Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2022 – 10:04 AM EST

PDB ID	:	7RFO
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 (i) symbol.

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

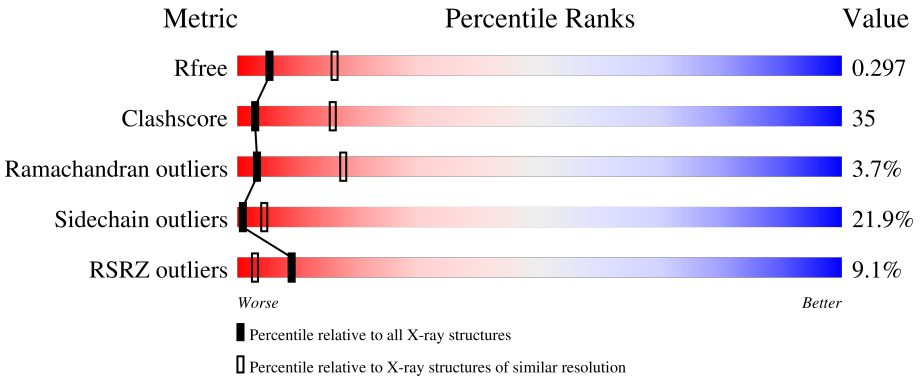
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (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 <=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	10% 47% 35% 14% .
1	B	341	9% 55% 33% 9% .
1	C	341	7% 47% 40% 9% 5%

2 Entry composition (i)

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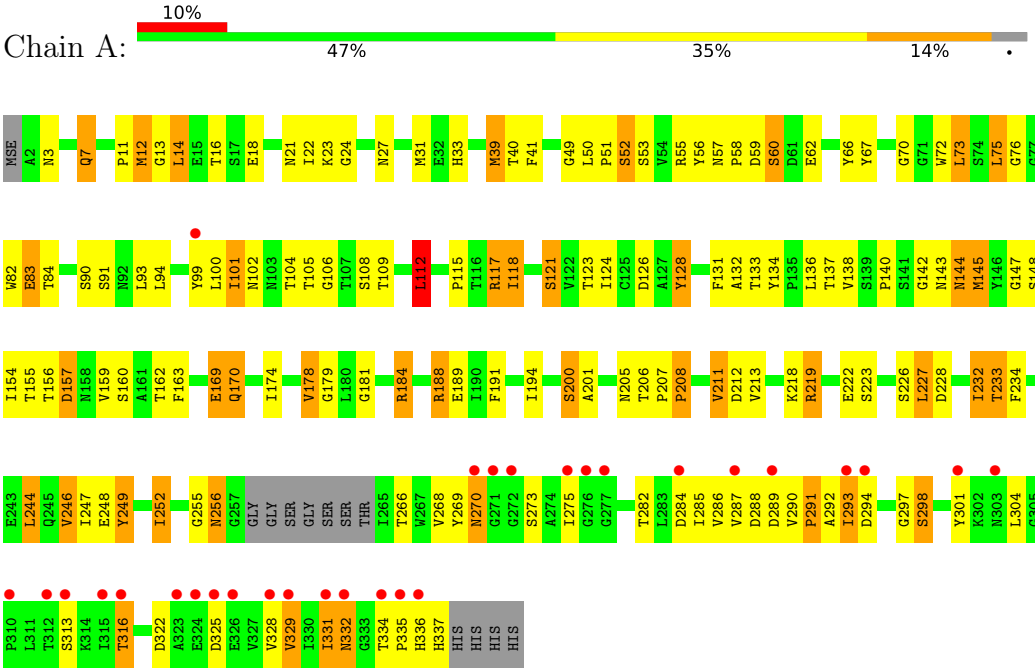
Chain	Residue	Modelled	Actual	Comment	Reference
C	338	HIS	-	expression tag	UNP G3M192
C	339	HIS	-	expression tag	UNP G3M192
C	340	HIS	-	expression tag	UNP G3M192
C	341	HIS	-	expression tag	UNP G3M192

