



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:12 AM UTC

PDB ID : 4UHV / pdb_00004uhv
Title : The structure of VgrG1, the needle tip of the bacterial Type VI Secretion System
Authors : Spinola-Amilibia, M.; Davo-Siguero, I.; Ruiz, F.M.; Santillana, E.; Medrano, F.J.; Romero, A.
Deposited on : 2015-03-25
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

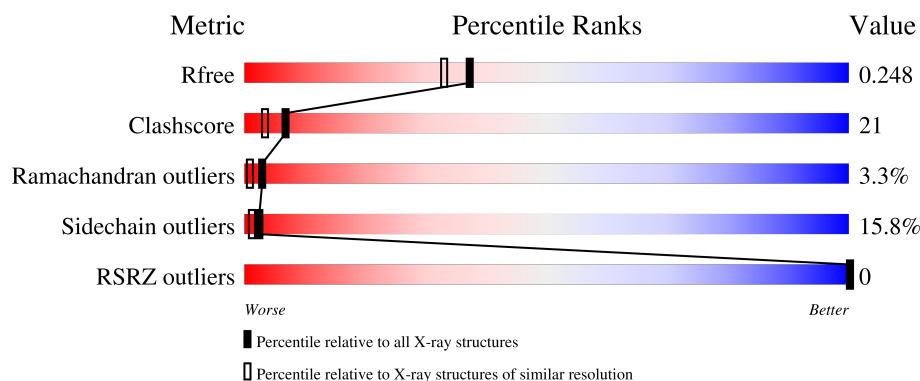
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	651	
1	B	651	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	1657	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10911 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 VGRG1, VALINE-GLYCINE REPEAT PROTEIN G1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	Se	0	3	0
			5107	3194	933	964	7	9			
1	B	645	Total	C	N	O	S	Se	0	3	0
			5109	3194	930	969	7	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	644	LEU	-	expression tag	UNP Q9I741
A	645	GLU	-	expression tag	UNP Q9I741
A	646	HIS	-	expression tag	UNP Q9I741
A	647	HIS	-	expression tag	UNP Q9I741
A	648	HIS	-	expression tag	UNP Q9I741
A	649	HIS	-	expression tag	UNP Q9I741
A	650	HIS	-	expression tag	UNP Q9I741
A	651	HIS	-	expression tag	UNP Q9I741
B	644	LEU	-	expression tag	UNP Q9I741
B	645	GLU	-	expression tag	UNP Q9I741
B	646	HIS	-	expression tag	UNP Q9I741
B	647	HIS	-	expression tag	UNP Q9I741
B	648	HIS	-	expression tag	UNP Q9I741
B	649	HIS	-	expression tag	UNP Q9I741
B	650	HIS	-	expression tag	UNP Q9I741
B	651	HIS	-	expression tag	UNP Q9I741

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	Cl	0	0
			13	13		
2	B	25	Total	Cl	0	0
			25	25		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	Na 6	0	0
3	B	7	Total 7	Na 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	268	Total 268	O 268	0	0
4	B	376	Total 376	O 376	0	0

H1S	S553	D554	S555	V556	Y560	E563	L570	V571	S575	V576	V577	F579	T584	I585	N586	I587	S588	F592	N593	L594	I602	L608	D609	L610	N611	V618	D619	K623	G624	V625	I629	D630	V633	Q634	A635	M636	F637	P638	P639	L644	E645	H1S	H1S	H1S	H1S				
	E453	Q454	T455	V456	P457	Y458	E459	L460	P461	A462	N463	A464	T465	S474	K475	G476	T477	T478	P479	A480	N481	F482	N483	M487	E488	D489	K490	L496	Y497	I498	H499	A500	E501	R502	N510	R520	S523	E528	L529	A530	R531	I532	N535	V540	R541	L542	N543	L546	L547
	R354	L355	V361	P362	V363	V371	V372	V373	Q374	P375	E378	E379	I380	D383	Q384	Y385	G386	R387	H391	F392	H393	D394	Y395	R396	H397	I398	Q399	S400	N403	W414	K417	S421	M422	Q423	I424	E427	G428	Q429	V433	L436	E437	T446	G447	R448	V449	A452			
	E269	R273	L276	E277	Q280	A281	Q282	H283	V286	R287	I295	G296	A297	G298	H299	L300	F301	G305	Y306	P307	R308	D309	D310	Q311	N312	Y315	L316	V317	R323	V324	V325	L328	Y329	G332	S333	G334	G335	F340	E341	S342	E343	L344	D345	C346	I347	Q351			
	F168	R169	Q172	K173	L176	L177	V178	L179	S180	D181	A182	Y183	G184	A185	H186	R187	S188	P189	G190	G191	Y192	V195	P196	Y197	Y198	P199	P200	T201	R205	E206	R207	D208	H209	D212	W213	Q220	L224	Q232	R237	L244	Y253	Y258	P259	V263	Q264	S265	Q266		

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	78.62Å 78.62Å 430.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.73 – 2.00 71.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (71.73-2.00) 94.0 (71.73-2.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.223 , 0.248 0.224 , 0.248	Depositor DCC
R_{free} test set	4702 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for K, H, -L	Depositor
Outliers	0 of 94822 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10911	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

