



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:53 AM UTC

PDB ID : 3EE1 / pdb_00003ee1
Title : Novel fold of VirA, a type III secretion system effector protein from *Shigella flexneri*
Authors : Davis, J.S.
Deposited on : 2008-09-03
Resolution : 3.01 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

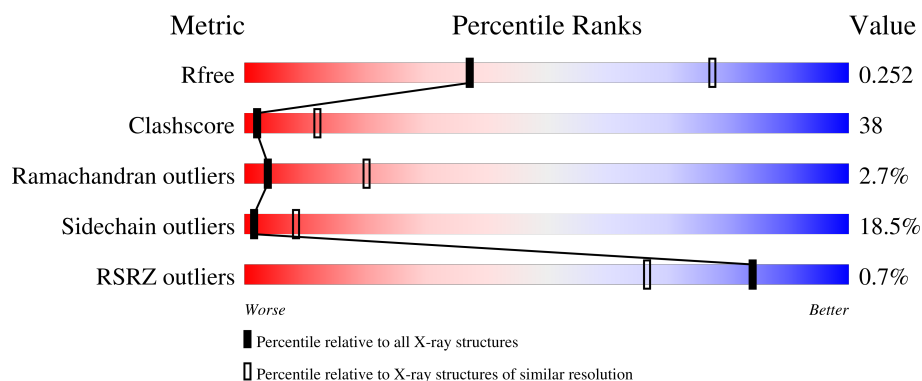
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	400	
1	B	400	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5244 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 Effector protein virA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	Se	0	0	0
			2622	1660	439	511	7	5			
1	B	341	Total	C	N	O	S	Se	0	0	0
			2622	1660	439	511	7	5			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP Q7BU69
A	2	VAL	-	expression tag	UNP Q7BU69
A	3	ALA	-	expression tag	UNP Q7BU69
A	4	SER	-	expression tag	UNP Q7BU69
A	5	TYR	-	expression tag	UNP Q7BU69
A	6	CYS	-	expression tag	UNP Q7BU69
A	7	ASP	-	expression tag	UNP Q7BU69
A	8	ARG	-	expression tag	UNP Q7BU69
A	9	VAL	-	expression tag	UNP Q7BU69
A	10	VAL	-	expression tag	UNP Q7BU69
A	11	ALA	-	expression tag	UNP Q7BU69
A	12	ALA	-	expression tag	UNP Q7BU69
A	13	VAL	-	expression tag	UNP Q7BU69
A	36	VAL	ILE	variant	UNP Q7BU69
A	56	TYR	HIS	variant	UNP Q7BU69
A	173	PRO	HIS	variant	UNP Q7BU69
A	239	LEU	VAL	variant	UNP Q7BU69
B	1	GLU	-	expression tag	UNP Q7BU69
B	2	VAL	-	expression tag	UNP Q7BU69
B	3	ALA	-	expression tag	UNP Q7BU69
B	4	SER	-	expression tag	UNP Q7BU69
B	5	TYR	-	expression tag	UNP Q7BU69
B	6	CYS	-	expression tag	UNP Q7BU69
B	7	ASP	-	expression tag	UNP Q7BU69
B	8	ARG	-	expression tag	UNP Q7BU69

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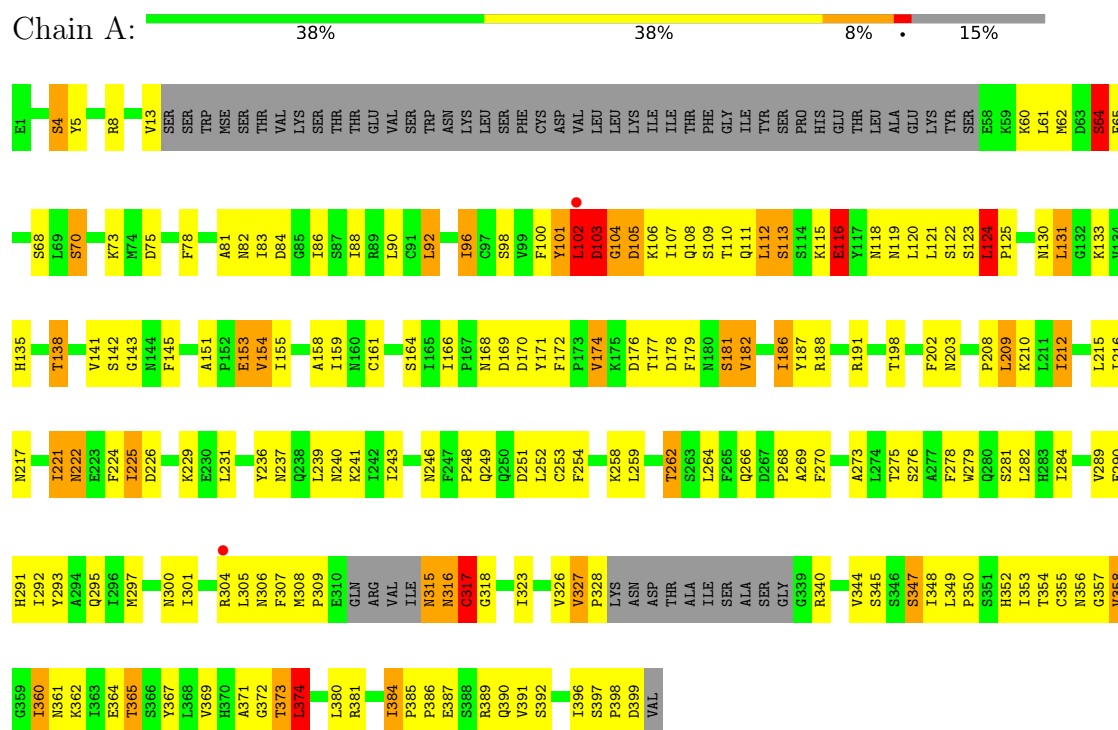
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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	VAL	-	expression tag	UNP Q7BU69
B	10	VAL	-	expression tag	UNP Q7BU69
B	11	ALA	-	expression tag	UNP Q7BU69
B	12	ALA	-	expression tag	UNP Q7BU69
B	13	VAL	-	expression tag	UNP Q7BU69
B	36	VAL	ILE	variant	UNP Q7BU69
B	56	TYR	HIS	variant	UNP Q7BU69
B	173	PRO	HIS	variant	UNP Q7BU69
B	239	LEU	VAL	variant	UNP Q7BU69

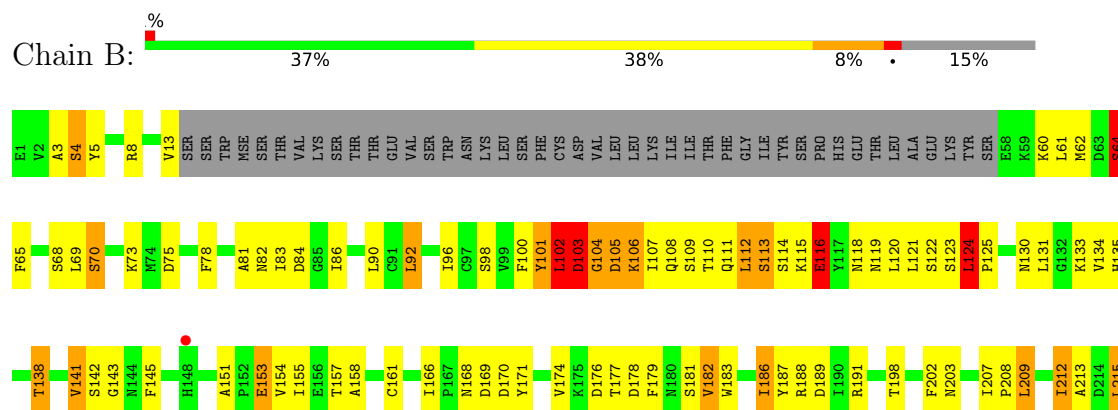
3 Residue-property plots

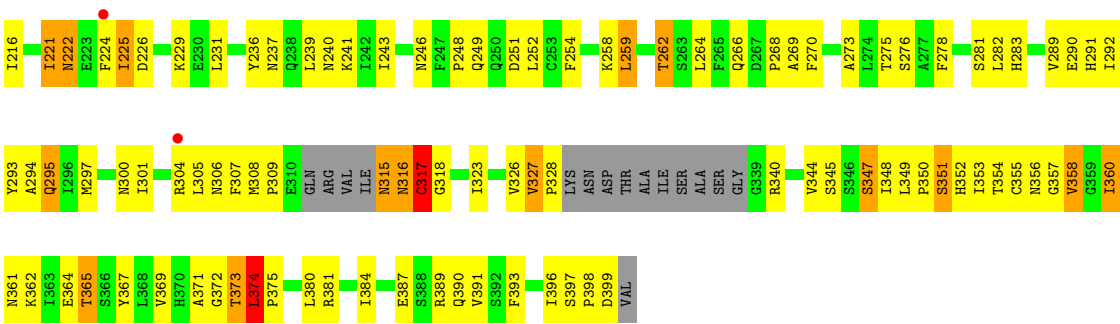
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Effector protein virA



• Molecule 1: Effector protein virA





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.25Å 170.91Å 46.16Å 90.00° 104.89° 90.00°	Depositor
