.72	122.95
1	D	144	PRO	C-N-CA	-5.83	115.72	122.95
1	B	468	ILE	CB-CA-C	-5.80	104.51	111.18
1	D	152	ASP	N-CA-C	5.70	120.35	113.17
1	E	465	GLN	N-CA-C	5.67	117.54	111.36
1	D	143	VAL	CA-C-N	5.56	125.88	119.93
1	D	143	VAL	C-N-CA	5.56	125.88	119.93
1	F	286	ARG	N-CA-C	5.54	115.97	109.60
1	E	464	LEU	N-CA-C	5.50	120.11	113.17
1	E	355	LEU	N-CA-C	-5.44	106.31	113.17
1	C	333	HIS	N-CA-C	5.43	117.88	110.55
1	D	466	GLU	N-CA-C	5.40	116.97	111.14
1	F	465	GLN	N-CA-C	5.35	118.27	111.69
1	B	188	VAL	N-CA-C	5.32	115.42	110.42
1	F	29	ASP	CA-C-N	5.30	124.91	119.56
1	F	29	ASP	C-N-CA	5.30	124.91	119.56
1	D	85	LEU	CB-CA-C	-5.26	110.49	116.54
1	F	280	HIS	N-CA-C	5.20	119.73	113.17
1	E	383	PHE	CA-C-N	5.18	124.80	119.05
1	E	383	PHE	C-N-CA	5.18	124.80	119.05
1	D	368	SER	N-CA-C	5.16	119.67	113.17
1	C	456	LEU	N-CA-C	5.14	118.71	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	339	GLU	N-CA-C	-5.13	105.76	111.36
1	A	151	VAL	N-CA-C	5.13	115.80	110.82
1	B	420	VAL	CB-CA-C	-5.13	105.70	111.45
1	C	331	SER	CA-C-N	5.10	124.71	119.56
1	C	331	SER	C-N-CA	5.10	124.71	119.56
1	A	418	ASP	N-CA-C	5.06	116.63	110.41
1	A	84	VAL	CA-C-N	-5.04	115.85	122.85
1	A	84	VAL	C-N-CA	-5.04	115.85	122.85
1	D	456	LEU	N-CA-C	5.03	118.56	112.23
1	D	151	VAL	N-CA-C	5.02	115.69	110.82
1	F	101	SER	N-CA-C	-5.01	106.43	112.54
1	C	452	VAL	CA-C-N	5.01	125.24	119.83
1	C	452	VAL	C-N-CA	5.01	125.24	119.83

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	3606	0	3584	129	0
1	B	3625	0	3600	134	0
1	C	3588	0	3506	157	0
1	D	3533	0	3483	130	0
1	E	3469	0	3414	117	0
1	F	3519	0	3465	121	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	756	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 (756) 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:A:344:MET:HE1	1:A:426:LEU:HB2	1.37	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:C:176:MET:HE2	1:C:474:ALA:HB2	1.49	0.92
1:A:412:GLN:O	1:A:412:GLN:HG3	1.66	0.92
1:E:327[A]:PHE:HZ	1:E:425:MET:HE3	1.31	0.90
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:PHE:HE2	1:E:323:LYS:HE3	1.44	0.83
1:C:176:MET:HE2	1:C:474:ALA:CB	2.08	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: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:C:327[A]:PHE:HZ	1:C:425:MET:HE3	1.47	0.79
1:E:188:VAL:HG13	1:F:229:MET:HE3	1.62	0.79
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: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:E:176:MET:HE2	1:E:470:PHE:CE1	2.23	0.74
1:B:276:ILE:HD12	1:B:327[B]:PHE:CE2	2.22	0.73
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:E:273:GLU:HB2	1:E:327[B]:PHE:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:172:ASP:HB3	1:C:176:MET:HE3	1.73	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:E:327[A]:PHE:CZ	1:E:425:MET:HE3	2.22	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:A:100:VAL:C	1:A:102:GLN:H	2.01	0.68
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:A:328:VAL:HG21	1:A:344:MET:HE2	1.75	0.67
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:A:229:MET:HE3	1:B:188:VAL:HG13	1.77	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:C:188:VAL:HG13	1:D:229:MET:HE3	1.75	0.67
