



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:46 AM UTC

PDB ID : 7RFO / pdb_00007rfo
Title : SeMet Tailspike protein 4 (TSP4) phage CBA120, residues 1-335, obtained in the presence of LiSO₄
Authors : Chao, K.; Shang, X.; Grenfield, J.; Linden, S.B.; Nelson, D.C.; Herzberg, O.
Deposited on : 2021-07-14
Resolution : 3.02 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)
Xtriage (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

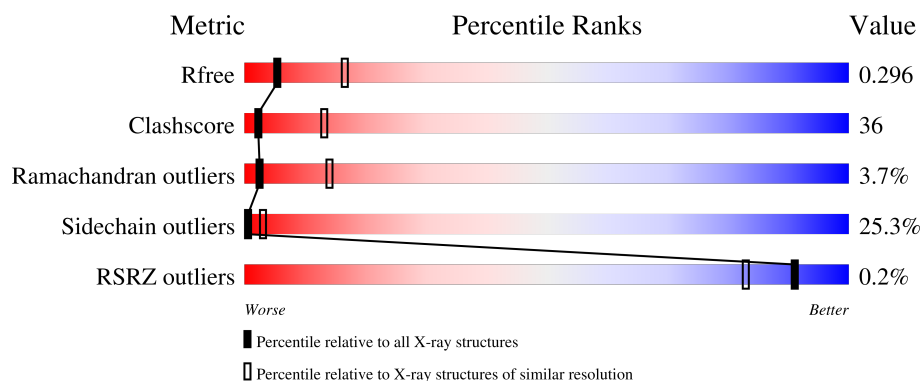
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

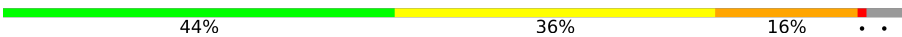
The reported resolution of this entry is 3.02 Å.

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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	341	 44% 36% 16% . .
1	B	341	 % 50% 34% 12% .
1	C	341	 43% 41% 10% . 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7077 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 Tailspike protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	Se	0	0	0
			2327	1445	388	488	1	5			
1	B	330	Total	C	N	O	S	Se	0	1	0
			2387	1488	388	505	1	5			
1	C	324	Total	C	N	O	S	Se	0	0	0
			2363	1475	383	498	1	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MSE	LEU	engineered mutation	UNP G3M192
A	31	MSE	ILE	engineered mutation	UNP G3M192
A	145	MSE	LEU	engineered mutation	UNP G3M192
A	336	HIS	-	expression tag	UNP G3M192
A	337	HIS	-	expression tag	UNP G3M192
A	338	HIS	-	expression tag	UNP G3M192
A	339	HIS	-	expression tag	UNP G3M192
A	340	HIS	-	expression tag	UNP G3M192
A	341	HIS	-	expression tag	UNP G3M192
B	12	MSE	LEU	engineered mutation	UNP G3M192
B	31	MSE	ILE	engineered mutation	UNP G3M192
B	145	MSE	LEU	engineered mutation	UNP G3M192
B	336	HIS	-	expression tag	UNP G3M192
B	337	HIS	-	expression tag	UNP G3M192
B	338	HIS	-	expression tag	UNP G3M192
B	339	HIS	-	expression tag	UNP G3M192
B	340	HIS	-	expression tag	UNP G3M192
B	341	HIS	-	expression tag	UNP G3M192
C	12	MSE	LEU	engineered mutation	UNP G3M192
C	31	MSE	ILE	engineered mutation	UNP G3M192
C	145	MSE	LEU	engineered mutation	UNP G3M192
C	336	HIS	-	expression tag	UNP G3M192
C	337	HIS	-	expression tag	UNP G3M192

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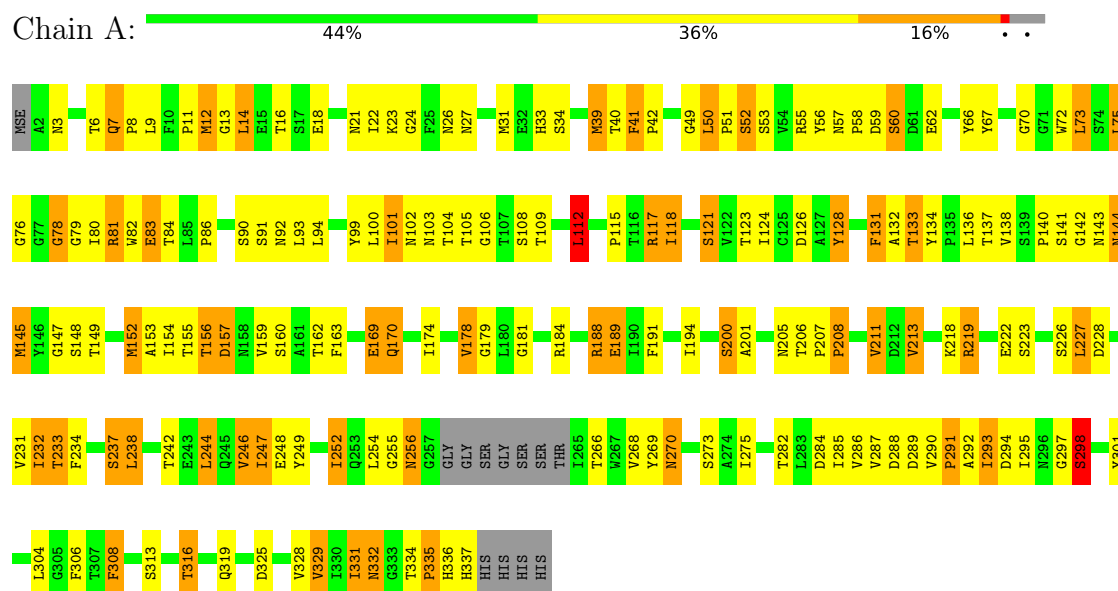
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Chain	Residue	Modelled	Actual	Comment	Reference
C	338	HIS	-	expression tag	UNP G3M192
C	339	HIS	-	expression tag	UNP G3M192
C	340	HIS	-	expression tag	UNP G3M192
C	341	HIS	-	expression tag	UNP G3M192

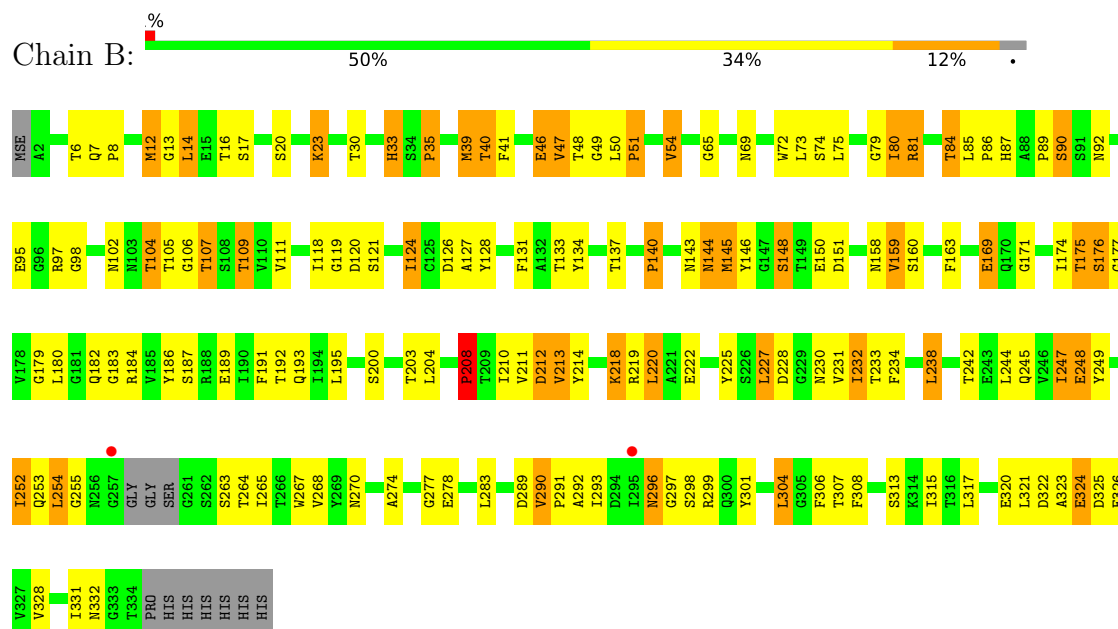
3 Residue-property plots

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.