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

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	0.72	1/5228 (0.0%)	1.07	21/7069 (0.3%)
1	B	0.77	1/5230 (0.0%)	1.12	27/7074 (0.4%)
All	All	0.75	2/10458 (0.0%)	1.09	48/14143 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	5
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	518	HIS	CA-C	7.59	1.56	1.52
1	B	510	ASN	CA-C	6.73	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	LEU	CA-C-N	18.68	143.19	119.84
1	A	460	LEU	C-N-CA	18.68	143.19	119.84
1	B	258	TYR	CA-C-N	11.43	134.13	119.84
1	B	258	TYR	C-N-CA	11.43	134.13	119.84
1	B	373	VAL	N-CA-C	9.75	123.86	108.85
1	A	460	LEU	C-N-CD	-9.55	85.84	125.00
1	B	543	ASN	N-CA-C	8.89	123.79	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	629	ILE	N-CA-C	-8.25	102.30	110.30
1	B	188	SER	N-CA-C	7.38	114.64	108.07
1	B	456	VAL	CA-C-N	6.72	126.67	119.28
1	B	456	VAL	C-N-CA	6.72	126.67	119.28
1	A	246	ARG	CA-C-N	6.65	128.16	119.84
1	A	246	ARG	C-N-CA	6.65	128.16	119.84
1	B	253	TYR	CA-C-N	6.43	126.96	120.14
1	B	253	TYR	C-N-CA	6.43	126.96	120.14
1	A	511	ASP	N-CA-C	6.37	119.27	107.99
1	B	535	ASN	N-CA-C	6.33	119.78	109.59
1	A	477	GLY	N-CA-C	6.32	118.55	111.85
1	A	209	HIS	N-CA-C	6.32	118.15	109.18
1	A	9	VAL	N-CA-C	6.26	118.13	109.80
1	B	263	VAL	N-CA-C	-6.25	105.61	111.48
1	A	59	SER	N-CA-C	6.19	118.02	110.41
1	A	328	LEU	N-CA-C	-6.12	104.31	112.94
1	B	176	ILE	N-CA-C	6.08	117.04	108.17
1	B	424	ILE	N-CA-CB	6.03	116.69	110.23
1	B	55	PRO	N-CA-C	5.94	119.83	111.33
1	B	335	GLY	N-CA-C	-5.76	99.53	113.18
1	A	74	VAL	N-CA-C	5.69	112.30	106.21
1	A	604	THR	N-CA-C	5.62	117.27	111.03
1	B	180	SER	N-CA-C	5.59	117.68	109.24
1	B	68	ARG	CA-C-N	-5.59	113.51	121.50
1	B	68	ARG	C-N-CA	-5.59	113.51	121.50
1	B	41	SER	N-CA-C	5.55	115.17	107.73
1	A	3	LEU	N-CA-C	5.53	117.71	109.25
1	B	1	MSE	CB-CA-C	-5.51	99.63	110.10
1	B	461	PRO	N-CA-C	-5.50	101.14	112.47
1	B	380	ILE	CB-CA-C	-5.50	104.19	110.73
1	A	474	SER	N-CA-C	5.45	118.15	109.81
1	B	69	PHE	N-CA-C	5.45	118.42	109.76
1	A	164	ILE	N-CA-C	5.34	116.26	108.58
1	B	308	ARG	N-CA-C	-5.31	100.37	108.76
1	B	452	ALA	N-CA-C	5.29	117.05	111.28
1	A	268	GLY	N-CA-C	-5.19	106.13	112.77
1	A	580	ASN	N-CA-C	5.18	118.13	110.46
1	A	598	GLY	N-CA-C	5.12	118.54	110.91
1	B	232	GLN	CB-CA-C	-5.09	102.66	110.81
1	A	330	GLU	N-CA-C	5.09	118.41	111.39
1	B	4	THR	N-CA-C	-5.01	100.14	110.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLN	Peptide
1	A	246	ARG	Peptide
1	A	258	TYR	Peptide
1	A	267	ASP	Peptide
1	A	299	HIS	Peptide
1	A	3	LEU	Peptide
1	A	329	TYR	Peptide
1	A	460	LEU	Peptide
1	A	602	ILE	Peptide
1	B	1	MSE	Peptide
1	B	114	VAL	Peptide
1	B	258	TYR	Peptide
1	B	334	GLY	Peptide
1	B	460	LEU	Peptide

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	5107	0	4940	228	3
1	B	5109	0	4932	202	2
2	A	13	0	0	3	0
2	B	25	0	0	8	0
3	A	6	0	0	0	0
3	B	7	0	0	0	0
4	A	268	0	0	30	1
4	B	376	0	0	29	0
All	All	10911	0	9872	431	5

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 21.