1:F:174:VAL:HG12	1:F:180:PHE:CB	2.23	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:MET:HE2	1:B:470:PHE:CD1	2.30	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:B:215:LEU:HG	1:B:430:MET:HE1	1.77	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:A:271:THR:HG22	1:A:323:LYS:HZ1	1.60	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:A:328:VAL:CG2	1:A:344:MET:HE2	2.27	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:D:241:SER:C	1:D:244:ASP:HB2	2.21	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:E:176:MET:HE2	1:E:470:PHE:CD1	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: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:B:229:MET:HB2	1:B:234:MET:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:229:MET:HE2	1:D:233:VAL:HG13	1.81	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:F:176:MET:HE2	1:F:470:PHE:CD2	2.38	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:E:321:PHE:CE2	1:E:323:LYS:HE3	2.32	0.59
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:C:71:LYS:C	1:C:72:GLU:HG2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:351:PHE:CD1	1:D:430:MET:HE3	2.38	0.58
1:A:379:LEU:HB3	1:A:393:VAL:HB	1.85	0.57
1:D:351:PHE:CG	1:D:430:MET:HE3	2.39	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: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:B:323:LYS:HZ1	1:B:429:THR:HG21	1.69	0.56
1:F:176:MET:HE2	1:F:470:PHE:CE2	2.41	0.56
1:C:333:HIS:HE2	1:C:421:GLU:CD	2.13	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:C:168:TYR:CD1	1:C:176:MET:HE1	2.41	0.56
1:E:303:GLN:OE1	1:F:252:GLY:HA2	2.05	0.56
1:A:344:MET:HE3	1:A:426:LEU:HD22	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:LYS:HD3	1:E:340:MET:HE1	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:C:272:SER:C	1:C:275:PRO:HD2	2.32	0.55
1:F:176:MET:SD	1:F:474:ALA:HB2	2.46	0.55
1:F:316:PHE:CZ	1:F:435:ARG:NH1	2.75	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: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:F:273:GLU:HB2	1:F:327[B]:PHE:HE1	1.71	0.54
1:F:379:LEU:HD23	1:F:379:LEU:C	2.32	0.54
1:A:177:VAL:HG12	1:A:199:VAL:CG2	2.33	0.54
1:F:64:ILE:CG2	1:F:68:MET:HE3	2.38	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: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: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:C:417:MET:HG2	1:C:417:MET:O	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:340:MET:HG3	1:A:344:MET:HE3	1.91	0.53
1:B:461:PRO:HG2	1:B:464:LEU:HB2	1.91	0.53
1:F:348:ALA:HA	1:F:430:MET:HE2	1.89	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
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:B:95:LEU:HD12	1:B:96:ALA:N	2.24	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: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:F:183:GLU:C	1:F:185:GLY:H	2.17	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:E:36:LEU:C	1:E:36:LEU:HD23	2.34	0.52
1:B:159:TRP:CZ2	1:B:353:GLN:HG3	2.45	0.52
1:B:272:SER:C	1:B:327[B]:PHE:CE2	2.88	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:C	1:A:102:GLN:N	2.68	0.51