3 Residue-property plots (i)

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

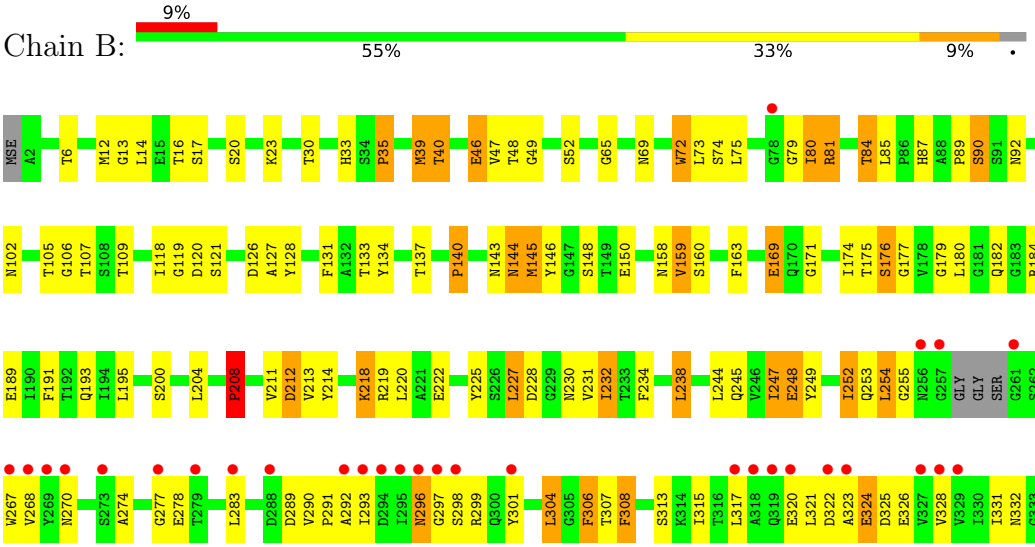
• Molecule 1: Tailspike protein

Chain A:



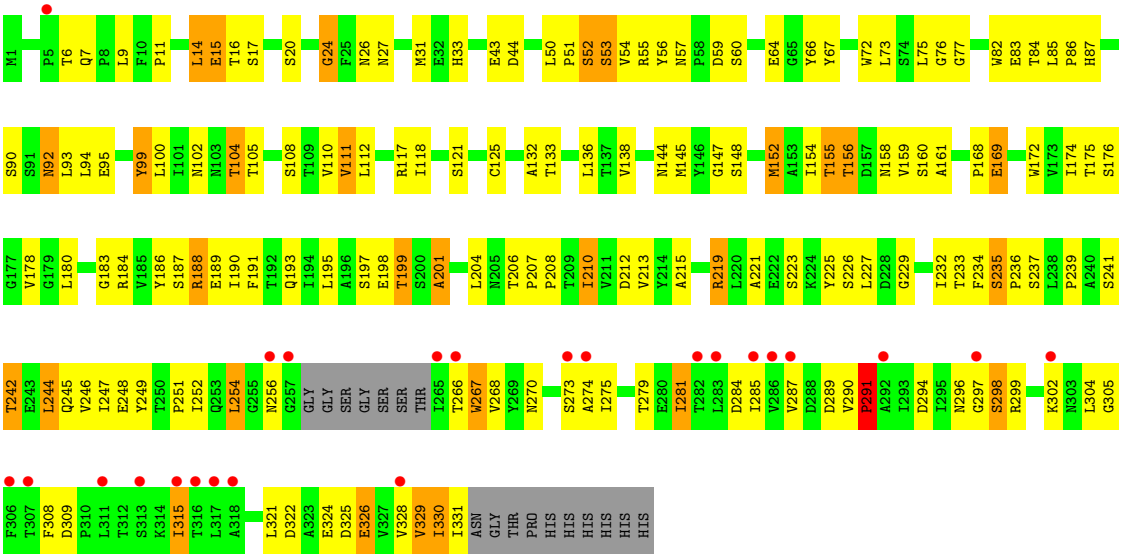
• Molecule 1: Tailspike protein

Chain B:



• Molecule 1: Tailspike protein

Chain C:



4 Data and refinement statistics (i)

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 48.01 – 3.02	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-3.02) 94.6 (48.01-3.02)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.225 , 0.296 0.237 , 0.297	Depositor DCC
R_{free} test set	1370 reflections (4.86%)	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)	0.31 , 115.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.75	0/2374	0.95	3/3250 (0.1%)
1	B	0.75	0/2436	0.96	2/3332 (0.1%)
1	C	0.75	0/2410	0.97	1/3296 (0.0%)
All	All	0.75	0/7220	0.96	6/9878 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	92	ASN	CB-CA-C	6.18	122.76	110.40
1	B	12	MSE	CG-SE-CE	6.16	112.46	98.90
1	A	39	MSE	CG-SE-CE	5.91	111.90	98.90
1	A	12	MSE	CG-SE-CE	5.80	111.67	98.90
1	A	256	ASN	CB-CA-C	5.64	121.67	110.40
1	C	99	TYR	CB-CA-C	5.39	121.17	110.40

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	188	0
1	B	2387	0	2163	176	0
1	C	2363	0	2180	173	0
All	All	7077	0	6413	468	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 35.

All (468) 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: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:B:47:VAL:C	1:B:72:TRP:HZ3	1.59	1.04
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: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:47:VAL:C	1:B:72:TRP:CZ3	2.50	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: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
1:C:266:THR:CG2	1:C:328:VAL:HG12	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:14:LEU:HD12	1:B:14:LEU:C	2.05	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:B:33:HIS:HE2	1:B:39:MSE:HE2	1.51	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:298:SER:HA	1:B:297:GLY:C	2.08	0.73
1:A:55:ARG:HD3	1:A:72:TRP:CE3	2.25	0.72
1:C:244:LEU:HD23	1:C:244:LEU:C	2.09	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: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
1:B:277:GLY:CA	1:B:320:GLU:OE2	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:124:ILE:C	1:A:124:ILE:HD12	2.12	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:B:298:SER:HB2	1:C:297:GLY:C	2.15	0.67
1:A:331:ILE:HD13	1:A:332:ASN:H	1.60	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: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:B:180:LEU:HB3	1:B:254:LEU:HD12	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:14:LEU:C	1:C:14:LEU:HD12	2.21	0.61
1:A:115:PRO:CD	1:A:143:ASN:OD1	2.48	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: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:252:ILE:HD12	1:B:252:ILE:C	2.22	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:A:189:GLU:H	1:A:189:GLU:CD	2.04	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
1:B:144:ASN:HD22	1:B:144:ASN:N	1.93	0.59
1:C:64:GLU:C	1:C:75:LEU:CD1	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:57:ASN:CG	1:A:60:SER:HB2	2.24	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: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:C:169:GLU:CD	1:C:169:GLU:H	2.07	0.57
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:48:THR:C	1:B:72:TRP:CH2	2.78	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:B:126:ASP:CG	1:B:131:PHE:CD1	2.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:64:GLU:C	1:C:75:LEU:HD12	2.28	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:267:TRP:CZ2	1:C:284:ASP:OD1	2.61	0.53
1:A:169:GLU:CD	1:A:169:GLU:H	2.10	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:A:298:SER:HA	1:B:298:SER:N	2.24	0.53
1:B:14:LEU:C	1:B:14:LEU:CD1	2.76	0.53
1:B:213:VAL:HG12	1:B:220:LEU:HB2	1.90	0.52
1:B:33:HIS:HE2	1:B:39:MSE:CE	2.22	0.52
1:A:14:LEU:CD1	1:A:14:LEU:C	2.78	0.52
1:A:244:LEU:HD23	1:A:244:LEU:C	2.29	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:C:191:PHE:CE1	1:C:244:LEU:CD2	2.93	0.52
1:C:87:HIS:HE2	1:C:108:SER:HB3	1.73	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:O	1:B:278:GLU:HG2	2.10	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: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: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:249:TYR:CD1	1:A:249:TYR:C	2.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PRO:HD2	1:C:169:GLU:CD	2.33	0.49
1:C:225:TYR:O	1:C:225:TYR:CD1	2.66	0.48
1:A:308:PHE:CD1	1:A:308:PHE:C	2.87	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: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:C:191:PHE:CD1	1:C:191:PHE:C	2.88	0.47
1:A:81:ARG:HH11	1:A:81:ARG:CG	2.27	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: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:A:306:PHE:CD1	1:A:306:PHE:C	2.88	0.47
1:B:20:SER:HB3	1:C:14:LEU:O	2.15	0.47
1:B:144:ASN:ND2	1:B:144:ASN:N	2.57	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:A:238:LEU:N	1:A:238:LEU:HD23	2.30	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
1:C:118:ILE:HD12	1:C:118:ILE:H	1.81	0.46
1:C:308:PHE:CD1	1:C:308:PHE:C	2.87	0.46
1:C:197:SER:O	1:C:199:THR:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:B:17:SER:HG	1:C:11:PRO:HA	1.75	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:144:ASN:OD1	1:A:147:GLY:C	2.57	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: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:A:124:ILE:C	1:A:124:ILE:CD1	2.83	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:B:33:HIS:NE2	1:B:39:MSE:CE	2.74	0.43
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: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:191:PHE:CD1	1:B:191:PHE:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LEU:HD11	1:B:232:ILE:CD1	2.47	0.42
1:C:147:GLY:O	1:C:148:SER:C	2.57	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: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:C:57:ASN:OD1	1:C:59:ASP:HB2	2.18	0.42
1:A:287:VAL:HG22	1:A:331:ILE:HD11	1.99	0.42
1:B:102:ASN:C	1:B:102:ASN:OD1	2.58	0.42
1:B:87:HIS:CD2	1:B:87:HIS:C	2.93	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: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
1:C:132:ALA:O	1:C:219:ARG:HD3	2.21	0.41
1:B:87:HIS:CE1	1:B:105:THR:HB	2.55	0.41
1:C:26:ASN:OD1	1:C:26:ASN:C	2.58	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: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:221:ALA:C	1:C:223:SER:N	2.74	0.41
1:A:75:LEU:HD12	1:A:75:LEU:N	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:249:TYR:CD1	1:B:249:TYR:C	2.94	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:A:126:ASP:CG	1:A:131:PHE:CD1	2.95	0.40
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: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: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 (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	325/341 (95%)	274 (84%)	40 (12%)	11 (3%)	3	19
1	B	327/341 (96%)	288 (88%)	29 (9%)	10 (3%)	4	21
1	C	320/341 (94%)	263 (82%)	42 (13%)	15 (5%)	2	13
All	All	972/1023 (95%)	825 (85%)	111 (11%)	36 (4%)	3	17