All (431) 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:B:397:HIS:HD2	4:B:2179:HOH:O	1.15	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TYR:CD2	1:B:259:PRO:HD2	1.88	1.09
1:A:11:CYS:SG	1:A:12:PRO:HD3	1.93	1.08
1:A:572:CYS:HA	4:A:2224:HOH:O	1.53	1.05
1:A:522:LYS:HE2	1:A:524:ILE:HD11	1.40	1.02
1:B:379:GLU:OE2	2:B:1657:CL:CL	2.19	0.97
1:A:387[B]:ARG:HH11	1:A:387[B]:ARG:HB2	1.29	0.96
1:B:205:ARG:HD3	1:B:207:ARG:HG3	1.43	0.96
1:A:111:ASN:O	1:A:112:GLN:HG2	1.64	0.95
1:B:379:GLU:OE1	4:B:2176:HOH:O	1.88	0.90
1:A:389:LYS:HB2	4:A:2165:HOH:O	1.72	0.89
1:A:189:PRO:HG3	1:A:300:LEU:HD21	1.55	0.89
1:A:11:CYS:SG	1:A:12:PRO:CD	2.62	0.86
1:B:397:HIS:CD2	4:B:2179:HOH:O	1.97	0.86
1:A:112:GLN:HG3	4:A:2049:HOH:O	1.74	0.85
1:B:396:ARG:N	4:B:2179:HOH:O	2.05	0.85
1:A:11:CYS:HG	1:A:12:PRO:HD3	1.38	0.84
1:A:189:PRO:CG	1:A:300:LEU:HD21	2.09	0.82
1:A:189:PRO:HG3	1:A:300:LEU:CD2	2.11	0.80
1:A:403:ASN:O	4:A:2185:HOH:O	1.99	0.80
1:A:189:PRO:CG	1:A:300:LEU:CD2	2.60	0.79
1:A:387[B]:ARG:HH11	1:A:387[B]:ARG:CB	1.94	0.79
1:B:258:TYR:CD2	1:B:259:PRO:CD	2.65	0.79
1:A:62:LEU:HB3	1:A:63:PRO:CD	2.12	0.79
1:B:378:GLU:OE2	4:B:2175:HOH:O	2.00	0.78
1:B:636:MSE:HG3	4:B:2114:HOH:O	1.82	0.78
1:B:465:THR:HG23	1:B:488:GLU:OE1	1.84	0.78
1:A:300:LEU:HD22	1:A:300:LEU:H	1.49	0.77
1:B:311:GLN:NE2	1:B:312:ASN:OD1	2.17	0.76
1:A:361:VAL:HG13	4:A:2161:HOH:O	1.86	0.75
1:A:300:LEU:HD22	1:A:300:LEU:N	2.03	0.74
1:B:11:CYS:HB3	1:B:12:PRO:CD	2.18	0.74
1:B:478:THR:O	1:B:480:ALA:N	2.21	0.73
1:A:35:TYR:HH	1:A:70:PHE:HE2	1.35	0.73
1:A:441:ASP:O	1:A:443:PRO:HD3	1.89	0.73
1:A:392:PHE:HB2	4:A:2179:HOH:O	1.88	0.72
1:B:399:GLN:NE2	4:B:2184:HOH:O	2.09	0.71
1:B:540:VAL:HG12	1:B:542:LEU:O	1.90	0.71
1:A:364:VAL:HG11	1:A:435:PHE:CD2	2.26	0.70
1:A:300:LEU:HD23	1:A:300:LEU:O	1.91	0.69
1:B:138:TYR:OH	1:B:181:ASP:OD2	2.09	0.69
1:A:167:TRP:CD1	1:A:180:SER:HG	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:SER:O	1:A:69:PHE:HA	1.93	0.68
1:A:624:GLY:O	4:A:2225:HOH:O	2.12	0.68
1:B:556:VAL:HG11	1:B:560:TYR:HB2	1.75	0.68
1:A:189:PRO:HG3	1:A:300:LEU:CG	2.25	0.67
1:A:599:ASN:ND2	4:A:2234:HOH:O	2.27	0.67
1:B:197:TYR:HB3	1:B:305:GLY:HA3	1.77	0.67
1:A:547:LEU:HB3	1:A:633:VAL:HG22	1.76	0.66
1:A:215:MSE:SE	1:A:217:ARG:HH21	2.28	0.66
1:A:380:ILE:HD11	1:A:474:SER:OG	1.94	0.66
1:A:510:ASN:OD1	4:A:2207:HOH:O	2.12	0.66
1:A:578:GLU:OE2	1:A:580:ASN:ND2	2.26	0.66
1:A:379:GLU:HB2	1:A:475:LYS:HA	1.77	0.66
1:A:394:TRP:CD2	4:A:2179:HOH:O	2.48	0.66
1:A:392:PHE:CB	4:A:2179:HOH:O	2.44	0.66
1:B:592:PHE:CD2	4:B:2236:HOH:O	2.48	0.66
1:A:312:ASN:ND2	4:A:2143:HOH:O	2.28	0.65
1:B:296:GLY:O	1:B:317:VAL:CG2	2.44	0.65
1:A:143:TYR:CD1	1:A:406:CYS:HB3	2.31	0.65
1:A:62:LEU:HB3	1:A:63:PRO:HD3	1.78	0.65
1:B:205:ARG:HD3	1:B:207:ARG:CG	2.22	0.65
1:B:307:PRO:O	1:B:308:ARG:HG3	1.97	0.64
1:B:265[A]:SER:OG	2:B:1653:CL:CL	2.49	0.64
1:A:136:ARG:NH2	1:A:270:GLN:OE1	2.30	0.63
1:B:2:GLN:HB2	1:B:16:ASP:CG	2.23	0.63
1:A:117:ILE:N	4:A:2049:HOH:O	2.30	0.63
1:A:395:ASP:N	4:A:2179:HOH:O	2.32	0.63
1:B:1:MSE:HG2	1:B:2:GLN:HG2	1.79	0.63
1:A:286:VAL:O	1:A:286:VAL:HG13	1.98	0.63
1:B:635:ALA:HB1	4:B:2279:HOH:O	1.99	0.63
1:A:75:ALA:CB	1:A:98:TRP:CZ3	2.81	0.62
1:A:210:PHE:CD1	1:A:290:GLY:HA2	2.34	0.62
1:B:31:ARG:NH2	4:B:2023:HOH:O	2.32	0.62
1:A:532:ILE:HG12	1:A:536:ARG:HG3	1.80	0.62
2:A:1705:CL:CL	4:A:2173:HOH:O	2.53	0.62
1:B:244:ILE:HD11	4:B:2147:HOH:O	1.98	0.62
1:B:258:TYR:CG	1:B:259:PRO:CD	2.83	0.62
1:A:37:LEU:N	1:A:91:ALA:O	2.32	0.61
1:A:582:ASP:O	1:A:584:THR:HG22	2.01	0.61
1:A:634:GLN:O	1:A:634:GLN:NE2	2.32	0.61
1:B:577:VAL:HG22	1:B:587:ILE:HG23	1.82	0.61
1:B:308:ARG:HB2	1:B:311:GLN:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG12	1:A:8:GLN:H	1.65	0.61
1:A:22:ARG:HB3	1:A:38:HIS:HB2	1.81	0.61
1:B:258:TYR:CG	1:B:259:PRO:HD2	2.36	0.61
1:A:259:PRO:HG3	1:A:437:GLU:HG2	1.83	0.61
1:A:215:MSE:SE	1:A:217:ARG:NH2	2.84	0.60
1:B:487:MSE:HG2	1:B:496:LEU:HD13	1.82	0.60
1:A:195:VAL:HG22	1:A:195:VAL:O	2.01	0.60
1:B:463:ASN:C	1:B:463:ASN:HD22	2.10	0.59
1:A:136:ARG:HG2	1:A:181:ASP:HB3	1.85	0.59
1:B:172:GLN:HE21	1:B:173:LYS:HE2	1.66	0.59
1:B:296:GLY:O	1:B:317:VAL:HG21	2.02	0.59
1:B:610:LEU:O	1:B:611:ASN:ND2	2.36	0.59
1:A:625:VAL:HG13	1:A:628:THR:HB	1.84	0.58
1:A:63:PRO:O	1:A:65:GLY:N	2.36	0.58
1:A:11:CYS:CB	1:A:12:PRO:CD	2.81	0.58
1:B:62:LEU:HD13	1:B:192:TYR:OH	2.03	0.58
1:B:592:PHE:HD2	4:B:2236:HOH:O	1.84	0.58
1:B:343:GLU:HG3	4:B:2150:HOH:O	2.03	0.58
1:A:434:SER:N	1:A:444:ILE:O	2.34	0.57
1:B:634:GLN:NE2	4:B:2259:HOH:O	2.37	0.57
1:A:62:LEU:CB	1:A:63:PRO:CD	2.81	0.57
1:B:477:GLY:CA	2:B:1657:CL:CL	2.89	0.57
1:B:27:GLU:HB2	1:B:33:PHE:HB3	1.86	0.57
1:B:618:VAL:HG13	1:B:618:VAL:O	2.05	0.57
1:B:30:GLY:HA3	1:B:355:LEU:HD21	1.87	0.57
1:B:453:GLU:HG3	1:B:454:GLN:HE21	1.69	0.57
1:A:55:PRO:HG3	4:A:2026:HOH:O	2.05	0.57
1:A:198:TYR:HB2	1:A:209:HIS:CD2	2.39	0.57
1:A:529:LEU:HG	1:A:531:ARG:HH11	1.69	0.57
1:A:44:PRO:CG	1:A:89:TYR:CE1	2.88	0.56
1:A:35:TYR:OH	1:A:70:PHE:HE2	1.88	0.56
1:B:547:LEU:HB3	1:B:633:VAL:HG22	1.87	0.56
1:A:311:GLN:O	1:A:311:GLN:NE2	2.39	0.56
1:B:630:ASP:OD1	1:B:634:GLN:HG3	2.05	0.56
1:A:44:PRO:HG2	1:A:89:TYR:CZ	2.41	0.56
1:A:578:GLU:CD	1:A:580:ASN:HD21	2.13	0.56
1:B:106:CYS:SG	1:B:148:ARG:HA	2.45	0.56
1:B:11:CYS:CB	1:B:12:PRO:CD	2.84	0.55
1:B:624:GLY:HA3	4:B:2228:HOH:O	2.07	0.55
1:A:295:ILE:HG22	1:A:299:HIS:HB2	1.89	0.55
1:A:329:TYR:HA	1:A:330:GLU:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ARG:CZ	4:B:2122:HOH:O	2.54	0.55
1:B:463:ASN:O	1:B:463:ASN:ND2	2.36	0.55
1:B:575:SER:HA	1:B:588:SER:O	2.07	0.55
1:B:224:LEU:N	1:B:276:ILE:HD11	2.23	0.54
1:B:181:ASP:N	1:B:181:ASP:OD1	2.40	0.54
1:A:4:THR:C	4:A:2004:HOH:O	2.49	0.54
1:A:595:TYR:O	1:A:596:ALA:HB2	2.07	0.54
1:B:212:ASP:OD2	1:B:287:ARG:NH2	2.40	0.54
1:A:131:GLU:OE1	1:A:169:ARG:NH2	2.40	0.54
1:B:29:LEU:HD12	1:B:167:TRP:HB3	1.89	0.54
1:B:296:GLY:O	1:B:299:HIS:ND1	2.34	0.54
1:A:546:LEU:HD11	1:A:548:VAL:CG2	2.37	0.54
1:A:391:HIS:CE1	1:A:398:ASP:OD1	2.62	0.53
1:A:394:TRP:CE3	4:A:2179:HOH:O	2.61	0.53
1:B:638:PRO:HA	4:B:2261:HOH:O	2.09	0.53
1:B:266:GLN:OE1	4:B:2140:HOH:O	2.19	0.53
1:B:65:GLY:HA3	1:B:192:TYR:OH	2.08	0.53
1:B:315:TYR:HA	1:B:347:ILE:O	2.08	0.53
1:A:389:LYS:HD3	1:A:402:GLU:O	2.09	0.53
1:B:623:LYS:O	1:B:625:VAL:N	2.42	0.53