1:A:100:VAL:HG12	1:A:101:SER:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:271:THR:C	1:C:273:GLU:H	2.19	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:F:173:LEU:HD22	1:F:450:ILE:HD11	1.93	0.51
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.76	0.51
1:E:326:GLN:NE2	1:E:430:MET:HE3	2.25	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: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: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:B:327[A]:PHE:HZ	1:B:425:MET:HE3	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:328:VAL:HB	1:A:344:MET:HE2	1.95	0.49
1:C:229:MET:HE1	1:C:233:VAL:HG12	1.93	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: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:A:328:VAL:CB	1:A:344:MET:HE2	2.43	0.49
1:B:327[B]:PHE:CE1	1:B:427:ASN:HB2	2.47	0.49
1:B:446:THR:OG1	1:B:447:GLU:N	2.35	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: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:272:SER:C	1:B:327[B]:PHE:CZ	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:91:THR:OG1	1:C:92:ALA:N	2.45	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:F:252:GLY:C	1:F:263:TYR:HD1	2.21	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: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: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:B:417:MET:HE3	1:B:417:MET:HB3	1.79	0.47
1:C:335:ASN:O	1:C:339:GLU:HG3	2.14	0.47
1:C:351:PHE:HB2	1:C:430:MET:HE2	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:PRO:CG	1:C:443:ASN:OD1	2.64	0.47
1:B:379:LEU:C	1:B:379:LEU:HD23	2.39	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
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: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:D:5:LEU:C	1:D:6:ASP:O	2.54	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:D:91:THR:C	1:D:93:ASP:N	2.73	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:E:348:ALA:HA	1:E:430:MET:HE2	1.98	0.45
1:A:272:SER:C	1:A:275:PRO:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:MET:HB2	1:C:234:MET:HE2	1.99	0.45
1:C:284:TRP:CE2	1:C:409:ARG:HD3	2.52	0.45
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:E:328:VAL:HG11	1:E:340:MET:HE2	1.98	0.45
1:E:379:LEU:C	1:E:379:LEU:HD23	2.42	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:F:70:LYS:HG3	1:F:70:LYS:O	2.16	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:C:327[A]:PHE:CZ	1:C:425:MET:HE3	2.38	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:165:ARG:C	1:D:166:LYS:HG2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:359:TYR:CD1	1:B:359:TYR:C	2.96	0.44
1:C:166:LYS:HG3	1:C:384:PRO:HB3	1.99	0.44
1:C:290:LEU:HA	1:C:291:PRO:C	2.42	0.44
1:D:359:TYR:CD1	1:D:359:TYR:C	2.95	0.44
1:E:272:SER:HB3	1:E:298:SER:HB3	1.99	0.44
1:F:359:TYR:CD1	1:F:359:TYR:C	2.95	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:E:90:LEU:HD23	1:E:90:LEU:C	2.42	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:A:460:MET:HE3	1:A:464:LEU:HB3	2.00	0.44
1:B:199:VAL:HG23	1:B:200:LEU:N	2.32	0.44
1:B:325:GLU:HB2	1:B:327[B]:PHE:CZ	2.52	0.44