Resolution (Å)	28.63 – 3.01 28.63 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.2 (28.63-3.01) 96.1 (28.63-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 3.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.256 0.212 , 0.252	Depositor DCC
R_{free} test set	1097 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	98.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 111.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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	0.74	0/2670	1.16	21/3618 (0.6%)
1	B	0.72	1/2670 (0.0%)	1.14	17/3618 (0.5%)
All	All	0.73	1/5340 (0.0%)	1.15	38/7236 (0.5%)

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	ALA	CA-CB	6.93	1.62	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	N-CA-C	-13.11	96.63	112.49
1	B	104	GLY	N-CA-C	-12.37	97.52	112.49
1	A	101	TYR	N-CA-C	-9.28	101.12	111.14
1	B	101	TYR	N-CA-C	-8.49	101.97	111.14
1	A	60	LYS	N-CA-C	-8.13	103.38	113.38
1	B	174	VAL	CB-CA-C	-7.91	102.69	111.23
1	B	124	LEU	CA-C-N	7.53	128.13	120.38
1	B	124	LEU	C-N-CA	7.53	128.13	120.38
1	B	60	LYS	N-CA-C	-7.50	104.12	113.28
1	A	374	LEU	CA-C-N	7.33	129.00	119.84
1	A	374	LEU	C-N-CA	7.33	129.00	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	LYS	N-CA-C	-7.23	102.25	113.02
1	B	64	SER	N-CA-C	-7.01	104.19	112.89
1	A	64	SER	N-CA-C	-6.96	104.26	112.89
1	B	115	LYS	N-CA-C	-6.87	102.79	113.02
1	A	124	LEU	CA-C-N	6.82	127.41	120.38
1	A	124	LEU	C-N-CA	6.82	127.41	120.38
1	A	174	VAL	CB-CA-C	-6.41	104.31	111.23
1	B	116	GLU	N-CA-C	-6.15	105.26	112.89
1	B	182	VAL	N-CA-C	6.08	116.55	110.23
1	B	374	LEU	CA-C-N	5.95	127.27	119.84
1	B	374	LEU	C-N-CA	5.95	127.27	119.84
1	A	385	PRO	CA-C-O	-5.82	116.71	120.90
1	A	116	GLU	N-CA-C	-5.78	105.73	112.89
1	A	385	PRO	O-C-N	5.76	123.96	121.31
1	B	207	ILE	CA-C-N	5.64	125.92	119.83
1	B	207	ILE	C-N-CA	5.64	125.92	119.83
1	A	318	GLY	N-CA-C	5.51	120.49	112.55
1	B	371	ALA	N-CA-C	5.48	116.93	111.07
1	A	371	ALA	N-CA-C	5.41	117.18	111.28
1	B	295	GLN	N-CA-C	-5.24	105.46	111.07
1	A	172	PHE	CA-C-N	-5.24	114.24	120.11
1	A	172	PHE	C-N-CA	-5.24	114.24	120.11
1	A	182	VAL	N-CA-C	5.20	115.64	110.23
1	A	384	ILE	CA-C-N	5.19	123.45	119.66
1	A	384	ILE	C-N-CA	5.19	123.45	119.66
1	A	154	VAL	N-CA-C	-5.10	106.71	111.45
1	B	318	GLY	N-CA-C	5.07	119.86	112.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Peptide
1	B	103	ASP	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	2622	0	2537	197	0
1	B	2622	0	2537	198	0
All	All	5244	0	5074	387	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 38.