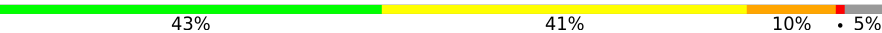
• Molecule 1: Tailspike protein

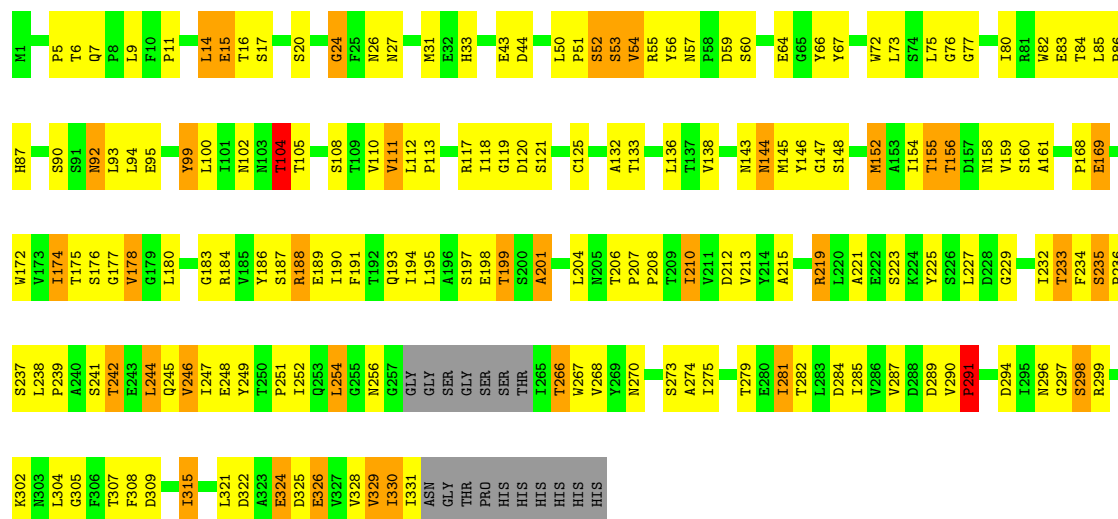


• Molecule 1: Tailspike protein



● Molecule 1: Tailspike protein

Chain C:  43% 41% 10% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	67.90Å 67.90Å 607.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.02 30.00 – 3.02	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-3.02) 94.8 (30.00-3.02)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.225 , 0.296 0.237 , 0.296	Depositor DCC
R_{free} test set	1370 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	118.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 110.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7077	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

5.1 Standard geometry

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	1.12	2/2374 (0.1%)	1.48	14/3250 (0.4%)
1	B	1.12	1/2436 (0.0%)	1.47	19/3332 (0.6%)
1	C	1.10	1/2410 (0.0%)	1.44	9/3296 (0.3%)
All	All	1.11	4/7220 (0.1%)	1.46	42/9878 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	ILE	C-O	6.96	1.30	1.24
1	A	42	PRO	C-O	-5.29	1.17	1.23
1	C	54	VAL	C-O	5.19	1.29	1.24
1	A	8	PRO	C-O	-5.12	1.18	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASN	CB-CA-C	7.18	122.76	109.54
1	C	5	PRO	N-CA-C	7.01	122.20	111.19
1	A	256	ASN	CB-CA-C	7.00	121.67	111.73
1	A	133	THR	CB-CA-C	6.96	121.01	110.08
1	B	192	THR	CA-CB-OG1	-6.86	99.31	109.60
1	C	99	TYR	CB-CA-C	6.62	121.17	109.72
1	C	104	THR	CA-CB-OG1	-6.59	99.71	109.60
1	A	92	ASN	CB-CA-C	6.38	120.25	109.84
1	B	7	GLN	CB-CA-C	-6.28	101.48	109.65
1	C	143	ASN	CA-CB-CG	-6.18	106.42	112.60
1	B	12	MSE	CG-SE-CE	6.15	112.46	98.92
1	C	104	THR	CB-CA-C	-6.14	100.98	110.81
1	B	151	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	97	ARG	CB-CA-C	6.01	120.34	109.83
1	A	39	MSE	CG-SE-CE	5.90	111.90	98.92
1	A	41	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	12	MSE	CG-SE-CE	5.79	111.67	98.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	THR	CA-CB-OG1	-5.75	100.97	109.60
1	A	131	PHE	N-CA-C	-5.71	105.13	111.36
1	C	113	PRO	CA-C-O	-5.69	114.92	121.86
1	B	109	THR	CB-CA-C	5.51	120.90	109.38
1	A	42	PRO	CA-C-O	-5.47	115.31	121.43
1	B	233	THR	CA-CB-OG1	-5.43	101.46	109.60
1	B	104	THR	CB-CA-C	5.43	119.80	110.79
1	B	8	PRO	CA-C-O	-5.40	115.26	121.36
1	C	194	ILE	CA-C-O	-5.39	114.58	120.84
1	B	107	THR	CA-CB-OG1	-5.39	101.52	109.60
1	B	148	SER	CA-C-N	5.38	129.21	120.60
1	B	148	SER	C-N-CA	5.38	129.21	120.60
1	C	233	THR	CA-CB-OG1	-5.38	101.53	109.60
1	B	86	PRO	N-CA-C	-5.34	102.73	110.80
1	A	156	THR	CA-C-O	-5.33	115.33	121.19
1	C	177	GLY	CA-C-O	-5.33	116.57	121.63
1	B	183	GLY	CA-C-O	-5.22	116.89	121.58
1	B	51	PRO	N-CA-C	-5.20	102.94	111.21
1	A	335	PRO	CB-CA-C	-5.20	104.09	111.68
1	A	103	ASN	N-CA-C	-5.15	107.51	112.97
1	B	208	PRO	N-CA-CB	-5.11	97.88	103.25
1	A	86	PRO	CB-CA-C	5.11	118.07	111.64
1	B	41	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	54	VAL	CA-C-O	-5.09	116.65	121.64
1	A	26	ASN	CA-CB-CG	5.01	117.61	112.60

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	2327	0	2070	194	0
1	B	2387	0	2163	178	0
1	C	2363	0	2180	182	0
All	All	7077	0	6413	484	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 36.