1:A:430:GLU:OE1	1:A:451:ASN:ND2	2.41	0.53
1:A:186:HIS:CB	1:A:300:LEU:HD12	2.39	0.53
1:A:210:PHE:HD1	1:A:290:GLY:HA2	1.73	0.53
1:B:264:GLN:OE1	1:B:264:GLN:HA	2.08	0.53
1:A:18:LEU:CB	1:A:41[A]:SER:OG	2.56	0.53
1:A:244:ILE:HD12	1:A:246:ARG:HG3	1.90	0.53
1:B:478:THR:C	1:B:480:ALA:H	2.17	0.53
1:A:380:ILE:HD11	1:A:474:SER:HG	1.72	0.53
1:A:186:HIS:HB3	1:A:300:LEU:CD1	2.38	0.52
1:A:364:VAL:HG13	1:A:368:GLN:NE2	2.23	0.52
1:A:361:VAL:HG23	1:A:362:PRO:HD2	1.91	0.52
1:A:111:ASN:C	1:A:112:GLN:HG2	2.34	0.52
1:B:28:GLU:HB2	1:B:31:ARG:HG3	1.91	0.52
1:B:50:GLN:NE2	4:B:2034:HOH:O	2.41	0.52
1:B:266:GLN:HE21	1:B:266:GLN:H	1.56	0.52
1:B:1:MSE:N	1:B:1:MSE:HE2	2.24	0.52
1:A:44:PRO:HG3	1:A:89:TYR:CE1	2.45	0.52
1:A:213:TRP:HA	1:A:288:LEU:HD23	1.92	0.52
1:B:75:ALA:HB1	1:B:98:TRP:CZ3	2.44	0.52
1:A:177:LEU:HD13	1:A:178:VAL:N	2.25	0.51
1:B:69:PHE:CE1	1:B:172:GLN:HB3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ARG:C	1:B:532:ILE:HD12	2.35	0.51
1:A:159:MSE:HE3	1:A:164:ILE:HG21	1.92	0.51
1:A:132:ASP:N	4:A:2063:HOH:O	2.40	0.51
1:A:189:PRO:CB	1:A:300:LEU:HD21	2.40	0.51
1:A:460:LEU:HD22	1:A:464:ALA:HA	1.93	0.51
1:B:391:HIS:CE1	1:B:392:PHE:O	2.64	0.51
1:A:11:CYS:SG	1:A:12:PRO:HD2	2.49	0.51
1:B:528:GLU:OE2	1:B:530:ALA:HB2	2.11	0.51
1:A:460:LEU:CB	1:A:461:PRO:CD	2.89	0.51
1:B:50:GLN:O	1:B:53:GLY:N	2.42	0.51
1:B:237:ARG:NH2	4:B:2122:HOH:O	2.43	0.51
1:A:29:LEU:HB3	1:A:318:VAL:HG13	1.92	0.51
1:A:224:LEU:HD22	1:A:272:ALA:O	2.11	0.51
1:A:387[B]:ARG:HH11	1:A:387[B]:ARG:CG	2.23	0.51
1:A:76:ARG:HB2	1:A:92:THR:OG1	2.12	0.50
1:A:37:LEU:HB2	1:A:91:ALA:HB3	1.93	0.50
1:B:11:CYS:HB3	1:B:12:PRO:HD3	1.92	0.50
1:B:168:PHE:HA	1:B:176:ILE:O	2.11	0.50
1:B:244:ILE:CD1	2:B:1706:CL:CL	2.96	0.50
1:B:386:GLY:HA3	1:B:422:MSE:HE1	1.94	0.50
1:A:300:LEU:CD2	1:A:300:LEU:N	2.70	0.50
1:B:26:ARG:HG2	1:B:27:GLU:N	2.27	0.50
1:A:39:LEU:HD12	1:A:89:TYR:C	2.37	0.50
1:A:387[A]:ARG:HG2	1:A:409:ARG:HA	1.93	0.50
1:B:150:THR:HG22	1:B:153:ASP:H	1.77	0.50
1:A:46:LEU:N	1:A:47:PRO:CD	2.74	0.50
1:A:578:GLU:HG2	1:A:580:ASN:ND2	2.26	0.50
1:B:11:CYS:SG	1:B:57:SER:OG	2.70	0.50
1:B:112:GLN:O	1:B:141:TRP:N	2.45	0.50
1:A:60:LEU:HA	1:A:68:ARG:O	2.12	0.49
1:A:189:PRO:HG3	1:A:300:LEU:HG	1.94	0.49
1:B:266:GLN:H	1:B:266:GLN:NE2	2.11	0.49
1:B:305:GLY:O	1:B:307:PRO:HD3	2.13	0.49
1:A:189:PRO:CG	1:A:300:LEU:HG	2.42	0.49
1:A:82:GLY:CA	1:A:87:ALA:HA	2.42	0.49
1:A:391:HIS:CE1	1:A:395:ASP:HB3	2.47	0.49
1:B:392:PHE:C	1:B:394:TRP:H	2.21	0.49
1:B:392:PHE:HB3	1:B:394:TRP:NE1	2.27	0.49
1:A:31:ARG:N	4:A:2017:HOH:O	2.46	0.49
1:A:580:ASN:HB2	1:A:584:THR:HG23	1.95	0.48
1:A:522:LYS:CE	1:A:524:ILE:HD11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:VAL:HG22	1:B:301:PHE:CD2	2.48	0.48
1:B:172:GLN:NE2	1:B:173:LYS:HE2	2.29	0.48
1:B:629:ILE:O	1:B:630:ASP:C	2.57	0.48
1:A:94:ARG:HB3	1:A:98:TRP:CD2	2.48	0.48
1:B:100:LEU:O	1:B:103:THR:HG22	2.13	0.48
1:A:198:TYR:CB	1:A:209:HIS:CD2	2.96	0.48
1:B:296:GLY:C	1:B:299:HIS:HD1	2.20	0.48
1:A:431:VAL:HG12	1:A:448:ARG:HD3	1.94	0.48
1:B:52:LEU:HD23	1:B:77:CYS:SG	2.54	0.48
1:A:273:ARG:O	1:A:276:ILE:HG22	2.13	0.48
1:B:374:GLY:O	1:B:427:ILE:HG21	2.14	0.47
1:A:71:HIS:NE2	1:A:172:GLN:O	2.47	0.47
1:B:34:ALA:HA	1:B:93:LEU:O	2.14	0.47
1:A:602:ILE:HG22	1:A:603:ASP:H	1.79	0.47
1:B:37:LEU:O	1:B:91:ALA:N	2.47	0.47
1:B:619:ASP:OD1	1:B:619:ASP:N	2.47	0.47
1:A:14:GLY:N	4:A:2010:HOH:O	2.46	0.47
1:A:56:MSE:SE	1:A:58:LEU:HD11	2.64	0.47
1:A:189:PRO:HB3	1:A:300:LEU:HD21	1.96	0.47
1:A:258:TYR:CD1	1:A:258:TYR:C	2.92	0.47
1:A:335:GLY:O	1:A:336:ALA:CB	2.63	0.47
1:A:5:ARG:N	4:A:2004:HOH:O	2.46	0.47
1:A:23:MSE:HE1	1:A:58:LEU:CD2	2.45	0.47
1:A:96:TRP:N	1:A:97:PRO:HD2	2.29	0.47
1:A:278:ALA:HB1	1:A:356:LEU:HB3	1.96	0.47
1:A:313:ARG:HG2	4:A:2148:HOH:O	2.14	0.47
1:A:189:PRO:HG2	1:A:300:LEU:CD2	2.40	0.47
1:A:242:SER:OG	1:A:243:ASN:N	2.46	0.47
1:A:248:HIS:O	1:A:249:ALA:HB2	2.15	0.47
1:A:299:HIS:HB3	1:A:300:LEU:HD22	1.97	0.47
1:B:111:ASN:ND2	1:B:142:GLU:OE1	2.47	0.47
1:A:335:GLY:O	1:A:336:ALA:HB3	2.14	0.47
1:A:36:GLU:HG3	1:A:92:THR:HG22	1.97	0.47
1:A:138:TYR:OH	1:A:164:ILE:CG1	2.63	0.47
1:B:332:GLY:O	1:B:333:SER:C	2.58	0.47
1:B:414:TRP:O	1:B:421:SER:N	2.48	0.47
1:B:32:LEU:HD13	1:B:95:PRO:HG2	1.98	0.46
1:A:189:PRO:CG	1:A:300:LEU:CG	2.91	0.46
1:B:96:TRP:CD2	1:B:97:PRO:HD3	2.50	0.46
1:B:166:TYR:HA	1:B:178:VAL:O	2.15	0.46
1:B:183:TYR:C	1:B:185:ALA:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLN:NE2	2:B:1655:CL:CL	2.86	0.46
1:A:329:TYR:C	1:A:330:GLU:HG3	2.41	0.46
1:B:2:GLN:HB2	1:B:16:ASP:OD2	2.16	0.46
1:B:379:GLU:CD	2:B:1657:CL:CL	2.95	0.46
1:A:56:MSE:O	1:A:71:HIS:CD2	2.69	0.46
1:A:31:ARG:HB2	4:A:2017:HOH:O	2.15	0.46
1:A:46:LEU:O	1:A:48:LEU:N	2.48	0.46
1:A:244:ILE:HG13	1:A:244:ILE:O	2.16	0.46
1:A:387[B]:ARG:HB2	1:A:387[B]:ARG:NH1	2.13	0.46
1:B:190:GLY:C	1:B:192:TYR:H	2.24	0.46
1:A:561:LEU:HD23	1:A:563:GLU:HB3	1.98	0.46
1:A:611:ASN:N	4:A:2241:HOH:O	2.48	0.46
1:B:299:HIS:O	1:B:317:VAL:HG22	2.16	0.46
1:B:571:VAL:HG13	1:B:576:VAL:HG22	1.98	0.46
1:B:52:LEU:O	1:B:74:VAL:O	2.33	0.45
1:A:224:LEU:HB2	1:A:276:ILE:HB	1.99	0.45
1:B:96:TRP:CG	1:B:97:PRO:HD3	2.51	0.45
1:A:300:LEU:CD2	1:A:300:LEU:O	2.63	0.45
1:B:189:PRO:HB2	1:B:192:TYR:HB2	1.98	0.45
1:A:114:VAL:N	1:A:115:PRO:HD2	2.31	0.45
1:A:192:TYR:CE1	1:A:302:ARG:HB2	2.52	0.45
1:B:146:GLN:O	1:B:146:GLN:HG2	2.16	0.45
1:B:460:LEU:HB2	4:B:2194:HOH:O	2.15	0.45
1:B:391:HIS:HB3	1:B:400:SER:HB2	1.98	0.45
1:B:497:TYR:CD1	1:B:497:TYR:C	2.95	0.45
1:A:226:LEU:CD2	1:A:257:ASP:HB3	2.45	0.45
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.83	0.45
1:B:456:VAL:HG11	1:B:460:LEU:HD22	1.97	0.45
1:A:82:GLY:HA2	1:A:86:PHE:O	2.17	0.45
1:A:486:ARG:NH1	4:A:2199:HOH:O	2.35	0.45
1:B:460:LEU:HA	1:B:462:ALA:H	1.81	0.45
1:A:186:HIS:HB3	1:A:300:LEU:HD12	1.98	0.45
1:A:578:GLU:O	1:A:585:ILE:HA	2.16	0.45
1:A:451:ASN:HB3	1:A:454:GLN:H	1.82	0.45
1:A:502:ARG:NH2	2:A:1645:CL:CL	2.87	0.45
1:A:580:ASN:ND2	1:A:584:THR:HG23	2.32	0.45
1:B:196:PRO:HG2	1:B:209:HIS:HA	1.99	0.45
1:B:264:GLN:NE2	4:B:2139:HOH:O	2.50	0.45
1:B:328:LEU:HD22	1:B:329:TYR:H	1.82	0.45
1:B:385:TYR:HB2	1:B:387:ARG:HD3	1.99	0.45
1:B:417:LYS:O	1:B:417:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLY:HA2	1:A:87:ALA:HA	1.99	0.44