1:B:402:GLN:HE21	1:B:425:MET:HE2	1.82	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:D:161:ASP:OD2	1:D:161:ASP:C	2.60	0.44
1:E:195:PHE:CE2	1:F:279:LEU:HD13	2.53	0.44
1:E:359:TYR:CD1	1:E:359:TYR:C	2.95	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:E:344:MET:HE2	1:E:395:CYS:SG	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:ASN:C	1:F:98:LEU:HD12	2.43	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:A:286:ARG:HB2	1:A:289:ASP:OD1	2.18	0.43
1:B:325:GLU:CD	1:B:429:THR:HG22	2.44	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:F:229:MET:HB2	1:F:234:MET:HE2	1.99	0.43
1:A:335:ASN:O	1:A:336:LYS:C	2.62	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:E:430:MET:HE3	1:E:430:MET: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: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
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:A:399:THR:OG1	1:A:400:ASP:N	2.50	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:67:LYS:HZ1	1:B:96:ALA:HA	1.82	0.43
1:B:131:ASN:O	1:B:135:ILE:HG13	2.19	0.43
1:A:344:MET:CE	1:A:426:LEU:HB2	2.27	0.43
1:D:157:ARG:C	1:D:158:ILE:HG12	2.44	0.43
1:F:9:ARG:HB2	1:F:12:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:ASP:OD1	1:F:15:ASP:C	2.62	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:A:359:TYR:CD1	1:A:359:TYR:C	2.97	0.42
1:B:191:SER:O	1:B:192:ARG:HB2	2.17	0.42
1:C:174:VAL:HG13	1:C:180:PHE:CB	2.49	0.42
1:C:303:GLN:O	1:C:304:GLU:C	2.62	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:C:176:MET:CE	1:C:474:ALA:HB2	2.33	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:C:360:HIS:HD1	1:C:360:HIS:C	2.26	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
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:F:194:TYR:CD1	1:F:194:TYR:C	2.97	0.42
1:A:95:LEU:O	1:A:103:ILE:HD11	2.19	0.42
1:D:153:ASN:OD1	1:D:365:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:348:ALA:HA	1:F:430:MET:HE1	2.00	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:288:GLU:OE1	1:F:288:GLU:N	2.45	0.41
1:B:215:LEU:CG	1:B:430:MET:HE1	2.49	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:A:64:ILE:O	1:A:68:MET:HE2	2.21	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
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:A:271:THR:HG22	1:A:323:LYS:HZ2	1.83	0.41
1:B:233:VAL:HG11	1:B:278:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:379:LEU:C	1:C:379:LEU:HD23	2.46	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:B:333:HIS:O	1:B:334:ASP:HB2	2.19	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:412:GLN:CD	1:B:412:GLN:O	2.65	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: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:176:MET:HE2	1:C:474:ALA:HB1	1.98	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%)	43	72
1	D	437/522 (84%)	420 (96%)	16 (4%)	1 (0%)	43	72
1	E	431/522 (83%)	422 (98%)	7 (2%)	2 (0%)	24	54
1	F	430/522 (82%)	410 (95%)	20 (5%)	0	100	100
All	All	2634/3132 (84%)	2526 (96%)	104 (4%)	4 (0%)	43	72

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%)	360 (93%)	28 (7%)	13	39