All (484) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MSE:HE1	1:A:252:ILE:HG21	1.21	1.19
1:A:287:VAL:HG23	1:A:335:PRO:CB	1.74	1.17
1:B:134:TYR:OH	1:B:218:LYS:HD2	1.44	1.15
1:A:70:GLY:HA3	1:A:73:LEU:HD11	1.24	1.15
1:B:47:VAL:C	1:B:72:TRP:HZ3	1.59	1.08
1:A:152:MSE:CE	1:A:252:ILE:HG21	1.84	1.07
1:A:40:THR:O	1:B:39:MSE:CE	2.04	1.06
1:A:287:VAL:CG2	1:A:335:PRO:HB3	1.85	1.05
1:C:152:MSE:HE2	1:C:252:ILE:HG21	1.38	1.04
1:B:252:ILE:HD11	1:B:254:LEU:HD23	1.40	1.02
1:A:41:PHE:HA	1:B:39:MSE:HE3	1.38	1.01
1:B:277:GLY:HA2	1:B:320:GLU:OE2	1.62	0.99
1:B:17:SER:OG	1:C:11:PRO:HA	1.63	0.99
1:C:152:MSE:CE	1:C:252:ILE:HG21	1.93	0.98
1:A:156:THR:HG21	1:A:179:GLY:O	1.64	0.95
1:B:267:TRP:O	1:B:328:VAL:HG13	1.67	0.95
1:A:40:THR:O	1:B:39:MSE:HE1	1.65	0.94
1:C:244:LEU:O	1:C:244:LEU:HD23	1.67	0.94
1:B:175:THR:HG21	1:C:82:TRP:HZ2	1.31	0.94
1:B:134:TYR:CZ	1:B:218:LYS:HD2	2.02	0.93
1:A:287:VAL:HG23	1:A:335:PRO:HB3	0.92	0.91
1:B:47:VAL:C	1:B:72:TRP:CZ3	2.50	0.89
1:C:267:TRP:HB3	1:C:329:VAL:HG22	1.53	0.88
1:C:206:THR:OG1	1:C:207:PRO:HD2	1.75	0.87
1:B:47:VAL:O	1:B:72:TRP:CZ3	2.29	0.86
1:A:132:ALA:CB	1:A:157:ASP:OD1	2.25	0.85
1:A:14:LEU:CD1	1:C:20:SER:HB3	2.07	0.85
1:A:287:VAL:HG21	1:A:331:ILE:HD12	1.57	0.84
1:B:144:ASN:HD22	1:B:144:ASN:H	1.25	0.84
1:A:33:HIS:NE2	1:A:39:MSE:HE3	1.92	0.83
1:B:33:HIS:NE2	1:B:39:MSE:HE2	1.93	0.83
1:B:33:HIS:CE1	1:B:39:MSE:HE2	2.13	0.83
1:A:287:VAL:CG2	1:A:331:ILE:HD12	2.07	0.83
1:B:14:LEU:HD12	1:B:14:LEU:C	2.05	0.81
1:A:170:GLN:HG2	1:B:127:ALA:O	1.80	0.81
1:C:290:VAL:HG22	1:C:331:ILE:HA	1.62	0.81
1:C:266:THR:HG22	1:C:328:VAL:HG12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:THR:CG2	1:C:328:VAL:HG12	2.10	0.80
1:A:200:SER:HA	1:A:237:SER:HB3	1.63	0.80
1:A:208:PRO:HG2	1:A:227:LEU:HD11	1.63	0.80
1:B:48:THR:O	1:B:72:TRP:HH2	1.65	0.80
1:B:299:ARG:O	1:C:297:GLY:HA2	1.82	0.79
1:C:294:ASP:HA	1:C:299:ARG:HA	1.64	0.79
1:A:132:ALA:HB3	1:A:157:ASP:OD1	1.82	0.79
1:B:252:ILE:CD1	1:B:254:LEU:HD23	2.13	0.78
1:C:102:ASN:OD1	1:C:104:THR:OG1	2.01	0.78
1:A:79:GLY:HA3	1:C:77:GLY:HA3	1.65	0.78
1:B:175:THR:HG21	1:C:82:TRP:CZ2	2.17	0.78
1:A:298:SER:HA	1:B:297:GLY:C	2.08	0.77
1:C:190:ILE:CG1	1:C:246:VAL:HG12	2.14	0.77
1:A:90:SER:HA	1:A:109:THR:O	1.85	0.77
1:C:50:LEU:O	1:C:53:SER:OG	2.03	0.77
1:C:232:ILE:CD1	1:C:246:VAL:HG21	2.14	0.77
1:C:244:LEU:HD23	1:C:244:LEU:C	2.09	0.77
1:B:47:VAL:O	1:B:72:TRP:HZ3	1.66	0.77
1:A:75:LEU:HD12	1:A:75:LEU:H	1.50	0.76
1:A:70:GLY:CA	1:A:73:LEU:HD11	2.11	0.76
1:B:145:MSE:SE	1:B:163:PHE:CE2	2.88	0.76
1:B:274:ALA:HB3	1:B:324:GLU:N	2.00	0.76
1:A:7:GLN:HG3	1:C:14:LEU:HA	1.65	0.76
1:A:81:ARG:HH11	1:A:81:ARG:CB	1.99	0.76
1:C:195:LEU:O	1:C:241:SER:N	2.19	0.75
1:A:270:ASN:O	1:A:270:ASN:ND2	2.18	0.75
1:A:124:ILE:C	1:A:124:ILE:HD12	2.12	0.74
1:B:252:ILE:HD11	1:B:254:LEU:CD2	2.17	0.74
1:C:239:PRO:O	1:C:242:THR:OG1	2.05	0.74
1:B:145:MSE:SE	1:B:163:PHE:HE2	2.21	0.73
1:C:92:ASN:HA	1:C:111:VAL:HG13	1.70	0.73
1:A:55:ARG:HD3	1:A:72:TRP:CE3	2.25	0.72
1:A:81:ARG:HH11	1:A:81:ARG:HB2	1.54	0.72
1:A:22:ILE:HA	1:B:16:THR:HG22	1.70	0.72
1:C:186:TYR:HD1	1:C:249:TYR:HB3	1.55	0.72
1:B:118:ILE:HD13	1:C:84:THR:HG23	1.72	0.71
1:B:298:SER:HB2	1:C:297:GLY:C	2.15	0.71
1:C:132:ALA:HA	1:C:155:THR:O	1.89	0.71
1:A:40:THR:O	1:B:39:MSE:HE2	1.89	0.71
1:C:152:MSE:HE2	1:C:252:ILE:CG2	2.19	0.71
1:A:21:ASN:ND2	1:C:7:GLN:HE22	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLY:CA	1:B:320:GLU:OE2	2.38	0.70
1:A:14:LEU:HD11	1:C:20:SER:HB3	1.71	0.70
1:A:244:LEU:O	1:A:244:LEU:HD23	1.91	0.70
1:C:87:HIS:ND1	1:C:105:THR:HG21	2.06	0.70
1:B:140:PRO:HB2	1:B:143:ASN:O	1.92	0.70
1:C:195:LEU:O	1:C:241:SER:CA	2.40	0.69
1:B:146:TYR:HE2	1:B:174:ILE:CD1	2.05	0.69
1:C:190:ILE:HD11	1:C:246:VAL:CG1	2.22	0.69
1:C:195:LEU:O	1:C:241:SER:HA	1.93	0.69
1:A:297:GLY:HA3	1:C:298:SER:HB3	1.74	0.68
1:A:108:SER:O	1:A:136:LEU:HD12	1.94	0.68
1:A:55:ARG:HD3	1:A:72:TRP:CZ3	2.29	0.68
1:B:204:LEU:HD11	1:B:232:ILE:HD11	1.76	0.68
1:B:146:TYR:CE2	1:B:174:ILE:HD12	2.28	0.68
1:B:274:ALA:HB3	1:B:324:GLU:H	1.59	0.68
1:A:201:ALA:HB2	1:A:233:THR:HG23	1.75	0.67
1:B:274:ALA:HB1	1:B:322:ASP:O	1.94	0.67
1:A:287:VAL:CG2	1:A:331:ILE:CD1	2.72	0.67
1:A:298:SER:HB2	1:B:297:GLY:HA3	1.76	0.67
1:C:281:ILE:HB	1:C:315:ILE:HB	1.75	0.67
1:B:134:TYR:OH	1:B:218:LYS:CD	2.35	0.67
1:C:266:THR:CG2	1:C:328:VAL:CG1	2.73	0.67
1:A:331:ILE:HD13	1:A:332:ASN:H	1.60	0.66
1:C:14:LEU:C	1:C:14:LEU:HD12	2.21	0.66
1:B:298:SER:HB2	1:C:298:SER:N	2.10	0.66
1:A:14:LEU:HD12	1:A:14:LEU:N	2.11	0.66
1:A:106:GLY:HA2	1:A:134:TYR:CD2	2.29	0.66
1:C:87:HIS:CG	1:C:105:THR:HG21	2.31	0.66
1:B:40:THR:O	1:C:33:HIS:NE2	2.29	0.65
1:B:106:GLY:HA2	1:B:134:TYR:CD1	2.31	0.65
1:B:180:LEU:HD22	1:B:254:LEU:HD13	1.78	0.65
1:C:212:ASP:OD1	1:C:249:TYR:HE2	1.79	0.65
1:B:252:ILE:HD12	1:B:252:ILE:C	2.22	0.65
1:B:180:LEU:HD22	1:B:254:LEU:CD1	2.26	0.65
1:C:201:ALA:HA	1:C:232:ILE:O	1.97	0.65
1:A:134:TYR:CZ	1:A:218:LYS:HG2	2.31	0.64
1:A:189:GLU:H	1:A:189:GLU:CD	2.04	0.64
1:B:180:LEU:HB3	1:B:254:LEU:HD12	1.79	0.64
1:C:64:GLU:C	1:C:75:LEU:CD1	2.71	0.64
1:B:290:VAL:HG21	1:B:308:PHE:CZ	2.32	0.63
1:C:184:ARG:NH2	1:C:249:TYR:OH	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:HA	1:A:149:THR:HA	1.77	0.63
1:B:144:ASN:H	1:B:144:ASN:ND2	1.96	0.63