All (387) 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:102:LEU:HA	1:A:108:GLN:HA	1.24	1.13
1:B:102:LEU:HA	1:B:108:GLN:HA	1.28	1.12
1:A:102:LEU:HD13	1:A:103:ASP:OD1	1.59	1.00
1:B:102:LEU:HD13	1:B:103:ASP:OD1	1.61	0.98
1:A:102:LEU:HB2	1:A:108:GLN:HG3	1.54	0.90
1:A:209:LEU:HA	1:A:212:ILE:HD11	1.56	0.88
1:B:158:ALA:O	1:B:362:LYS:HE3	1.74	0.87
1:B:349:LEU:HB3	1:B:360:ILE:CD1	2.05	0.87
1:B:209:LEU:HA	1:B:212:ILE:HD11	1.57	0.86
1:A:349:LEU:HB3	1:A:360:ILE:CD1	2.05	0.86
1:B:104:GLY:HA3	1:B:107:ILE:HD12	1.56	0.86
1:B:143:GLY:HA3	1:B:356:ASN:O	1.76	0.85
1:B:102:LEU:HB2	1:B:108:GLN:HG3	1.58	0.85
1:B:326:VAL:HG22	1:B:327:VAL:H	1.39	0.85
1:A:344:VAL:HG11	1:A:367:TYR:CE2	2.11	0.85
1:A:104:GLY:HA3	1:A:107:ILE:HD12	1.57	0.84
1:A:143:GLY:HA3	1:A:356:ASN:O	1.78	0.83
1:A:326:VAL:HG22	1:A:327:VAL:H	1.43	0.83
1:B:344:VAL:HG11	1:B:367:TYR:CE2	2.14	0.82
1:A:349:LEU:HB3	1:A:360:ILE:HD12	1.63	0.80
1:A:102:LEU:HA	1:A:108:GLN:CA	2.11	0.80
1:A:158:ALA:O	1:A:362:LYS:HE3	1.82	0.80
1:A:226:ASP:HB3	1:A:229:LYS:HG2	1.64	0.79
1:A:350:PRO:HD2	1:A:361:ASN:O	1.83	0.79
1:A:100:PHE:O	1:A:102:LEU:HD12	1.83	0.79
1:A:65:PHE:CD2	1:A:81:ALA:HB2	2.19	0.78
1:A:297:MSE:O	1:A:301:ILE:HD13	1.85	0.76
1:B:226:ASP:HB3	1:B:229:LYS:HG2	1.65	0.76
1:A:216:ILE:HB	1:A:221:ILE:HG12	1.67	0.76
1:A:221:ILE:HG13	1:A:221:ILE:O	1.86	0.76
1:B:239:LEU:HD11	1:B:262:THR:HA	1.67	0.76
1:B:350:PRO:HD2	1:B:361:ASN:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:MSE:O	1:B:301:ILE:HD13	1.86	0.75
1:B:348:ILE:HG23	1:B:350:PRO:HD3	1.68	0.75
1:A:239:LEU:HD11	1:A:262:THR:HA	1.67	0.75
1:B:349:LEU:HB3	1:B:360:ILE:HD11	1.69	0.74
1:B:349:LEU:HB3	1:B:360:ILE:HD12	1.69	0.74
1:A:102:LEU:HD22	1:A:103:ASP:OD2	1.87	0.74
1:B:65:PHE:CD2	1:B:81:ALA:HB2	2.23	0.73
1:B:216:ILE:HB	1:B:221:ILE:HG12	1.71	0.73
1:A:208:PRO:O	1:A:212:ILE:HD13	1.89	0.72
1:B:100:PHE:O	1:B:102:LEU:HD12	1.89	0.72
1:B:317:CYS:HB3	1:B:349:LEU:O	1.90	0.72
1:A:317:CYS:HB3	1:A:349:LEU:O	1.90	0.72
1:B:326:VAL:HG22	1:B:327:VAL:N	2.05	0.72
1:A:348:ILE:HG23	1:A:350:PRO:HD3	1.70	0.71
1:A:306:ASN:HD21	1:B:188:ARG:NE	1.88	0.71
1:B:208:PRO:O	1:B:212:ILE:HD13	1.91	0.70
1:A:102:LEU:C	1:A:103:ASP:OD1	2.34	0.70
1:A:100:PHE:C	1:A:102:LEU:HD12	2.15	0.70
1:B:153:GLU:CD	1:B:153:GLU:H	2.00	0.70
1:B:221:ILE:O	1:B:221:ILE:HG13	1.92	0.69
1:B:102:LEU:HA	1:B:108:GLN:CA	2.17	0.69
1:A:304:ARG:HA	1:A:353:ILE:HD12	1.75	0.69
1:A:349:LEU:HD22	1:A:360:ILE:HD11	1.73	0.69
1:A:326:VAL:HG22	1:A:327:VAL:N	2.08	0.68
1:A:237:ASN:O	1:A:241:LYS:HG2	1.94	0.67
1:A:349:LEU:HB3	1:A:360:ILE:HD11	1.76	0.67
1:B:102:LEU:HD22	1:B:103:ASP:OD2	1.95	0.66
1:A:102:LEU:C	1:A:103:ASP:CG	2.63	0.66
1:A:101:TYR:O	1:A:103:ASP:N	2.28	0.66
1:B:237:ASN:O	1:B:241:LYS:HG2	1.94	0.66
1:B:300:ASN:ND2	1:B:353:ILE:H	1.93	0.66