1:A:100:LEU:C	1:A:152:PHE:HB2	2.42	0.44
1:A:136:ARG:HG2	1:A:181:ASP:CB	2.46	0.44
1:B:116:GLU:HA	1:B:119:LYS:HG3	1.99	0.44
1:B:371:VAL:O	1:B:373:VAL:HG13	2.17	0.44
1:A:285:ARG:HD2	1:A:347:ILE:HG22	1.99	0.44
1:A:402:GLU:HG3	1:A:403:ASN:N	2.31	0.44
1:A:532:ILE:HG21	1:A:536:ARG:HG3	1.99	0.44
1:B:150:THR:HB	1:B:153:ASP:OD2	2.17	0.44
1:B:277:GLU:HB3	1:B:354:ARG:HG3	1.99	0.44
1:B:579:PHE:CD1	1:B:585:ILE:HG23	2.52	0.44
1:A:33:PHE:CD1	1:A:33:PHE:C	2.96	0.44
1:A:88:GLY:C	1:A:89:TYR:CD1	2.96	0.44
1:A:595:TYR:CD1	1:A:595:TYR:C	2.95	0.44
1:B:396:ARG:C	4:B:2179:HOH:O	2.59	0.44
1:B:457:PRO:HG2	1:B:458:TYR:CE2	2.51	0.44
1:A:107:ARG:NE	4:A:2044:HOH:O	2.51	0.44
1:B:47:PRO:O	1:B:51:LEU:HD21	2.17	0.44
1:A:532:ILE:HG12	1:A:536:ARG:CG	2.47	0.44
1:B:5:ARG:O	1:B:6:LEU:CB	2.65	0.44
1:B:296:GLY:O	1:B:297:ALA:C	2.60	0.44
1:A:75:ALA:HB1	1:A:98:TRP:CZ3	2.52	0.44
1:B:373:VAL:HG11	1:B:391:HIS:HB3	2.00	0.44
1:A:18:LEU:HB2	1:A:41[A]:SER:OG	2.17	0.44
1:A:22:ARG:HB3	1:A:38:HIS:CB	2.46	0.43
1:A:410:VAL:HG11	1:A:425:PRO:HG3	2.00	0.43
1:A:580:ASN:HD22	1:A:584:THR:HG23	1.83	0.43
1:B:147:TYR:C	1:B:149:GLU:H	2.24	0.43
1:A:111:ASN:OD1	1:A:143:TYR:N	2.51	0.43
1:B:183:TYR:C	1:B:183:TYR:CD1	2.96	0.43
1:A:58:LEU:HD22	1:A:70:PHE:O	2.18	0.43
1:A:560:TYR:CD1	1:A:560:TYR:C	2.96	0.43
1:B:258:TYR:CE2	1:B:259:PRO:CD	3.01	0.43
1:A:7:VAL:HG12	1:A:9:VAL:HG13	1.99	0.43
1:B:55:PRO:HA	1:B:73:ILE:HA	1.99	0.43
1:B:139:ARG:HG2	1:B:141:TRP:CD1	2.54	0.43
1:B:312:ASN:HA	1:B:315:TYR:OH	2.18	0.43
1:B:18:LEU:HD23	1:B:18:LEU:O	2.18	0.43
1:B:73:ILE:HD13	1:B:99:LEU:CD1	2.49	0.43
1:A:379:GLU:HB3	1:A:380:ILE:HD12	2.00	0.43
1:B:414:TRP:HA	1:B:414:TRP:CE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:HB2	1:A:289:ARG:HB2	2.01	0.43
1:A:364:VAL:HG13	1:A:368:GLN:HE21	1.84	0.43
1:B:306:TYR:CD1	1:B:306:TYR:C	2.97	0.43
1:A:122:PHE:O	1:A:126:GLY:HA3	2.18	0.43
1:A:186:HIS:HB2	1:A:300:LEU:HD12	2.01	0.43
1:A:201:THR:HG22	1:A:202:LEU:HD12	2.01	0.43
1:A:226:LEU:HD12	1:A:272:ALA:HB2	2.01	0.43
1:A:532:ILE:CG1	1:A:536:ARG:HG3	2.45	0.43
1:B:27:GLU:CG	1:B:28:GLU:N	2.81	0.43
1:B:124:ASN:OD1	1:B:125:LEU:N	2.52	0.43
1:A:546:LEU:HG	1:A:548:VAL:HG23	2.00	0.43
1:B:32:LEU:CD1	1:B:98:TRP:HB2	2.48	0.43
1:B:69:PHE:HE1	1:B:172:GLN:CB	2.32	0.43
1:B:125:LEU:HB2	4:B:2068:HOH:O	2.18	0.43
1:B:199:PRO:O	1:B:201:THR:N	2.51	0.43
1:B:644:LEU:C	1:B:644:LEU:HD22	2.44	0.43
1:A:74:VAL:HG23	1:A:76:ARG:O	2.19	0.43
1:B:456:VAL:CG1	1:B:457:PRO:HD2	2.49	0.43
1:B:457:PRO:HG2	1:B:458:TYR:CD2	2.54	0.43
1:B:114:VAL:O	1:B:118:ILE:CD1	2.67	0.42
1:B:340:PHE:CG	1:B:341:GLU:N	2.87	0.42
1:B:475:LYS:HA	4:B:2176:HOH:O	2.19	0.42
1:B:5:ARG:O	1:B:6:LEU:HB2	2.18	0.42
1:B:169:ARG:HB2	1:B:178:VAL:CG2	2.48	0.42
1:B:361:VAL:O	1:B:362:PRO:C	2.62	0.42
1:A:47:PRO:O	1:A:51:LEU:CD2	2.67	0.42
1:A:118:ILE:HG23	1:A:155:ILE:HG22	2.01	0.42
1:A:315:TYR:HA	1:A:349:ALA:HB2	2.01	0.42
1:B:1:MSE:HE2	1:B:1:MSE:H3	1.83	0.42
1:A:37:LEU:HB2	1:A:91:ALA:O	2.19	0.42
1:A:75:ALA:CB	1:A:98:TRP:HZ3	2.29	0.42
1:B:12:PRO:HD2	1:B:71:HIS:HE1	1.83	0.42
1:B:383:ASP:OD1	1:B:383:ASP:C	2.63	0.42
1:B:483:ASN:HA	1:B:499:HIS:O	2.20	0.42
1:A:328:LEU:HG	1:A:328:LEU:O	2.20	0.42
1:A:387[B]:ARG:NH1	1:A:407:TRP:HB3	2.33	0.42
1:B:237:ARG:NH1	4:B:2122:HOH:O	2.52	0.42
1:A:17:VAL:HG13	1:A:18:LEU:N	2.34	0.42
1:A:390:VAL:HG22	1:A:408:ILE:CD1	2.50	0.42
1:B:186:HIS:HB2	1:B:300:LEU:HD11	2.01	0.42
1:A:57:SER:CB	1:A:172:GLN:HE21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLU:HB2	2:A:1646:CL:CL	2.56	0.42
1:A:595:TYR:O	1:A:596:ALA:CB	2.68	0.42
1:B:4:THR:C	1:B:5:ARG:HD2	2.44	0.42
1:B:147:TYR:O	1:B:149:GLU:N	2.44	0.42
1:A:11:CYS:HB2	1:A:18:LEU:HD11	2.01	0.42
1:A:95:PRO:O	1:A:98:TRP:HB3	2.20	0.42
1:B:488:GLU:OE1	1:B:489:ASP:N	2.53	0.42
1:B:644:LEU:HD22	1:B:645:GLU:N	2.35	0.42
1:A:258:TYR:HD1	1:A:258:TYR:O	2.03	0.42
1:A:387[B]:ARG:NH1	4:A:2168:HOH:O	2.52	0.41
1:B:101:THR:HA	1:B:150:THR:CG2	2.50	0.41
1:B:414:TRP:HA	1:B:414:TRP:HE3	1.84	0.41
1:A:258:TYR:CD1	1:A:258:TYR:O	2.73	0.41
1:B:18:LEU:HD23	1:B:18:LEU:C	2.45	0.41
1:B:586:ASN:N	1:B:586:ASN:HD22	2.18	0.41
1:A:101:THR:HG23	1:A:102:ARG:CZ	2.50	0.41
1:A:195:VAL:O	1:A:195:VAL:CG2	2.67	0.41
1:A:641:ALA:HB3	4:A:2261:HOH:O	2.20	0.41
1:B:11:CYS:HB3	1:B:12:PRO:HD2	1.97	0.41
1:B:13:LEU:HD12	2:B:1646:CL:CL	2.57	0.41
1:B:306:TYR:HB3	4:B:2158:HOH:O	2.20	0.41
1:A:624:GLY:CA	4:A:2224:HOH:O	2.68	0.41
1:B:101:THR:HA	1:B:150:THR:HG21	2.01	0.41
1:B:183:TYR:O	1:B:185:ALA:N	2.52	0.41
1:B:287:ARG:HG2	4:B:2150:HOH:O	2.19	0.41
1:B:532:ILE:HD12	1:B:532:ILE:N	2.35	0.41
1:A:173:LYS:HD2	1:A:174:ARG:NH1	2.36	0.41
1:A:578:GLU:CG	1:A:580:ASN:HD21	2.34	0.41
1:B:478:THR:C	1:B:480:ALA:N	2.77	0.41
1:A:313:ARG:NH1	1:A:348:ASP:OD1	2.54	0.41
1:A:578:GLU:HG2	1:A:580:ASN:HD21	1.85	0.41
1:B:220:GLN:NE2	1:B:282:GLN:HG2	2.36	0.41
1:B:540:VAL:CG1	1:B:542:LEU:O	2.65	0.41
1:A:120:GLN:O	1:A:123:ARG:HD2	2.21	0.41
1:B:277:GLU:CB	1:B:354:ARG:HG3	2.49	0.41
1:A:62:LEU:O	1:A:63:PRO:C	2.63	0.41
1:A:112:GLN:HG3	1:A:113:SER:H	1.86	0.41
1:A:186:HIS:ND1	1:A:298:GLY:O	2.54	0.41
1:A:187:ARG:O	1:A:188:SER:C	2.64	0.41
1:A:587:ILE:HG22	1:A:592:PHE:HZ	1.86	0.41
1:B:54:LYS:HG2	1:B:55:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LEU:HD22	1:B:329:TYR:N	2.36	0.41
1:B:448:ARG:O	1:B:449:VAL:HG13	2.20	0.41
1:B:637:PHE:O	1:B:639:PRO:HD3	2.21	0.41
1:B:307:PRO:HD2	4:B:2154:HOH:O	2.21	0.41
1:B:403:ASN:ND2	2:B:1660:CL:CL	2.80	0.41
1:A:225:THR:HG22	1:A:241:ARG:HB2	2.02	0.40
1:A:240:VAL:O	1:A:240:VAL:HG23	2.21	0.40
1:B:1:MSE:HB2	1:B:2:GLN:HA	2.03	0.40
1:B:296:GLY:O	1:B:317:VAL:HG23	2.17	0.40
1:A:413:ALA:HB3	1:A:421:SER:OG	2.22	0.40
1:A:587:ILE:HG22	1:A:592:PHE:CZ	2.56	0.40
1:B:46:LEU:HD13	1:B:51:LEU:CD2	2.51	0.40
1:A:481:ASN:HA	1:A:501:GLU:CD	2.47	0.40
1:B:75:ALA:HB1	1:B:98:TRP:CH2	2.56	0.40
1:B:308:ARG:O	1:B:309:ASP:C	2.63	0.40
1:A:136:ARG:HD3	1:A:137:PRO:O	2.20	0.40
1:B:22:ARG:HE	1:B:38:HIS:CD2	2.40	0.40
1:A:31:ARG:NH2	1:A:160:GLU:OE2	2.54	0.40
1:B:482:PHE:C	1:B:501:GLU:HB2	2.46	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ALA:O	4:A:2224:HOH:O[3_765]	1.76	0.44
1:A:503:ASN:ND2	1:A:511:ASP:O[3_765]	1.99	0.21
1:A:45:ASN:OD1	1:A:66:SER:OG[2_755]	2.04	0.16
1:B:465:THR:OG1	1:B:474:SER:OG[2_755]	2.12	0.08
1:B:523:SER:OG	1:B:531:ARG:NH2[2_755]	2.19	0.01