1:C:145:MSE:HB3	1:C:172:TRP:HB2	1.80	0.63
1:C:190:ILE:HG13	1:C:246:VAL:HG12	1.79	0.63
1:A:121:SER:HB3	1:A:163:PHE:O	1.98	0.63
1:B:174:ILE:HG21	1:B:180:LEU:HD11	1.79	0.63
1:C:85:LEU:HD12	1:C:86:PRO:HD2	1.79	0.63
1:A:55:ARG:HD3	1:A:72:TRP:CD2	2.34	0.63
1:A:287:VAL:HG22	1:A:331:ILE:CD1	2.28	0.63
1:A:124:ILE:HD12	1:A:124:ILE:O	1.98	0.63
1:A:188:ARG:HD3	1:A:248:GLU:HB2	1.81	0.63
1:A:14:LEU:HD12	1:C:20:SER:HB3	1.81	0.62
1:A:57:ASN:CG	1:A:60:SER:HB2	2.24	0.62
1:B:90:SER:HA	1:B:109:THR:O	2.00	0.62
1:A:78:GLY:H	1:B:79:GLY:HA2	1.65	0.61
1:A:152:MSE:HE1	1:A:252:ILE:CG2	2.14	0.61
1:C:169:GLU:CD	1:C:169:GLU:H	2.07	0.61
1:A:115:PRO:CD	1:A:143:ASN:OD1	2.48	0.61
1:B:48:THR:C	1:B:72:TRP:CH2	2.78	0.61
1:B:219:ARG:NH2	1:B:222:GLU:OE1	2.34	0.61
1:C:266:THR:HG22	1:C:328:VAL:CG1	2.31	0.61
1:C:204:LEU:HD11	1:C:232:ILE:HD11	1.82	0.61
1:A:108:SER:O	1:A:136:LEU:CD1	2.48	0.61
1:A:289:ASP:HB3	1:A:332:ASN:HB2	1.83	0.61
1:B:126:ASP:CG	1:B:131:PHE:CD1	2.79	0.60
1:B:48:THR:O	1:B:72:TRP:CH2	2.50	0.60
1:B:219:ARG:HG2	1:B:219:ARG:HH11	1.66	0.60
1:C:125:CYS:HB2	1:C:160:SER:OG	2.01	0.60
1:A:252:ILE:O	1:A:252:ILE:HG23	2.01	0.60
1:B:195:LEU:N	1:B:195:LEU:HD23	2.16	0.60
1:C:266:THR:HG21	1:C:328:VAL:CG1	2.32	0.60
1:A:14:LEU:HD12	1:A:14:LEU:H	1.67	0.60
1:A:79:GLY:CA	1:C:77:GLY:HA3	2.32	0.60
1:B:118:ILE:HD13	1:C:84:THR:CG2	2.30	0.60
1:C:186:TYR:CD1	1:C:249:TYR:HB3	2.36	0.60
1:B:208:PRO:HG2	1:B:227:LEU:CD1	2.31	0.60
1:B:47:VAL:CA	1:B:72:TRP:HZ3	2.15	0.59
1:B:146:TYR:HE2	1:B:174:ILE:HD12	1.65	0.59
1:A:154:ILE:HG21	1:A:159:VAL:HG11	1.84	0.59
1:C:212:ASP:OD1	1:C:249:TYR:CE2	2.55	0.59
1:C:204:LEU:HD11	1:C:232:ILE:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HD22	1:B:144:ASN:N	1.93	0.59
1:C:330:ILE:HD13	1:C:330:ILE:N	2.18	0.59
1:A:41:PHE:HA	1:B:39:MSE:CE	2.24	0.59
1:B:146:TYR:CE2	1:B:174:ILE:CD1	2.85	0.59
1:B:274:ALA:CB	1:B:325:ASP:H	2.15	0.59
1:C:64:GLU:C	1:C:75:LEU:HD12	2.28	0.59
1:A:169:GLU:CD	1:A:169:GLU:H	2.10	0.58
1:A:291:PRO:HD2	1:A:331:ILE:HA	1.84	0.58
1:B:175:THR:CG2	1:C:82:TRP:HZ2	2.11	0.58
1:B:219:ARG:HG2	1:B:219:ARG:NH1	2.18	0.58
1:C:87:HIS:NE2	1:C:108:SER:HB3	2.17	0.58
1:A:132:ALA:HB2	1:A:157:ASP:OD1	2.01	0.58
1:B:102:ASN:ND2	1:B:128:TYR:CE2	2.71	0.58
1:A:115:PRO:HD2	1:A:143:ASN:OD1	2.04	0.58
1:A:21:ASN:HD22	1:C:7:GLN:HE22	1.50	0.58
1:B:40:THR:O	1:C:33:HIS:CD2	2.56	0.58
1:A:287:VAL:HG23	1:A:335:PRO:CG	2.34	0.58
1:A:287:VAL:HG22	1:A:331:ILE:HD12	1.86	0.58
1:A:21:ASN:HD22	1:C:7:GLN:NE2	2.02	0.57
1:A:287:VAL:HG13	1:A:331:ILE:HD11	1.86	0.57
1:C:266:THR:HG21	1:C:328:VAL:HG12	1.86	0.57
1:C:87:HIS:ND1	1:C:105:THR:CG2	2.67	0.57
1:B:14:LEU:C	1:B:14:LEU:CD1	2.76	0.57
1:B:208:PRO:HG2	1:B:227:LEU:HD11	1.86	0.57
1:A:118:ILE:CD1	1:B:84:THR:HG23	2.34	0.57
1:A:289:ASP:O	1:A:331:ILE:HG12	2.05	0.57
1:B:65:GLY:N	1:B:75:LEU:HD21	2.19	0.57
1:A:14:LEU:CD1	1:A:14:LEU:C	2.78	0.57
1:A:244:LEU:HD23	1:A:244:LEU:C	2.29	0.56
1:C:84:THR:HA	1:C:100:LEU:HB2	1.86	0.56
1:B:304:LEU:CB	1:C:326:GLU:OE2	2.53	0.56
1:A:82:TRP:O	1:A:83:GLU:HB3	2.06	0.56
1:A:255:GLY:HA2	1:B:179:GLY:HA2	1.88	0.56
1:B:238:LEU:HD23	1:B:238:LEU:N	2.20	0.56
1:C:85:LEU:HD12	1:C:86:PRO:CD	2.35	0.56
1:A:117:ARG:HB2	1:A:117:ARG:NH1	2.21	0.56
1:B:301:TYR:CE2	1:C:328:VAL:HG11	2.40	0.56
1:C:55:ARG:HD3	1:C:72:TRP:CE3	2.41	0.56
1:C:296:ASN:HA	1:C:326:GLU:HB2	1.87	0.56
1:A:191:PHE:HD2	1:A:244:LEU:HD21	1.71	0.56
1:C:197:SER:O	1:C:199:THR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:HD12	1:B:80:ILE:H	1.70	0.55
1:B:109:THR:HB	1:B:137:THR:HB	1.89	0.55
1:C:152:MSE:HE1	1:C:252:ILE:HG21	1.84	0.55
1:A:268:VAL:HG22	1:A:328:VAL:HG13	1.87	0.55
1:C:87:HIS:CG	1:C:105:THR:CG2	2.89	0.55
1:C:169:GLU:OE1	1:C:169:GLU:N	2.37	0.55
1:A:41:PHE:CE1	1:C:54:VAL:HG21	2.42	0.55
1:B:65:GLY:N	1:B:75:LEU:CD2	2.69	0.55
1:B:301:TYR:CZ	1:C:328:VAL:HG11	2.41	0.55
1:A:227:LEU:HG	1:A:232:ILE:HD13	1.89	0.55
1:C:27:ASN:ND2	1:C:31:MSE:HG3	2.23	0.54
1:A:287:VAL:HG11	1:A:331:ILE:HG13	1.88	0.54
1:B:306:PHE:HB3	1:B:317:LEU:HA	1.88	0.54
1:B:274:ALA:CB	1:B:322:ASP:O	2.56	0.54
1:C:9:LEU:HG	1:C:11:PRO:HD3	1.89	0.54
1:A:268:VAL:HG12	1:A:269:TYR:N	2.22	0.54
1:B:291:PRO:HD3	1:B:332:ASN:CB	2.37	0.54
1:A:249:TYR:CD1	1:A:249:TYR:C	2.86	0.54
1:B:274:ALA:HB2	1:B:325:ASP:N	2.23	0.54
1:C:55:ARG:HD3	1:C:72:TRP:CZ3	2.43	0.53
1:C:213:VAL:HG22	1:C:246:VAL:HG22	1.90	0.53
1:A:152:MSE:HE2	1:A:252:ILE:HG21	1.81	0.53
1:C:168:PRO:HD2	1:C:169:GLU:CD	2.33	0.53
1:C:267:TRP:CZ2	1:C:284:ASP:OD1	2.61	0.53
1:A:308:PHE:CD1	1:A:308:PHE:C	2.87	0.53
1:A:55:ARG:HD3	1:A:72:TRP:CH2	2.44	0.53
1:A:126:ASP:OD2	1:A:157:ASP:O	2.27	0.53
1:A:142:GLY:HA2	1:A:149:THR:CG2	2.39	0.53
1:A:293:ILE:HG13	1:A:329:VAL:HA	1.91	0.53
1:B:213:VAL:HG12	1:B:220:LEU:HB2	1.90	0.52
1:C:191:PHE:CD1	1:C:191:PHE:C	2.88	0.52
1:A:290:VAL:HG12	1:A:290:VAL:O	2.10	0.52
1:B:227:LEU:O	1:B:227:LEU:HD23	2.09	0.52
1:A:53:SER:HA	1:B:39:MSE:O	2.09	0.52
1:A:213:VAL:HG13	1:A:246:VAL:HG23	1.92	0.52
1:B:234:PHE:CD1	1:B:234:PHE:N	2.77	0.52
1:C:190:ILE:HD11	1:C:246:VAL:HG11	1.92	0.52
1:A:247:ILE:HD12	1:A:247:ILE:N	2.24	0.52
1:A:298:SER:HA	1:B:298:SER:N	2.24	0.52
1:A:306:PHE:CD1	1:A:306:PHE:C	2.88	0.52
1:C:191:PHE:CE1	1:C:244:LEU:CD2	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:OE1	1:A:169:GLU:N	2.43	0.51