1:B:100:PHE:C	1:B:102:LEU:HD12	2.20	0.66
1:B:349:LEU:HD22	1:B:360:ILE:HD11	1.76	0.66
1:A:101:TYR:O	1:A:103:ASP:OD1	2.14	0.66
1:A:306:ASN:HD21	1:B:188:ARG:HE	1.44	0.66
1:B:315:ASN:N	1:B:351:SER:HG	1.95	0.65
1:A:65:PHE:CE2	1:A:81:ALA:HB2	2.32	0.65
1:A:68:SER:HB2	1:A:73:LYS:HE2	1.78	0.65
1:B:62:MSE:HG3	1:B:123:SER:O	1.95	0.65
1:B:101:TYR:O	1:B:103:ASP:N	2.30	0.64
1:B:304:ARG:HA	1:B:353:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:SER:CB	1:A:73:LYS:HE2	2.28	0.63
1:B:209:LEU:HD23	1:B:212:ILE:HD11	1.80	0.63
1:A:61:LEU:O	1:A:64:SER:OG	2.17	0.63
1:A:293:TYR:OH	1:A:297:MSE:HE3	1.99	0.63
1:B:273:ALA:HA	1:B:369:VAL:HG21	1.82	0.62
1:A:209:LEU:HD23	1:A:212:ILE:HD11	1.80	0.62
1:A:84:ASP:C	1:A:86:ILE:H	2.08	0.62
1:A:153:GLU:H	1:A:153:GLU:CD	2.07	0.62
1:A:216:ILE:HD12	1:A:221:ILE:HD11	1.80	0.62
1:B:365:THR:HB	1:B:391:VAL:HG22	1.81	0.62
1:A:365:THR:HB	1:A:391:VAL:HG22	1.80	0.62
1:A:68:SER:CA	1:A:73:LYS:HE2	2.31	0.61
1:B:102:LEU:C	1:B:103:ASP:CG	2.69	0.60
1:A:13:VAL:H	1:A:119:ASN:HD22	1.50	0.60
1:B:216:ILE:HD12	1:B:221:ILE:HD11	1.81	0.60
1:A:226:ASP:HB3	1:A:229:LYS:CG	2.31	0.60
1:A:300:ASN:ND2	1:A:353:ILE:H	1.99	0.60
1:B:68:SER:HB2	1:B:73:LYS:HE2	1.84	0.60
1:B:300:ASN:HB2	1:B:352:HIS:CD2	2.37	0.60
1:B:293:TYR:OH	1:B:297:MSE:HE3	2.02	0.59
1:B:353:ILE:HG22	1:B:354:THR:O	2.02	0.59
1:B:239:LEU:CD1	1:B:262:THR:HA	2.33	0.59
1:B:13:VAL:H	1:B:119:ASN:HD22	1.51	0.58
1:B:326:VAL:CG2	1:B:327:VAL:H	2.11	0.58
1:A:83:ILE:O	1:A:86:ILE:HB	2.02	0.58
1:B:68:SER:CB	1:B:73:LYS:HE2	2.33	0.58
1:A:100:PHE:HB3	1:A:102:LEU:HD12	1.84	0.58
1:B:65:PHE:CE2	1:B:81:ALA:HB2	2.37	0.58
1:B:84:ASP:C	1:B:86:ILE:H	2.12	0.58
1:A:344:VAL:HG11	1:A:367:TYR:CD2	2.39	0.57
1:B:68:SER:HB2	1:B:73:LYS:HG3	1.85	0.57
1:B:101:TYR:O	1:B:103:ASP:OD1	2.22	0.57
1:B:300:ASN:HD22	1:B:353:ILE:H	1.51	0.57
1:A:62:MSE:HG3	1:A:123:SER:O	2.04	0.57
1:B:68:SER:CA	1:B:73:LYS:HE2	2.34	0.57
1:A:326:VAL:CG2	1:A:327:VAL:H	2.13	0.57
1:B:83:ILE:O	1:B:86:ILE:HB	2.04	0.57
1:B:226:ASP:HB3	1:B:229:LYS:CG	2.33	0.57
1:A:239:LEU:CD1	1:A:262:THR:HA	2.34	0.57
1:A:273:ALA:HA	1:A:369:VAL:HG21	1.86	0.57
1:A:209:LEU:HA	1:A:212:ILE:CD1	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HA	1:A:124:LEU:HD23	1.87	0.56
1:B:111:GLN:HG3	1:B:112:LEU:H	1.69	0.56
1:A:300:ASN:HB2	1:A:352:HIS:CD2	2.41	0.56
1:B:168:ASN:HD21	1:B:289:VAL:HG23	1.70	0.56
1:B:102:LEU:C	1:B:103:ASP:OD1	2.48	0.56
1:B:254:PHE:O	1:B:258:LYS:HG3	2.05	0.56
1:A:315:ASN:O	1:A:317:CYS:N	2.39	0.56
1:B:316:ASN:O	1:B:317:CYS:O	2.23	0.56
1:B:61:LEU:O	1:B:64:SER:OG	2.21	0.55
1:A:102:LEU:O	1:A:103:ASP:CG	2.49	0.55
1:B:100:PHE:HB3	1:B:102:LEU:HD12	1.88	0.55
1:A:316:ASN:O	1:A:317:CYS:O	2.25	0.55
1:B:90:LEU:HD13	1:B:120:LEU:HD21	1.88	0.55
1:A:291:HIS:CD2	1:B:290:GLU:OE1	2.60	0.55
1:B:243:ILE:HD12	1:B:258:LYS:HB3	1.89	0.55