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	645/651 (99%)	519 (80%)	103 (16%)	23 (4%)	2	1
1	B	646/651 (99%)	538 (83%)	88 (14%)	20 (3%)	3	1
All	All	1291/1302 (99%)	1057 (82%)	191 (15%)	43 (3%)	3	1

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	63	PRO
1	A	64	GLY
1	A	234	PRO
1	A	249	ALA
1	A	259	PRO
1	A	461	PRO
1	A	583	GLY
1	A	596	ALA
1	B	6	LEU
1	B	11	CYS
1	B	259	PRO
1	B	461	PRO
1	A	5	ARG
1	A	11	CYS
1	A	14	GLY
1	A	247	PRO
1	A	296	GLY
1	A	336	ALA
1	A	611	ASN
1	B	400	SER
1	B	479	PRO
1	B	624	GLY
1	A	111	ASN
1	A	201	THR
1	B	10	ASP
1	B	399	GLN
1	B	638	PRO
1	A	205	ARG
1	B	44	PRO
1	B	148	ARG
1	B	362	PRO
1	B	393	HIS
1	B	417	LYS
1	A	15	PRO

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Mol	Chain	Res	Type
1	A	443	PRO
1	B	115	PRO
1	A	32	LEU
1	B	305	GLY
1	B	114	VAL
1	B	184	GLY
1	B	375	PRO
1	A	240	VAL