1:B:214:TYR:CE1	1:B:219:ARG:HB2	2.45	0.51
1:A:7:GLN:HG3	1:C:14:LEU:CA	2.39	0.51
1:B:33:HIS:CE1	1:C:31:MSE:CE	2.92	0.51
1:B:180:LEU:HB3	1:B:254:LEU:CD1	2.40	0.51
1:A:55:ARG:HD3	1:A:72:TRP:CE2	2.46	0.51
1:B:40:THR:HB	1:C:31:MSE:O	2.11	0.51
1:C:161:ALA:HB1	1:C:174:ILE:HD13	1.92	0.51
1:C:291:PRO:HA	1:C:302:LYS:CB	2.41	0.51
1:C:308:PHE:CD1	1:C:308:PHE:C	2.87	0.51
1:B:175:THR:CG2	1:C:82:TRP:CZ2	2.89	0.51
1:B:291:PRO:CD	1:B:332:ASN:CB	2.88	0.51
1:C:138:VAL:HG12	1:C:145:MSE:HE1	1.93	0.51
1:B:186:TYR:CD1	1:B:249:TYR:HB3	2.46	0.51
1:A:132:ALA:HA	1:A:155:THR:O	2.11	0.51
1:A:13:GLY:HA2	1:C:16:THR:CG2	2.42	0.50
1:B:33:HIS:HE1	1:C:31:MSE:CE	2.23	0.50
1:A:298:SER:CB	1:B:297:GLY:HA3	2.39	0.50
1:B:159:VAL:HG22	1:B:160:SER:H	1.77	0.50
1:B:278:GLU:O	1:B:278:GLU:HG2	2.10	0.50
1:A:11:PRO:HA	1:C:17:SER:HB2	1.93	0.50
1:C:191:PHE:HE1	1:C:244:LEU:CD2	2.24	0.50
1:A:137:THR:HA	1:A:153:ALA:HA	1.93	0.50
1:C:112:LEU:HD12	1:C:172:TRP:CD1	2.46	0.50
1:B:265:ILE:CB	1:B:331:ILE:CB	2.89	0.50
1:A:102:ASN:OD1	1:A:104:THR:HB	2.11	0.50
1:A:206:THR:HG23	1:A:207:PRO:HD2	1.93	0.50
1:A:118:ILE:HD13	1:B:84:THR:HG23	1.94	0.50
1:A:145:MSE:N	1:A:148:SER:O	2.41	0.50
1:C:186:TYR:HD1	1:C:249:TYR:CB	2.25	0.50
1:C:66:TYR:HD1	1:C:72:TRP:CD1	2.30	0.49
1:C:156:THR:O	1:C:159:VAL:HG12	2.12	0.49
1:B:106:GLY:HA2	1:B:134:TYR:CG	2.47	0.49
1:A:13:GLY:HA2	1:C:16:THR:HG23	1.95	0.49
1:A:286:VAL:HA	1:A:313:SER:HB3	1.94	0.49
1:B:182:GLN:HE22	1:B:253:GLN:HB2	1.78	0.49
1:B:121:SER:HA	1:B:163:PHE:O	2.12	0.49
1:B:296:ASN:HA	1:B:326:GLU:HB3	1.95	0.49
1:A:51:PRO:O	1:A:52:SER:OG	2.28	0.49
1:A:78:GLY:HA2	1:B:80:ILE:HD11	1.93	0.49
1:A:287:VAL:CG2	1:A:335:PRO:CG	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:VAL:HG23	1:B:328:VAL:HG22	1.95	0.49
1:B:292:ALA:HA	1:B:306:PHE:HZ	1.78	0.49
1:C:225:TYR:O	1:C:225:TYR:CD1	2.66	0.48
1:A:286:VAL:HG12	1:A:313:SER:HB3	1.95	0.48
1:C:125:CYS:CB	1:C:160:SER:OG	2.61	0.48
1:C:201:ALA:HB2	1:C:233:THR:HA	1.95	0.48
1:C:321:LEU:HD11	1:C:325:ASP:HB2	1.96	0.48
1:A:144:ASN:OD1	1:A:147:GLY:C	2.57	0.48
1:B:14:LEU:HD12	1:B:14:LEU:O	2.13	0.48
1:B:274:ALA:HB2	1:B:325:ASP:H	1.77	0.48
1:B:293:ILE:CB	1:B:306:PHE:HE2	2.27	0.48
1:C:252:ILE:HG23	1:C:254:LEU:HD21	1.94	0.48
1:B:81:ARG:O	1:B:98:GLY:N	2.25	0.48
1:C:191:PHE:CE1	1:C:193:GLN:HB2	2.48	0.48
1:B:222:GLU:HA	1:B:225:TYR:CE1	2.49	0.48
1:A:287:VAL:HG22	1:A:288:ASP:H	1.78	0.47
1:B:191:PHE:CE1	1:B:244:LEU:HD23	2.48	0.47
1:A:81:ARG:HH11	1:A:81:ARG:CG	2.27	0.47
1:A:124:ILE:C	1:A:124:ILE:CD1	2.83	0.47
1:C:138:VAL:CG1	1:C:145:MSE:HE1	2.44	0.47
1:A:67:TYR:CD2	1:A:73:LEU:HD12	2.50	0.47
1:A:78:GLY:H	1:B:79:GLY:CA	2.28	0.47
1:A:336:HIS:CG	1:A:336:HIS:O	2.67	0.47
1:B:278:GLU:OE1	1:B:321:LEU:CB	2.62	0.47
1:C:252:ILE:HG23	1:C:252:ILE:O	2.13	0.47
1:A:76:GLY:HA3	1:B:75:LEU:O	2.14	0.47
1:A:178:VAL:HG12	1:C:180:LEU:HD12	1.96	0.47
1:B:191:PHE:CD1	1:B:191:PHE:C	2.92	0.47
1:C:147:GLY:O	1:C:148:SER:C	2.57	0.47
1:A:49:GLY:HA3	1:A:66:TYR:CD2	2.49	0.47
1:A:117:ARG:CB	1:A:117:ARG:CZ	2.92	0.47
1:A:285:ILE:CB	1:A:337:HIS:O	2.62	0.47
1:B:20:SER:HB3	1:C:14:LEU:O	2.15	0.47
1:C:51:PRO:O	1:C:52:SER:HB3	2.15	0.47
1:A:308:PHE:CE2	1:A:313:SER:HA	2.49	0.47
1:C:204:LEU:HD11	1:C:232:ILE:HG13	1.97	0.47
1:B:144:ASN:ND2	1:B:144:ASN:N	2.57	0.47
1:A:238:LEU:N	1:A:238:LEU:HD23	2.30	0.46
1:B:102:ASN:C	1:B:102:ASN:OD1	2.58	0.46
1:B:308:PHE:CE2	1:B:313:SER:HA	2.51	0.46
1:A:118:ILE:HD11	1:B:84:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:HIS:C	1:B:87:HIS:CD2	2.93	0.46
1:C:118:ILE:HD12	1:C:118:ILE:H	1.81	0.46
1:C:197:SER:O	1:C:199:THR:HG23	2.14	0.46
1:C:154:ILE:HG22	1:C:159:VAL:HG11	1.97	0.46
1:A:144:ASN:HA	1:A:148:SER:O	2.15	0.46
1:A:292:ALA:HB2	1:A:301:TYR:HA	1.97	0.46
1:B:186:TYR:HE1	1:B:212:ASP:HB2	1.79	0.46
1:C:26:ASN:C	1:C:26:ASN:OD1	2.58	0.46
1:A:93:LEU:O	1:A:94:LEU:HD23	2.15	0.46
1:A:154:ILE:CG2	1:A:159:VAL:HG11	2.45	0.46
1:A:27:ASN:ND2	1:A:31:MSE:HE3	2.31	0.46
1:A:112:LEU:HD22	1:A:138:VAL:CG1	2.45	0.46
1:B:289:ASP:CB	1:B:332:ASN:O	2.63	0.46
1:A:181:GLY:HA3	1:C:256:ASN:ND2	2.31	0.46
1:B:17:SER:HG	1:C:11:PRO:HA	1.74	0.46
1:A:93:LEU:HG	1:A:99:TYR:CD1	2.51	0.46
1:A:206:THR:CG2	1:A:207:PRO:HD2	2.45	0.46
1:B:33:HIS:NE2	1:B:39:MSE:CE	2.74	0.46
1:B:119:GLY:HA3	1:C:82:TRP:HB2	1.97	0.46
1:B:191:PHE:HE1	1:B:244:LEU:HD23	1.78	0.46
1:B:290:VAL:HG21	1:B:308:PHE:CE2	2.51	0.46
1:C:190:ILE:CD1	1:C:246:VAL:HG12	2.46	0.46
1:C:168:PRO:HD2	1:C:169:GLU:OE1	2.16	0.45
1:B:47:VAL:CA	1:B:72:TRP:CZ3	2.97	0.45
1:B:189:GLU:HA	1:B:247:ILE:HG23	1.98	0.45
1:B:249:TYR:CD1	1:B:249:TYR:C	2.94	0.45
1:A:126:ASP:CG	1:A:131:PHE:CD1	2.95	0.45
1:B:33:HIS:CE1	1:C:31:MSE:HE3	2.51	0.45
1:C:154:ILE:CG2	1:C:159:VAL:HG11	2.47	0.45
1:A:115:PRO:HD3	1:A:143:ASN:OD1	2.16	0.45
1:C:232:ILE:HD13	1:C:246:VAL:HG21	1.94	0.45
1:A:189:GLU:N	1:A:189:GLU:OE1	2.49	0.45
1:A:287:VAL:CG2	1:A:335:PRO:CB	2.65	0.45
1:B:290:VAL:CG2	1:B:308:PHE:CZ	2.99	0.45
1:B:144:ASN:O	1:B:171:GLY:HA3	2.16	0.45
1:C:93:LEU:HD22	1:C:99:TYR:CD2	2.51	0.45
1:C:187:SER:HB3	1:C:248:GLU:O	2.17	0.45
1:A:16:THR:HB	1:B:13:GLY:HA2	1.99	0.45
1:A:57:ASN:HB3	1:A:60:SER:CB	2.47	0.45
1:B:40:THR:O	1:B:40:THR:HG22	2.16	0.44
1:C:112:LEU:HD13	1:C:172:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:HG12	1:A:145:MSE:HE1	1.99	0.44