1:B:300:ASN:HB2	1:B:352:HIS:HD2	1.72	0.55
1:A:254:PHE:O	1:A:258:LYS:HG3	2.06	0.55
1:A:104:GLY:O	1:A:105:ASP:HB2	2.06	0.54
1:B:151:ALA:O	1:B:154:VAL:HB	2.07	0.54
1:A:209:LEU:O	1:A:212:ILE:HG12	2.07	0.54
1:A:102:LEU:HD22	1:A:103:ASP:CG	2.32	0.54
1:A:171:TYR:CD1	1:A:387:GLU:HA	2.43	0.54
1:A:151:ALA:O	1:A:154:VAL:HB	2.06	0.54
1:A:101:TYR:HB3	1:A:109:SER:HB2	1.90	0.54
1:A:102:LEU:C	1:A:107:ILE:O	2.50	0.54
1:B:121:LEU:HA	1:B:124:LEU:HD23	1.89	0.54
1:B:315:ASN:O	1:B:317:CYS:N	2.41	0.54
1:B:153:GLU:CD	1:B:153:GLU:N	2.65	0.54
1:A:315:ASN:N	1:A:315:ASN:HD22	2.04	0.53
1:A:68:SER:HB2	1:A:73:LYS:HG3	1.88	0.53
1:A:243:ILE:HD12	1:A:258:LYS:HB3	1.90	0.53
1:B:304:ARG:CA	1:B:353:ILE:HD12	2.38	0.53
1:B:102:LEU:C	1:B:107:ILE:O	2.51	0.53
1:A:300:ASN:HD22	1:A:353:ILE:H	1.57	0.53
1:A:186:ILE:HD13	1:A:275:THR:HG22	1.90	0.53
1:A:373:THR:C	1:A:374:LEU:HD23	2.33	0.53
1:A:353:ILE:HG22	1:A:354:THR:O	2.08	0.53
1:B:111:GLN:HG3	1:B:112:LEU:N	2.22	0.53
1:A:225:ILE:HG12	1:A:226:ASP:N	2.24	0.53
1:B:101:TYR:HB3	1:B:109:SER:HB2	1.91	0.52
1:B:225:ILE:HG12	1:B:226:ASP:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:SER:O	1:B:101:TYR:HE1	1.93	0.52
1:B:104:GLY:O	1:B:105:ASP:HB2	2.08	0.52
1:B:344:VAL:HG11	1:B:367:TYR:CD2	2.44	0.52
1:A:62:MSE:O	1:A:65:PHE:HB2	2.10	0.52
1:A:168:ASN:HD21	1:A:289:VAL:HG23	1.75	0.52
1:A:186:ILE:HG23	1:A:278:PHE:CD2	2.44	0.52
1:A:306:ASN:ND2	1:B:188:ARG:NE	2.57	0.52
1:B:249:GLN:H	1:B:249:GLN:CD	2.17	0.52
1:A:158:ALA:HA	1:A:396:ILE:HG13	1.92	0.52
1:B:102:LEU:HD22	1:B:103:ASP:CG	2.35	0.51
1:B:5:TYR:O	1:B:8:ARG:N	2.44	0.51
1:A:249:GLN:CD	1:A:249:GLN:H	2.18	0.51
1:B:171:TYR:CD1	1:B:387:GLU:HA	2.45	0.51
1:B:304:ARG:HE	1:B:353:ILE:CD1	2.24	0.51
1:B:354:THR:HG22	1:B:357:GLY:O	2.10	0.51
1:B:4:SER:HA	1:B:101:TYR:OH	2.10	0.51
1:B:153:GLU:N	1:B:153:GLU:OE2	2.43	0.51
1:B:349:LEU:CB	1:B:360:ILE:HD11	2.40	0.51
1:A:304:ARG:CA	1:A:353:ILE:HD12	2.40	0.51
1:B:304:ARG:HE	1:B:353:ILE:HD11	1.75	0.51
1:B:4:SER:HA	1:B:101:TYR:CE1	2.45	0.51
1:B:209:LEU:O	1:B:212:ILE:HG12	2.11	0.51
1:A:103:ASP:OD1	1:A:103:ASP:N	2.44	0.50
1:B:102:LEU:O	1:B:103:ASP:CG	2.54	0.50
1:B:142:SER:HA	1:B:399:ASP:C	2.36	0.50
1:A:297:MSE:O	1:A:301:ILE:CD1	2.57	0.50
1:B:186:ILE:HG23	1:B:278:PHE:CD2	2.46	0.50
1:A:168:ASN:HB2	1:A:171:TYR:CZ	2.47	0.50
1:A:4:SER:HA	1:A:101:TYR:CE1	2.46	0.50
1:B:158:ALA:HA	1:B:396:ILE:HG13	1.94	0.50
1:A:161:CYS:SG	1:A:396:ILE:HD11	2.52	0.50
1:B:373:THR:C	1:B:374:LEU:HD23	2.36	0.50
1:A:111:GLN:HG3	1:A:112:LEU:H	1.77	0.50
1:B:145:PHE:HZ	1:B:355:CYS:O	1.95	0.50
1:A:246:ASN:C	1:A:248:PRO:HD3	2.37	0.49
1:A:300:ASN:HB2	1:A:352:HIS:HD2	1.74	0.49
1:A:178:ASP:O	1:A:179:PHE:HB2	2.13	0.49
1:A:202:PHE:CE2	1:A:264:LEU:HD11	2.48	0.49
1:A:4:SER:HA	1:A:101:TYR:OH	2.13	0.49