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	539/534 (101%)	444 (82%)	95 (18%)	2	1
1	B	540/534 (101%)	465 (86%)	75 (14%)	3	2
All	All	1079/1068 (101%)	909 (84%)	170 (16%)	2	1

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	THR
1	A	5	ARG
1	A	7	VAL
1	A	8	GLN
1	A	11	CYS
1	A	18	LEU
1	A	24	GLU
1	A	27	GLU
1	A	37	LEU
1	A	39	LEU
1	A	45	ASN
1	A	46	LEU
1	A	48	LEU
1	A	49	GLU

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Mol	Chain	Res	Type
1	A	54	LYS
1	A	61	GLU
1	A	62	LEU
1	A	63	PRO
1	A	68	ARG
1	A	71	HIS
1	A	73	ILE
1	A	83	HIS
1	A	92	THR
1	A	101	THR
1	A	103	THR
1	A	110	GLN
1	A	121	VAL
1	A	125	LEU
1	A	134	LEU
1	A	136	ARG
1	A	144	CYS
1	A	158	LEU
1	A	165	TYR
1	A	173	LYS
1	A	175	HIS
1	A	177	LEU
1	A	179	LEU
1	A	194	SER
1	A	195	VAL
1	A	201	THR
1	A	220	GLN
1	A	223	SER
1	A	224	LEU
1	A	227	ASN
1	A	232	GLN
1	A	233	ARG
1	A	238	LEU
1	A	241	ARG
1	A	261	GLU
1	A	287	ARG
1	A	300	LEU
1	A	311	GLN
1	A	313	ARG
1	A	329	TYR
1	A	330	GLU
1	A	341	GLU

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Mol	Chain	Res	Type
1	A	346	CYS
1	A	351	GLN
1	A	353	PHE
1	A	369	THR
1	A	379	GLU
1	A	404	SER
1	A	409	ARG
1	A	414	TRP
1	A	423	GLN
1	A	434	SER
1	A	442	ARG
1	A	444	ILE
1	A	446	THR
1	A	449	VAL
1	A	451	ASN
1	A	465	THR
1	A	467	SER
1	A	469	MSE
1	A	513	SER
1	A	521	ASN
1	A	536	ARG
1	A	537	THR
1	A	541	LYS
1	A	542	LEU
1	A	557	THR
1	A	559	THR
1	A	561	LEU
1	A	567	GLN
1	A	584	THR
1	A	595	TYR
1	A	597	SER
1	A	601	ASN
1	A	604	THR
1	A	609	ASP
1	A	611	ASN
1	A	619	ASP
1	A	621	LYS
1	A	644	LEU
1	B	1	MSE
1	B	5	ARG
1	B	6	LEU
1	B	7	VAL