1:A:287:VAL:CG1	1:A:331:ILE:HD11	2.47	0.44
1:B:274:ALA:O	1:B:323:ALA:HA	2.17	0.44
1:C:51:PRO:O	1:C:52:SER:CB	2.65	0.44
1:C:221:ALA:C	1:C:223:SER:N	2.74	0.44
1:C:225:TYR:HB3	1:C:234:PHE:HD1	1.81	0.44
1:A:287:VAL:HG21	1:A:335:PRO:HG3	2.00	0.44
1:A:293:ILE:HD11	1:A:329:VAL:HG13	2.00	0.44
1:B:180:LEU:HD12	1:C:178:VAL:HG22	1.98	0.44
1:C:14:LEU:HD12	1:C:15:GLU:N	2.32	0.44
1:A:93:LEU:C	1:A:94:LEU:HD23	2.42	0.44
1:A:149:THR:HG22	1:A:149:THR:O	2.16	0.44
1:A:286:VAL:HA	1:A:313:SER:CB	2.48	0.44
1:A:102:ASN:ND2	1:A:128:TYR:CE2	2.86	0.44
1:A:134:TYR:CZ	1:A:218:LYS:CG	2.99	0.44
1:A:234:PHE:CD2	1:A:238:LEU:HD21	2.52	0.44
1:A:268:VAL:CG2	1:A:328:VAL:HG13	2.48	0.44
1:B:30:THR:O	1:C:24:GLY:HA3	2.17	0.44
1:B:252:ILE:HD12	1:B:253:GLN:N	2.33	0.44
1:C:112:LEU:HD13	1:C:172:TRP:CE2	2.53	0.44
1:A:155:THR:HG23	1:A:184:ARG:HG3	1.99	0.44
1:B:182:GLN:NE2	1:B:253:GLN:OE1	2.51	0.44
1:B:180:LEU:O	1:B:255:GLY:HA3	2.18	0.44
1:C:43:GLU:HA	1:C:56:TYR:O	2.18	0.44
1:C:93:LEU:HD13	1:C:99:TYR:CD2	2.53	0.44
1:A:268:VAL:CG1	1:A:269:TYR:N	2.81	0.43
1:B:40:THR:HG22	1:C:33:HIS:HD2	1.83	0.43
1:C:189:GLU:HG2	1:C:247:ILE:HG12	2.00	0.43
1:C:191:PHE:CZ	1:C:193:GLN:HB2	2.53	0.43
1:A:56:TYR:CE1	1:A:58:PRO:HA	2.53	0.43
1:B:290:VAL:HG23	1:B:308:PHE:CE1	2.54	0.43
1:C:144:ASN:OD1	1:C:144:ASN:C	2.62	0.43
1:B:267:TRP:CZ3	1:B:283:LEU:CD2	3.02	0.43
1:B:292:ALA:HA	1:B:306:PHE:CZ	2.53	0.43
1:C:188:ARG:O	1:C:188:ARG:HG3	2.19	0.43
1:C:204:LEU:HD11	1:C:232:ILE:CG1	2.48	0.43
1:A:22:ILE:HG23	1:B:16:THR:CG2	2.49	0.43
1:A:55:ARG:HD3	1:A:72:TRP:CZ2	2.54	0.43
1:C:119:GLY:C	1:C:120:ASP:O	2.60	0.43
1:C:212:ASP:CG	1:C:249:TYR:CE2	2.96	0.43
1:B:50:LEU:O	1:B:51:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:THR:HA	1:B:331:ILE:O	2.19	0.43
1:C:95:GLU:HG2	1:C:121:SER:H	1.83	0.43
1:C:190:ILE:CD1	1:C:246:VAL:CG1	2.94	0.43
1:C:270:ASN:O	1:C:270:ASN:ND2	2.52	0.43
1:C:87:HIS:CD2	1:C:108:SER:HB3	2.53	0.42
1:A:52:SER:O	1:B:40:THR:HA	2.18	0.42
1:A:132:ALA:CB	1:A:157:ASP:CG	2.92	0.42
1:A:163:PHE:CE2	1:A:174:ILE:HD11	2.55	0.42
1:A:211:VAL:HG12	1:A:248:GLU:HA	2.01	0.42
1:B:176:SER:OG	1:B:177:GLY:N	2.48	0.42
1:B:204:LEU:HD11	1:B:232:ILE:CD1	2.47	0.42
1:A:51:PRO:C	1:A:52:SER:OG	2.61	0.42
1:C:110:VAL:HG13	1:C:136:LEU:HD11	2.00	0.42
1:C:274:ALA:H	1:C:324:GLU:HA	1.83	0.42
1:A:75:LEU:O	1:C:76:GLY:HA3	2.19	0.42
1:A:82:TRP:CZ2	1:C:175:THR:HG21	2.54	0.42
1:B:252:ILE:HG13	1:B:252:ILE:O	2.19	0.42
1:B:254:LEU:HD12	1:B:255:GLY:H	1.85	0.42
1:A:31:MSE:HE3	1:A:31:MSE:HB2	1.81	0.42
1:A:123:THR:OG1	1:A:162:THR:OG1	2.32	0.42
1:C:119:GLY:O	1:C:120:ASP:C	2.62	0.42
1:C:232:ILE:CG2	1:C:234:PHE:CE1	3.03	0.42
1:A:55:ARG:CD	1:A:72:TRP:CE3	3.01	0.42
1:B:308:PHE:HB2	1:B:315:ILE:HA	2.01	0.42
1:C:201:ALA:HB2	1:C:233:THR:HG23	2.02	0.42
1:C:206:THR:OG1	1:C:207:PRO:CD	2.58	0.42
1:C:268:VAL:HG13	1:C:268:VAL:O	2.19	0.42
1:A:50:LEU:O	1:A:51:PRO:C	2.60	0.42
1:C:57:ASN:OD1	1:C:59:ASP:HB2	2.18	0.42
1:A:14:LEU:C	1:A:14:LEU:HD13	2.45	0.42
1:A:287:VAL:HG22	1:A:331:ILE:HD11	1.99	0.42
1:B:211:VAL:HG12	1:B:248:GLU:HA	2.02	0.41
1:A:101:ILE:HG21	1:A:136:LEU:HD22	2.02	0.41
1:A:128:TYR:CD1	1:A:128:TYR:N	2.88	0.41
1:B:46:GLU:HA	1:B:46:GLU:OE1	2.20	0.41
1:B:80:ILE:H	1:B:80:ILE:CD1	2.32	0.41
1:C:145:MSE:O	1:C:146:TYR:C	2.63	0.41
1:C:235:SER:HA	1:C:236:PRO:HA	1.87	0.41
1:B:159:VAL:HG13	1:B:160:SER:N	2.35	0.41
1:A:57:ASN:HB3	1:A:60:SER:HB3	2.01	0.41
1:A:219:ARG:O	1:A:219:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ALA:O	1:C:219:ARG:HD3	2.21	0.41
1:C:221:ALA:C	1:C:223:SER:H	2.28	0.41
1:B:87:HIS:CE1	1:B:105:THR:HB	2.55	0.41
1:B:158:ASN:C	1:B:159:VAL:O	2.63	0.41
1:C:208:PRO:CG	1:C:227:LEU:HD11	2.51	0.41
1:A:123:THR:OG1	1:A:162:THR:HG23	2.19	0.41
1:A:178:VAL:CG1	1:C:180:LEU:HD12	2.51	0.41
1:B:80:ILE:HD12	1:B:80:ILE:N	2.35	0.41
1:A:298:SER:CA	1:B:297:GLY:C	2.89	0.41
1:B:274:ALA:HB3	1:B:325:ASP:H	1.84	0.41
1:C:183:GLY:O	1:C:252:ILE:HG22	2.21	0.41
1:A:22:ILE:HG23	1:B:16:THR:HG21	2.02	0.41
1:C:102:ASN:OD1	1:C:102:ASN:C	2.64	0.41
1:A:75:LEU:HD12	1:A:75:LEU:N	2.27	0.41
1:A:102:ASN:ND2	1:A:128:TYR:CZ	2.89	0.41
1:A:138:VAL:N	1:A:152:MSE:O	2.50	0.41
1:A:156:THR:HB	1:A:159:VAL:HB	2.02	0.41
1:A:268:VAL:HG12	1:A:269:TYR:H	1.83	0.41
1:B:102:ASN:CG	1:B:128:TYR:CD2	2.99	0.41
1:C:249:TYR:CD1	1:C:249:TYR:C	2.98	0.41
1:B:182:GLN:NE2	1:B:253:GLN:HB2	2.35	0.41
1:B:274:ALA:CB	1:B:325:ASP:N	2.81	0.41
1:C:64:GLU:O	1:C:75:LEU:CD1	2.69	0.41
1:C:267:TRP:N	1:C:329:VAL:O	2.42	0.41
1:B:95:GLU:HG2	1:B:120:ASP:HB3	2.03	0.40
1:C:210:ILE:HG13	1:C:249:TYR:O	2.21	0.40
1:C:212:ASP:CG	1:C:249:TYR:HE2	2.28	0.40
1:A:93:LEU:HG	1:A:99:TYR:CE1	2.57	0.40
1:A:268:VAL:CG1	1:A:269:TYR:H	2.33	0.40
1:B:49:GLY:CA	1:B:72:TRP:CH2	3.03	0.40
1:B:249:TYR:CD1	1:B:249:TYR:O	2.75	0.40
1:C:85:LEU:HD12	1:C:86:PRO:N	2.36	0.40
1:C:14:LEU:C	1:C:14:LEU:CD1	2.90	0.40
1:C:67:TYR:CD2	1:C:73:LEU:HB2	2.56	0.40
1:A:106:GLY:HA2	1:A:134:TYR:CE2	2.55	0.40
1:A:142:GLY:HA2	1:A:149:THR:HG23	2.04	0.40
1:A:316:THR:O	1:A:316:THR:OG1	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/341 (95%)	274 (84%)	40 (12%)	11 (3%)	3	15
1	B	327/341 (96%)	288 (88%)	29 (9%)	10 (3%)	3	17
1	C	320/341 (94%)	263 (82%)	42 (13%)	15 (5%)	2	10
All	All	972/1023 (95%)	825 (85%)	111 (11%)	36 (4%)	2	14