1	B	388/461 (84%)	352 (91%)	36 (9%)	8	27
1	C	379/461 (82%)	355 (94%)	24 (6%)	16	45
1	D	370/461 (80%)	334 (90%)	36 (10%)	8	25
1	E	365/461 (79%)	333 (91%)	32 (9%)	9	29
1	F	373/461 (81%)	347 (93%)	26 (7%)	14	40
All	All	2263/2766 (82%)	2081 (92%)	182 (8%)	11	34

All (182) 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	106	VAL
1	A	108	LEU
1	A	123	LYS
1	A	133	ARG
1	A	149	GLU
1	A	156	GLU
1	A	174	VAL
1	A	197	LYS
1	A	201	VAL
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	412	GLN
1	A	413	THR
1	A	420	VAL
1	A	426	LEU
1	B	2	VAL
1	B	7	LEU
1	B	10	VAL
1	B	32	LEU
1	B	49	ARG
1	B	60	CYS
1	B	66	GLU
1	B	69	LYS
1	B	77	ASP
1	B	85	LEU
1	B	97	ASN
1	B	122	ILE
1	B	123	LYS
1	B	157	ARG
1	B	169	SER

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Mol	Chain	Res	Type
1	B	218	ARG
1	B	225	THR
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	346	THR
1	B	353	GLN
1	B	391	GLU
1	B	394	SER
1	B	418	ASP
1	B	420	VAL
1	B	421	GLU
1	B	426	LEU
1	B	458	GLU
1	C	36	LEU
1	C	63	THR
1	C	64	ILE
1	C	91	THR
1	C	106	VAL
1	C	115	LEU
1	C	122	ILE
1	C	149	GLU
1	C	163	THR
1	C	164	VAL
1	C	174	VAL
1	C	199	VAL
1	C	223	ILE
1	C	243	PHE
1	C	250	VAL
1	C	290	LEU
1	C	353	GLN
1	C	360	HIS
1	C	374	SER
1	C	394	SER
1	C	420	VAL

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Mol	Chain	Res	Type
1	C	445	GLN
1	C	446	THR
1	C	447	GLU
1	D	2	VAL
1	D	63	THR
1	D	64	ILE
1	D	71	LYS
1	D	86	SER
1	D	95	LEU
1	D	106	VAL
1	D	111	ASP
1	D	112	GLU
1	D	127	GLU
1	D	158	ILE
1	D	166	LYS
1	D	181	GLU
1	D	199	VAL
1	D	212	LEU
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	251	ILE
1	D	271	THR
1	D	272	SER
1	D	274	GLN
1	D	324	ILE
1	D	337	SER
1	D	353	GLN
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	471	VAL
1	D	472	LYS
1	E	2	VAL
1	E	5	LEU
1	E	10	VAL

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Mol	Chain	Res	Type
1	E	57	LYS
1	E	62	LYS
1	E	90	LEU
1	E	100	VAL
1	E	106	VAL
1	E	115	LEU
1	E	120	GLU
1	E	122	ILE
1	E	158	ILE
1	E	167	LYS
1	E	171	VAL
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
1	E	361	ILE
1	E	374	SER
1	E	412	GLN
1	E	418	ASP
1	E	420	VAL
1	E	421	GLU
1	E	429	THR
1	E	430	MET
1	E	445	GLN
1	E	459	PHE
1	E	467	LEU
1	F	64	ILE
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	154	LYS
1	F	177	VAL
1	F	228	PHE
1	F	233	VAL
1	F	239	GLN
1	F	246	GLU

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Mol	Chain	Res	Type
1	F	264	ASP
1	F	271	THR
1	F	274	GLN
1	F	276	ILE
1	F	285	LEU
1	F	286	ARG
1	F	305	VAL
1	F	325	GLU
1	F	346	THR
1	F	360	HIS
1	F	420	VAL
1	F	430	MET
1	F	450	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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
1	B	320	GLN
1	B	326	GLN
1	B	360	HIS
1	B	402	GLN
1	B	412	GLN
1	C	102	GLN
1	C	131	ASN
1	C	320	GLN
1	C	402	GLN
1	C	445	GLN
1	C	465	GLN
1	D	54	ASN
1	D	326	GLN
1	D	402	GLN
1	D	412	GLN
1	E	35	GLN
1	E	205	GLN
1	E	235	GLN
1	E	320	GLN
1	F	102	GLN

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Mol	Chain	Res	Type
1	F	170	HIS
1	F	319	HIS
1	F	320	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 oligosaccharides 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	D	601	-	4,4,4	0.76	0	6,6,6	0.61	0