1:B:161:CYS:SG	1:B:396:ILE:HD11	2.52	0.49
1:B:168:ASN:HB2	1:B:171:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:HG	1:A:279:TRP:CD1	2.31	0.48
1:B:138:THR:HA	1:B:397:SER:O	2.13	0.48
1:B:178:ASP:O	1:B:179:PHE:HB2	2.12	0.48
1:A:153:GLU:CD	1:A:153:GLU:N	2.71	0.48
1:B:354:THR:HG23	1:B:355:CYS:N	2.28	0.48
1:A:306:ASN:ND2	1:B:188:ARG:HE	2.10	0.48
1:B:246:ASN:C	1:B:248:PRO:HD3	2.39	0.48
1:A:202:PHE:O	1:A:203:ASN:C	2.57	0.48
1:B:202:PHE:O	1:B:203:ASN:C	2.56	0.48
1:B:113:SER:CB	1:B:116:GLU:HG3	2.44	0.48
1:A:142:SER:HA	1:A:399:ASP:C	2.39	0.48
1:A:166:ILE:HD12	1:A:292:ILE:HG13	1.96	0.48
1:A:354:THR:HG23	1:A:356:ASN:H	1.79	0.47
1:A:4:SER:O	1:A:101:TYR:HE1	1.97	0.47
1:A:226:ASP:CB	1:A:229:LYS:HE2	2.45	0.47
1:B:316:ASN:O	1:B:317:CYS:C	2.58	0.47
1:A:13:VAL:N	1:A:119:ASN:HD22	2.11	0.47
1:B:102:LEU:CD1	1:B:103:ASP:OD1	2.49	0.47
1:A:5:TYR:O	1:A:8:ARG:N	2.47	0.47
1:A:111:GLN:HG3	1:A:112:LEU:N	2.29	0.47
1:A:153:GLU:N	1:A:153:GLU:OE2	2.46	0.47
1:B:70:SER:O	1:B:73:LYS:HD3	2.15	0.47
1:A:100:PHE:HB3	1:A:102:LEU:CD1	2.45	0.47
1:A:252:LEU:O	1:A:252:LEU:HD12	2.14	0.47
1:B:354:THR:HG23	1:B:356:ASN:H	1.79	0.47
1:A:90:LEU:HD13	1:A:120:LEU:HD21	1.97	0.47
1:B:145:PHE:HD2	1:B:308:MSE:CG	2.28	0.47
1:B:186:ILE:HD13	1:B:275:THR:HG22	1.96	0.47
1:B:209:LEU:HA	1:B:212:ILE:CD1	2.35	0.47
1:A:316:ASN:O	1:A:317:CYS:C	2.58	0.46
1:B:202:PHE:HA	1:B:323:ILE:O	2.15	0.46
1:A:100:PHE:CB	1:A:102:LEU:HD12	2.45	0.46
1:A:226:ASP:HB3	1:A:229:LYS:CE	2.44	0.46
1:A:187:TYR:CE1	1:A:222:ASN:HA	2.50	0.46
1:A:188:ARG:HE	1:B:306:ASN:HD21	1.63	0.46
1:B:187:TYR:CE1	1:B:222:ASN:HA	2.51	0.46
1:A:84:ASP:C	1:A:86:ILE:N	2.72	0.46
1:A:202:PHE:HA	1:A:323:ILE:O	2.15	0.46
1:A:304:ARG:HE	1:A:353:ILE:HD11	1.81	0.46
1:A:70:SER:O	1:A:73:LYS:HD3	2.15	0.46
1:B:268:PRO:O	1:B:269:ALA:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:CD2	1:B:360:ILE:HD11	2.45	0.46
1:A:358:VAL:O	1:A:358:VAL:HG22	2.15	0.46
1:B:78:PHE:CD2	1:B:92:LEU:HD12	2.51	0.46
1:A:182:VAL:O	1:A:186:ILE:HG13	2.16	0.46
1:A:354:THR:HG22	1:A:357:GLY:O	2.15	0.46
1:B:226:ASP:HB3	1:B:229:LYS:HE2	1.97	0.46
1:B:259:LEU:HD13	1:B:259:LEU:HA	1.87	0.46
1:A:100:PHE:O	1:A:102:LEU:CD1	2.61	0.46
1:A:349:LEU:CD2	1:A:360:ILE:HD11	2.42	0.46
1:B:62:MSE:O	1:B:65:PHE:HB2	2.15	0.46
1:B:315:ASN:N	1:B:315:ASN:HD22	2.13	0.46
1:B:13:VAL:N	1:B:119:ASN:HD22	2.12	0.46
1:B:84:ASP:C	1:B:86:ILE:N	2.74	0.46
1:B:104:GLY:H	1:B:107:ILE:HB	1.79	0.45
1:B:106:LYS:HB2	1:B:106:LYS:HE3	1.71	0.45
1:B:354:THR:HG23	1:B:356:ASN:N	2.31	0.45
1:A:372:GLY:O	1:A:373:THR:O	2.35	0.45
1:B:226:ASP:HB3	1:B:229:LYS:CE	2.46	0.45
1:A:138:THR:HA	1:A:397:SER:O	2.16	0.45
1:A:354:THR:HG23	1:A:355:CYS:N	2.32	0.45
1:A:124:LEU:HD12	1:A:125:PRO:CD	2.47	0.45
1:B:226:ASP:CB	1:B:229:LYS:HE2	2.46	0.45
1:B:297:MSE:O	1:B:300:ASN:HB3	2.17	0.45