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	298	SER
1	B	169	GLU
1	C	188	ARG
1	C	198	GLU
1	A	24	GLY
1	A	78	GLY
1	A	291	PRO
1	A	304	LEU
1	C	215	ALA
1	B	23	LYS
1	B	263	SER
1	B	296	ASN
1	B	304	LEU
1	C	24	GLY
1	C	44	ASP
1	C	201	ALA
1	C	304	LEU
1	A	275	ILE
1	B	69	ASN
1	C	52	SER
1	A	105	THR
1	B	35	PRO
1	B	159	VAL

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Mol	Chain	Res	Type
1	C	291	PRO
1	A	112	LEU
1	B	46	GLU
1	C	251	PRO
1	C	326	GLU
1	A	140	PRO
1	A	208	PRO
1	B	208	PRO
1	C	229	GLY
1	C	287	VAL
1	C	305	GLY
1	C	285	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/280 (84%)	157 (67%)	78 (33%)	0	1
1	B	249/280 (89%)	191 (77%)	58 (23%)	1	4
1	C	252/280 (90%)	202 (80%)	50 (20%)	1	7
All	All	736/840 (88%)	550 (75%)	186 (25%)	0	3

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	7	GLN
1	A	9	LEU
1	A	12	MSE
1	A	14	LEU
1	A	18	GLU
1	A	23	LYS
1	A	34	SER
1	A	50	LEU
1	A	52	SER