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
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 (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	235/280 (84%)	164 (70%)	71 (30%)	0 1
1	B	249/280 (89%)	202 (81%)	47 (19%)	1 7
1	C	252/280 (90%)	209 (83%)	43 (17%)	2 9
All	All	736/840 (88%)	575 (78%)	161 (22%)	1 4

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	7	GLN
1	A	12	MSE
1	A	14	LEU
1	A	18	GLU
1	A	23	LYS
1	A	50	LEU
1	A	52	SER
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	144	ASN
1	A	145	MSE
1	A	152	MSE
1	A	157	ASP
1	A	160	SER
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	170	GLN
1	A	178	VAL
1	A	184	ARG
1	A	188	ARG
1	A	194	ILE
1	A	200	SER
1	A	205	ASN
1	A	211	VAL
1	A	212	ASP
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	232	ILE
1	A	233	THR
1	A	237	SER
1	A	238	LEU
1	A	242	THR
1	A	244	LEU
1	A	246	VAL
1	A	249	TYR
1	A	252	ILE
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	308	PHE
1	A	316	THR
1	A	322	ASP
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	35	PRO

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Mol	Chain	Res	Type
1	B	39	MSE
1	B	40	THR
1	B	52	SER
1	B	72	TRP
1	B	73	LEU
1	B	74	SER
1	B	80	ILE
1	B	81	ARG
1	B	84	THR
1	B	85	LEU
1	B	89	PRO
1	B	90	SER
1	B	107	THR
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	158	ASN
1	B	169	GLU
1	B	176	SER
1	B	184	ARG
1	B	187	SER
1	B	193	GLN
1	B	200	SER
1	B	208	PRO
1	B	212	ASP
1	B	218	LYS
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	245	GLN
1	B	247	ILE
1	B	248	GLU
1	B	252	ILE
1	B	254	LEU
1	B	270	ASN
1	B	306	PHE