1:A:239:LEU:C	1:A:239:LEU:HD12	2.41	0.45
1:A:145:PHE:HD2	1:A:308:MSE:CG	2.29	0.45
1:A:304:ARG:HE	1:A:353:ILE:CD1	2.29	0.45
1:B:145:PHE:CE2	1:B:307:PHE:HB3	2.51	0.45
1:B:157:THR:O	1:B:161:CYS:HB3	2.16	0.45
1:A:248:PRO:HD2	1:A:249:GLN:OE1	2.16	0.45
1:B:248:PRO:HD2	1:B:249:GLN:OE1	2.17	0.45
1:A:226:ASP:HB3	1:A:229:LYS:HE2	1.97	0.45
1:A:367:TYR:CE2	1:A:384:ILE:HD13	2.52	0.45
1:A:209:LEU:HA	1:A:209:LEU:HD23	1.61	0.45
1:A:82:ASN:C	1:A:83:ILE:HG13	2.42	0.44
1:A:293:TYR:CZ	1:A:297:MSE:HE3	2.52	0.44
1:A:349:LEU:CB	1:A:360:ILE:HD11	2.46	0.44
1:A:104:GLY:H	1:A:107:ILE:HB	1.81	0.44
1:A:347:SER:HA	1:A:364:GLU:HA	1.98	0.44
1:A:133:LYS:HE3	1:A:135:HIS:CE1	2.52	0.44
1:A:145:PHE:HZ	1:A:355:CYS:O	1.99	0.44
1:A:264:LEU:HD22	1:A:270:PHE:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LEU:HA	1:B:375:PRO:HD3	1.74	0.44
1:B:186:ILE:O	1:B:187:TYR:C	2.59	0.44
1:B:297:MSE:O	1:B:301:ILE:CD1	2.63	0.44
1:A:290:GLU:OE1	1:B:291:HIS:CD2	2.71	0.44
1:A:100:PHE:HB3	1:A:102:LEU:HG	1.98	0.44
1:A:291:HIS:HE1	1:A:295:GLN:OE1	2.00	0.44
1:A:354:THR:HG23	1:A:356:ASN:N	2.32	0.44
1:B:202:PHE:CE2	1:B:264:LEU:HD11	2.53	0.44
1:B:252:LEU:HD12	1:B:252:LEU:O	2.17	0.44
1:A:344:VAL:CG1	1:A:367:TYR:CD2	3.01	0.44
1:B:293:TYR:CZ	1:B:297:MSE:HE3	2.52	0.44
1:A:113:SER:CB	1:A:116:GLU:HG3	2.48	0.44
1:B:326:VAL:CG2	1:B:327:VAL:N	2.73	0.44
1:A:88:ILE:HD12	1:A:88:ILE:N	2.33	0.44
1:A:4:SER:HA	1:A:101:TYR:HE1	1.83	0.43
1:A:102:LEU:CD1	1:A:103:ASP:OD1	2.48	0.43
1:A:62:MSE:HE2	1:A:123:SER:C	2.43	0.43
1:A:384:ILE:O	1:A:389:ARG:NH1	2.51	0.43
1:B:294:ALA:O	1:B:295:GLN:C	2.59	0.43
1:A:100:PHE:HB3	1:A:102:LEU:CG	2.48	0.43
1:A:264:LEU:HA	1:A:264:LEU:HD23	1.80	0.43
1:A:297:MSE:O	1:A:300:ASN:HB3	2.18	0.43
1:B:315:ASN:CG	1:B:316:ASN:N	2.76	0.43
1:A:308:MSE:N	1:A:309:PRO:HD3	2.33	0.43
1:B:182:VAL:O	1:B:186:ILE:HG13	2.19	0.43
1:B:264:LEU:HD22	1:B:270:PHE:CD1	2.54	0.43
1:B:276:SER:C	1:B:278:PHE:N	2.76	0.43
1:A:186:ILE:O	1:A:187:TYR:C	2.61	0.43
1:A:236:TYR:O	1:A:240:ASN:HB2	2.19	0.43
1:B:102:LEU:HD22	1:B:102:LEU:O	2.18	0.43
1:B:283:HIS:CD2	1:B:283:HIS:H	2.36	0.43
1:B:178:ASP:HB2	1:B:381:ARG:HB2	2.00	0.43
1:B:182:VAL:HG13	1:B:183:TRP:N	2.33	0.43
1:B:347:SER:HA	1:B:364:GLU:HA	1.99	0.43
1:A:78:PHE:CD2	1:A:92:LEU:HD12	2.54	0.43
1:A:239:LEU:CD2	1:A:266:GLN:HG3	2.49	0.43
1:B:308:MSE:N	1:B:309:PRO:HD3	2.34	0.43
1:B:367:TYR:CE2	1:B:384:ILE:HD13	2.54	0.42
1:A:210:LYS:HD3	1:A:210:LYS:HA	1.65	0.42
1:B:358:VAL:O	1:B:358:VAL:HG22	2.18	0.42
1:A:174:VAL:HG22	1:A:386:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:O	1:A:284:ILE:HG22	2.20	0.42
1:B:133:LYS:HE3	1:B:135:HIS:CE1	2.54	0.42
1:A:217:ASN:HD22	1:A:217:ASN:HA	1.70	0.42
1:A:276:SER:C	1:A:278:PHE:N	2.78	0.42
1:B:82:ASN:C	1:B:83:ILE:HG13	2.43	0.42
1:B:344:VAL:HG11	1:B:367:TYR:CZ	2.54	0.42