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Mol	Chain	Res	Type
1	B	19	LEU
1	B	23	MSE
1	B	32	LEU
1	B	46	LEU
1	B	50	GLN
1	B	51	LEU
1	B	52	LEU
1	B	56	MSE
1	B	67	ARG
1	B	80	VAL
1	B	85	GLN
1	B	90	GLN
1	B	94	ARG
1	B	114	VAL
1	B	136	ARG
1	B	139	ARG
1	B	150	THR
1	B	151	SER
1	B	173	LYS
1	B	180	SER
1	B	205	ARG
1	B	213	TRP
1	B	259	PRO
1	B	263	VAL
1	B	266	GLN
1	B	269	GLU
1	B	273	ARG
1	B	280	GLN
1	B	283	HIS
1	B	286	VAL
1	B	295	ILE
1	B	310	ASP
1	B	311	GLN
1	B	323	ARG
1	B	325	VAL
1	B	328	LEU
1	B	345	ASP
1	B	351	GLN
1	B	363	VAL
1	B	391	HIS
1	B	414	TRP
1	B	424	ILE

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Mol	Chain	Res	Type
1	B	427	ILE
1	B	429	GLN
1	B	433	VAL
1	B	437	GLU
1	B	446	THR
1	B	460	LEU
1	B	463	ASN
1	B	465	THR
1	B	488	GLU
1	B	490	LYS
1	B	497	TYR
1	B	502	ARG
1	B	520	ARG
1	B	542	LEU
1	B	546	LEU
1	B	547	LEU
1	B	553	SER
1	B	555	SER
1	B	563	GLU
1	B	570	LEU
1	B	584	THR
1	B	586	ASN
1	B	587	ILE
1	B	594	LEU
1	B	602	ILE
1	B	608	LEU
1	B	610	LEU
1	B	619	ASP
1	B	644	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	172	GLN
1	A	214	GLN
1	A	220	GLN
1	A	299	HIS
1	A	423	GLN
1	A	518	HIS
1	A	567	GLN
1	A	580	ASN

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Mol	Chain	Res	Type
1	A	599	ASN
1	B	2	GLN
1	B	8	GLN
1	B	50	GLN
1	B	71	HIS
1	B	83	HIS
1	B	90	GLN
1	B	172	GLN
1	B	243	ASN
1	B	266	GLN
1	B	339	GLN
1	B	393	HIS
1	B	397	HIS
1	B	403	ASN
1	B	412	GLN
1	B	429	GLN
1	B	463	ASN
1	B	466	GLN
1	B	521	ASN
1	B	526	HIS
1	B	586	ASN
1	B	634	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

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 [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	635/651 (97%)	-1.10	0 100 100	10, 41, 63, 78	3 (0%)
1	B	636/651 (97%)	-1.23	0 100 100	10, 33, 54, 63	3 (0%)
All	All	1271/1302 (97%)	-1.17	0 100 100	10, 37, 59, 78	6 (0%)

There are no RSRZ outliers to report.

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
2	CL	B	1707	1/1	0.97	0.06	75,75,75,75	0
2	CL	B	1655	1/1	0.98	0.06	68,68,68,68	0
2	CL	B	1656	1/1	0.98	0.05	59,59,59,59	0
2	CL	B	1648	1/1	0.98	0.07	70,70,70,70	0
3	NA	B	1663	1/1	0.98	0.06	60,60,60,60	0
3	NA	B	1711	1/1	0.98	0.07	48,48,48,48	0
3	NA	B	1712	1/1	0.98	0.04	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	1704	1/1	0.99	0.03	42,42,42,42	0
2	CL	A	1705	1/1	0.99	0.03	40,40,40,40	0
2	CL	B	1646	1/1	0.99	0.03	49,49,49,49	0
2	CL	B	1647	1/1	0.99	0.06	63,63,63,63	0
2	CL	A	1647	1/1	0.99	0.03	44,44,44,44	0
2	CL	B	1649	1/1	0.99	0.04	55,55,55,55	0
2	CL	B	1650	1/1	0.99	0.03	37,37,37,37	0
2	CL	B	1651	1/1	0.99	0.02	44,44,44,44	0
2	CL	B	1653	1/1	0.99	0.03	43,43,43,43	0
2	CL	B	1654	1/1	0.99	0.03	52,52,52,52	0
2	CL	A	1649	1/1	0.99	0.03	43,43,43,43	0
2	CL	A	1650	1/1	0.99	0.02	57,57,57,57	0
2	CL	B	1658	1/1	0.99	0.02	46,46,46,46	0
2	CL	B	1659	1/1	0.99	0.03	53,53,53,53	0
2	CL	B	1660	1/1	0.99	0.04	50,50,50,50	0
2	CL	B	1661	1/1	0.99	0.03	39,39,39,39	0
2	CL	B	1701	1/1	0.99	0.03	46,46,46,46	0
2	CL	B	1704	1/1	0.99	0.04	48,48,48,48	0
2	CL	B	1705	1/1	0.99	0.02	42,42,42,42	0
2	CL	B	1706	1/1	0.99	0.03	46,46,46,46	0
2	CL	A	1651	1/1	0.99	0.02	45,45,45,45	0
2	CL	B	1708	1/1	0.99	0.03	50,50,50,50	0
3	NA	A	1652	1/1	0.99	0.03	34,34,34,34	0
3	NA	A	1653	1/1	0.99	0.02	35,35,35,35	0
3	NA	A	1654	1/1	0.99	0.06	41,41,41,41	0
3	NA	A	1655	1/1	0.99	0.03	34,34,34,34	0
3	NA	A	1710	1/1	0.99	0.03	36,36,36,36	0
2	CL	A	1700	1/1	0.99	0.02	38,38,38,38	0
3	NA	B	1710	1/1	0.99	0.03	32,32,32,32	0
2	CL	A	1701	1/1	0.99	0.04	40,40,40,40	0
2	CL	A	1703	1/1	0.99	0.04	51,51,51,51	0
3	NA	B	1713	1/1	0.99	0.03	43,43,43,43	0
3	NA	B	1714	1/1	0.99	0.04	36,36,36,36	0
2	CL	B	1702	1/1	1.00	0.02	35,35,35,35	0
2	CL	B	1703	1/1	1.00	0.02	41,41,41,41	0
2	CL	B	1657	1/1	1.00	0.02	42,42,42,42	0
3	NA	A	1711	1/1	1.00	0.01	33,33,33,33	0
3	NA	B	1662	1/1	1.00	0.01	20,20,20,20	0
2	CL	B	1652	1/1	1.00	0.02	43,43,43,43	0
2	CL	A	1646	1/1	1.00	0.02	41,41,41,41	0
2	CL	A	1645	1/1	1.00	0.01	31,31,31,31	0
2	CL	A	1702	1/1	1.00	0.02	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	1700	1/1	1.00	0.01	26,26,26,26	0
2	CL	A	1648	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.