3	PO4	A	602	-	4,4,4	0.90	0	6,6,6	0.41	0
3	PO4	B	602	-	4,4,4	0.86	0	6,6,6	0.52	0
3	PO4	E	601	-	4,4,4	0.81	0	6,6,6	0.44	0
3	PO4	F	601	-	4,4,4	0.78	0	6,6,6	0.59	0
3	PO4	C	601	-	4,4,4	0.89	0	6,6,6	0.35	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, 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	451/522 (86%)	0.02	11 (2%) 59 50	35, 74, 146, 167	2 (0%)
1	B	454/522 (86%)	-0.10	12 (2%) 57 48	36, 70, 126, 153	1 (0%)
1	C	456/522 (87%)	0.14	21 (4%) 37 29	39, 78, 147, 165	2 (0%)
1	D	450/522 (86%)	0.18	23 (5%) 33 26	36, 72, 140, 156	4 (0%)
1	E	440/522 (84%)	0.09	19 (4%) 40 31	38, 72, 133, 149	2 (0%)
1	F	443/522 (84%)	0.10	21 (4%) 36 28	35, 71, 150, 176	4 (0%)
All	All	2694/3132 (86%)	0.07	107 (3%) 42 34	35, 73, 142, 176	15 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	240	LEU	5.6
1	E	240	LEU	5.5
1	E	307	SER	5.3
1	D	305	VAL	5.1
1	D	90	LEU	4.8
1	D	78	GLU	4.6
1	A	307	SER	4.3
1	D	83	ASN	4.2
1	F	63	THR	3.8
1	E	476	ILE	3.7
1	F	476	ILE	3.5
1	B	79	SER	3.5
1	C	412	GLN	3.4
1	E	182	GLY	3.3
1	D	92	ALA	3.3
1	A	476	ILE	3.3
1	F	94	ALA	3.3
1	E	85	LEU	3.2
1	F	305	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	85	LEU	3.2
1	B	80	VAL	3.2
1	E	230	ARG	3.2
1	D	476	ILE	3.2
1	A	63	THR	3.1
1	A	243	PHE	3.1
1	C	78	GLU	3.1
1	F	312	THR	3.1
1	D	264	ASP	3.0
1	F	85	LEU	3.0
1	E	246	GLU	3.0
1	C	263	TYR	3.0
1	D	64	ILE	3.0
1	F	88	ASP	3.0
1	D	240	LEU	2.9
1	C	73	PRO	2.9
1	D	96	ALA	2.9
1	E	413	THR	2.9
1	A	240	LEU	2.9
1	C	413	THR	2.9
1	C	253	LYS	2.9
1	F	238	ALA	2.8
1	D	253	LYS	2.8
1	C	313	ARG	2.8
1	E	313	ARG	2.8
1	F	84	VAL	2.8
1	F	64	ILE	2.8
1	B	70	LYS	2.8
1	F	81	PRO	2.8
1	F	83	ASN	2.7
1	E	272	SER	2.7
1	B	312	THR	2.7
1	E	263	TYR	2.7
1	D	238	ALA	2.7
1	E	253	LYS	2.7
1	B	89	ASP	2.7
1	D	72	GLU	2.6
1	C	475	PRO	2.6
1	F	100	VAL	2.6
1	B	309	GLY	2.6
1	D	100	VAL	2.6
1	D	82	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	84	VAL	2.5
1	D	181	GLU	2.5
1	A	247	LEU	2.5
1	D	187	VAL	2.5
1	B	81	PRO	2.5
1	C	77	ASP	2.4
1	F	284	TRP	2.4
1	A	413	THR	2.4
1	F	184	LYS	2.4
1	F	80	VAL	2.3
1	F	98	LEU	2.3
1	D	75	GLY	2.3
1	A	312	THR	2.3
1	C	266	LYS	2.3
1	E	193	GLY	2.3
1	F	104	LYS	2.3
1	C	186	ALA	2.2
1	C	238	ALA	2.2
1	E	273	GLU	2.2
1	B	240	LEU	2.2
1	A	402	GLN	2.2
1	F	68	MET	2.2
1	F	87	PHE	2.2
1	A	417	MET	2.2
1	B	85	LEU	2.2
1	C	251	ILE	2.2
1	E	305	VAL	2.2
1	E	87	PHE	2.2
1	C	265	GLU	2.2
1	C	239	GLN	2.1
1	E	237	VAL	2.1
1	D	416	MET	2.1
1	B	413	THR	2.1
1	E	306	GLY	2.1
1	B	60	CYS	2.1
1	F	70	LYS	2.1
1	C	247	LEU	2.1
1	D	312	THR	2.1
1	C	100	VAL	2.1
1	C	64	ILE	2.1
1	B	84	VAL	2.0
1	D	98	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	264	ASP	2.0
1	C	273	GLU	2.0
1	D	284	TRP	2.0
1	C	419	LYS	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	PO4	D	601	5/5	0.65	0.15	117,134,150,164	0
3	PO4	E	601	5/5	0.66	0.15	125,128,143,154	0
3	PO4	B	602	5/5	0.67	0.12	134,146,154,159	0
3	PO4	C	601	5/5	0.69	0.15	126,131,151,163	0
3	PO4	F	601	5/5	0.69	0.14	121,124,146,155	0
3	PO4	A	602	5/5	0.77	0.13	115,118,145,154	0
2	MG	A	601	1/1	0.86	0.26	86,86,86,86	0
2	MG	B	601	1/1	0.91	0.19	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.