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Mol	Chain	Res	Type
1	A	59	ASP
1	A	60	SER
1	A	62	GLU
1	A	73	LEU
1	A	75	LEU
1	A	80	ILE
1	A	81	ARG
1	A	84	THR
1	A	91	SER
1	A	100	LEU
1	A	101	ILE
1	A	112	LEU
1	A	117	ARG
1	A	118	ILE
1	A	121	SER
1	A	128	TYR
1	A	133	THR
1	A	141	SER
1	A	144	ASN
1	A	145	MSE
1	A	152	MSE
1	A	157	ASP
1	A	160	SER
1	A	169	GLU
1	A	170	GLN
1	A	178	VAL
1	A	188	ARG
1	A	189	GLU
1	A	194	ILE
1	A	200	SER
1	A	205	ASN
1	A	211	VAL
1	A	213	VAL
1	A	219	ARG
1	A	222	GLU
1	A	223	SER
1	A	226	SER
1	A	227	LEU
1	A	228	ASP
1	A	231	VAL
1	A	232	ILE
1	A	233	THR

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Mol	Chain	Res	Type
1	A	237	SER
1	A	238	LEU
1	A	242	THR
1	A	244	LEU
1	A	246	VAL
1	A	247	ILE
1	A	252	ILE
1	A	254	LEU
1	A	256	ASN
1	A	266	THR
1	A	270	ASN
1	A	273	SER
1	A	282	THR
1	A	284	ASP
1	A	293	ILE
1	A	294	ASP
1	A	295	ILE
1	A	298	SER
1	A	308	PHE
1	A	316	THR
1	A	319	GLN
1	A	325	ASP
1	A	329	VAL
1	A	331	ILE
1	A	332	ASN
1	A	334	THR
1	B	6	THR
1	B	12	MSE
1	B	14	LEU
1	B	23	LYS
1	B	33	HIS
1	B	35	PRO
1	B	39	MSE
1	B	40	THR
1	B	47	VAL
1	B	54	VAL
1	B	73	LEU
1	B	74	SER
1	B	80	ILE
1	B	81	ARG
1	B	84	THR
1	B	85	LEU

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Mol	Chain	Res	Type
1	B	89	PRO
1	B	90	SER
1	B	104	THR
1	B	107	THR
1	B	111	VAL
1	B	124	ILE
1	B	133	THR
1	B	140	PRO
1	B	144	ASN
1	B	145	MSE
1	B	148	SER
1	B	150	GLU
1	B	169	GLU
1	B	175	THR
1	B	176	SER
1	B	184	ARG
1	B	187	SER
1	B	193	GLN
1	B	200	SER
1	B	203	THR
1	B	208	PRO
1	B	210	ILE
1	B	212	ASP
1	B	213	VAL
1	B	218	LYS
1	B	220	LEU
1	B	227	LEU
1	B	228	ASP
1	B	230	ASN
1	B	231	VAL
1	B	232	ILE
1	B	238	LEU
1	B	242	THR
1	B	245	GLN
1	B	247	ILE
1	B	248	GLU
1	B	252	ILE
1	B	254	LEU
1	B	270	ASN
1	B	290	VAL
1	B	307	THR
1	B	324	GLU

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Mol	Chain	Res	Type
1	C	6	THR
1	C	14	LEU
1	C	15	GLU
1	C	53	SER
1	C	60	SER
1	C	80	ILE
1	C	83	GLU
1	C	90	SER
1	C	92	ASN
1	C	94	LEU
1	C	104	THR
1	C	111	VAL
1	C	117	ARG
1	C	133	THR
1	C	144	ASN
1	C	152	MSE
1	C	155	THR
1	C	156	THR
1	C	158	ASN
1	C	169	GLU
1	C	174	ILE
1	C	176	SER
1	C	178	VAL
1	C	199	THR
1	C	210	ILE
1	C	219	ARG
1	C	235	SER
1	C	237	SER
1	C	238	LEU
1	C	242	THR
1	C	244	LEU
1	C	245	GLN
1	C	246	VAL
1	C	254	LEU
1	C	266	THR
1	C	273	SER
1	C	275	ILE
1	C	279	THR
1	C	281	ILE
1	C	282	THR
1	C	289	ASP
1	C	291	PRO

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Mol	Chain	Res	Type
1	C	298	SER
1	C	307	THR
1	C	309	ASP
1	C	315	ILE
1	C	322	ASP
1	C	324	GLU
1	C	329	VAL
1	C	330	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	69	ASN
1	A	332	ASN
1	B	21	ASN
1	B	143	ASN
1	B	144	ASN
1	B	182	GLN
1	B	193	GLN
1	B	245	GLN
1	B	253	GLN
1	B	270	ASN
1	C	7	GLN
1	C	21	ASN
1	C	158	ASN
1	C	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	324/341 (95%)	-0.37	0 100 100	84, 132, 234, 313	0
1	B	325/341 (95%)	-0.40	2 (0%) 85 69	68, 120, 255, 288	1 (0%)
1	C	318/341 (93%)	-0.45	0 100 100	83, 118, 224, 266	0
All	All	967/1023 (94%)	-0.40	2 (0%) 91 83	68, 122, 239, 313	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	ILE	2.1
1	B	257	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.