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Mol	Chain	Res	Type
1	B	307	THR
1	B	308	PHE
1	B	324	GLU
1	C	6	THR
1	C	14	LEU
1	C	15	GLU
1	C	53	SER
1	C	60	SER
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	176	SER
1	C	199	THR
1	C	210	ILE
1	C	219	ARG
1	C	226	SER
1	C	235	SER
1	C	237	SER
1	C	242	THR
1	C	244	LEU
1	C	245	GLN
1	C	254	LEU
1	C	267	TRP
1	C	273	SER
1	C	275	ILE
1	C	279	THR
1	C	281	ILE
1	C	289	ASP
1	C	291	PRO
1	C	298	SER
1	C	309	ASP

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Mol	Chain	Res	Type
1	C	315	ILE
1	C	322	ASP
1	C	329	VAL
1	C	330	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	332	ASN
1	B	21	ASN
1	B	143	ASN
1	B	144	ASN
1	B	182	GLN
1	B	253	GLN
1	B	270	ASN
1	B	300	GLN
1	C	158	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 monosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	324/341 (95%)	0.40	33 (10%) 6 2	84, 132, 234, 313	0
1	B	325/341 (95%)	0.25	31 (9%) 8 2	81, 120, 255, 288	0
1	C	318/341 (93%)	0.38	24 (7%) 14 4	83, 118, 224, 266	0
All	All	967/1023 (94%)	0.34	88 (9%) 9 3	81, 122, 239, 313	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	GLY	11.0
1	C	256	ASN	9.3
1	C	318	ALA	7.9
1	B	257	GLY	7.6
1	B	292	ALA	7.1
1	A	335	PRO	6.3
1	B	327	VAL	6.2
1	C	316	THR	6.2
1	A	312	THR	6.2
1	A	309	ASP	6.1
1	C	265	ILE	6.1
1	A	326	GLU	6.0
1	B	261	GLY	5.9
1	C	317	LEU	5.6
1	B	296	ASN	5.4
1	A	284	ASP	5.2
1	C	286	VAL	5.0
1	C	307	THR	4.9
1	C	292	ALA	4.9
1	B	319	GLN	4.7
1	B	328	VAL	4.7
1	A	324	GLU	4.7
1	A	325	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	297	GLY	4.4
1	B	294	ASP	4.4
1	C	5	PRO	4.4
1	B	273	SER	4.3
1	A	328	VAL	4.2
1	A	316	THR	4.2
1	B	269	TYR	3.9
1	A	276	GLY	3.7
1	A	293	ILE	3.7
1	B	334	THR	3.6
1	C	274	ALA	3.6
1	A	301	TYR	3.6
1	B	293	ILE	3.6
1	A	315	ILE	3.5
1	C	313	SER	3.5
1	A	310	PRO	3.5
1	B	317	LEU	3.4
1	A	272	GLY	3.4
1	A	332	ASN	3.3
1	C	282	THR	3.3
1	A	334	THR	3.2
1	C	266	THR	3.1
1	B	267	TRP	3.1
1	A	336	HIS	3.1
1	C	283	LEU	3.1
1	C	273	SER	3.0
1	A	313	SER	3.0
1	B	301	TYR	3.0
1	A	271	GLY	2.9
1	B	329	VAL	2.8
1	A	289	ASP	2.8
1	A	323	ALA	2.8
1	B	318	ALA	2.8
1	A	275	ILE	2.7
1	A	329	VAL	2.7
1	B	322	ASP	2.7
1	C	315	ILE	2.7
1	A	303	ASN	2.7
1	B	270	ASN	2.7
1	B	78	GLY	2.6
1	A	331	ILE	2.6
1	C	285	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	308	PHE	2.6
1	A	277	GLY	2.6
1	C	287	VAL	2.5
1	B	298	SER	2.5
1	B	295	ILE	2.5
1	A	287	VAL	2.5
1	B	277	GLY	2.5
1	C	311	LEU	2.4
1	B	256	ASN	2.3
1	C	302	LYS	2.3
1	B	279	THR	2.3
1	A	99	TYR	2.3
1	B	323	ALA	2.3
1	A	270	ASN	2.2
1	A	79	GLY	2.2
1	B	288	ASP	2.2
1	B	320	GLU	2.2
1	C	306	PHE	2.2
1	B	283	LEU	2.1
1	A	294	ASP	2.1
1	B	297	GLY	2.0
1	B	268	VAL	2.0
1	C	328	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.