1:A:116:GLU:H	1:A:116:GLU:HG2	1.53	0.42
1:B:100:PHE:CB	1:B:102:LEU:HD12	2.50	0.42
1:B:276:SER:C	1:B:278:PHE:H	2.27	0.42
1:B:116:GLU:H	1:B:116:GLU:HG2	1.52	0.42
1:A:374:LEU:HD23	1:A:374:LEU:N	2.35	0.42
1:B:236:TYR:O	1:B:240:ASN:HB2	2.19	0.42
1:A:65:PHE:CE2	1:A:81:ALA:CB	3.02	0.42
1:A:145:PHE:CE2	1:A:307:PHE:HB3	2.55	0.42
1:B:209:LEU:HA	1:B:209:LEU:HD23	1.63	0.42
1:B:384:ILE:O	1:B:389:ARG:NH1	2.53	0.42
1:A:84:ASP:O	1:A:86:ILE:N	2.44	0.41
1:A:96:ILE:H	1:A:96:ILE:HG13	1.73	0.41
1:A:301:ILE:HD12	1:A:301:ILE:N	2.35	0.41
1:B:254:PHE:H	1:B:254:PHE:HD1	1.66	0.41
1:A:102:LEU:HD22	1:A:102:LEU:O	2.20	0.41
1:A:102:LEU:CB	1:A:108:GLN:HG3	2.37	0.41
1:A:124:LEU:HD12	1:A:125:PRO:HD3	2.01	0.41
1:A:168:ASN:CB	1:A:171:TYR:CZ	3.03	0.41
1:B:124:LEU:HD12	1:B:125:PRO:CD	2.50	0.41
1:B:209:LEU:CD2	1:B:212:ILE:HD11	2.50	0.41
1:B:241:LYS:N	1:B:241:LYS:HD3	2.35	0.41
1:B:291:HIS:HE1	1:B:295:GLN:OE1	2.02	0.41
1:A:131:LEU:HD13	1:A:131:LEU:N	2.35	0.41
1:A:315:ASN:CG	1:A:316:ASN:N	2.77	0.41
1:A:326:VAL:O	1:A:328:PRO:HD3	2.20	0.41
1:B:4:SER:HA	1:B:101:TYR:HE1	1.84	0.41
1:B:213:ALA:O	1:B:216:ILE:HG12	2.20	0.41
1:B:304:ARG:CB	1:B:353:ILE:HD12	2.51	0.41
1:A:268:PRO:O	1:A:269:ALA:C	2.62	0.41
1:B:141:VAL:HG22	1:B:142:SER:O	2.21	0.41
1:B:168:ASN:CB	1:B:171:TYR:CZ	3.04	0.41
1:B:374:LEU:HD23	1:B:374:LEU:N	2.35	0.41
1:A:251:ASP:HB2	1:A:254:PHE:CD1	2.56	0.41
1:B:124:LEU:HA	1:B:125:PRO:HD3	1.85	0.41
1:B:134:VAL:CG2	1:B:393:PHE:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:SER:C	1:A:278:PHE:H	2.28	0.41
1:B:372:GLY:O	1:B:373:THR:O	2.38	0.41
1:A:131:LEU:HB2	1:A:164:SER:HB2	2.01	0.41
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.69	0.41
1:B:251:ASP:HB2	1:B:254:PHE:CD1	2.55	0.41
1:A:164:SER:C	1:A:392:SER:HB2	2.46	0.41
1:A:178:ASP:HB2	1:A:381:ARG:HB2	2.02	0.41
1:A:216:ILE:HB	1:A:221:ILE:CG1	2.44	0.41
1:A:254:PHE:H	1:A:254:PHE:HD1	1.68	0.41
1:A:295:GLN:HE21	1:A:295:GLN:HB3	1.70	0.41
1:A:384:ILE:HG22	1:A:389:ARG:HD3	2.03	0.41
1:B:68:SER:HB2	1:B:73:LYS:CG	2.48	0.41
1:B:100:PHE:HB3	1:B:102:LEU:CD1	2.51	0.41
1:B:114:SER:H	1:B:116:GLU:CG	2.34	0.41
1:B:188:ARG:NH1	1:B:189:ASP:OD1	2.53	0.41
1:B:166:ILE:HD12	1:B:292:ILE:HG13	2.01	0.41
1:B:239:LEU:HD12	1:B:239:LEU:C	2.47	0.40
1:B:114:SER:H	1:B:116:GLU:HG3	1.86	0.40
1:B:326:VAL:O	1:B:328:PRO:HD3	2.21	0.40
1:A:188:ARG:NE	1:B:306:ASN:HD21	2.19	0.40
1:B:69:LEU:H	1:B:73:LYS:HZ3	1.68	0.40
1:B:307:PHE:C	1:B:308:MSE:HG3	2.47	0.40
1:A:68:SER:HA	1:A:73:LYS:HE2	2.04	0.40
1:B:68:SER:OG	1:B:78:PHE:C	2.65	0.40
1:B:111:GLN:CG	1:B:112:LEU:H	2.34	0.40
1:B:239:LEU:CD2	1:B:266:GLN:HG3	2.51	0.40
1:B:295:GLN:HE21	1:B:295:GLN:HB3	1.71	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	333/400 (83%)	283 (85%)	41 (12%)	9 (3%)	4	20
1	B	333/400 (83%)	285 (86%)	39 (12%)	9 (3%)	4	20
All	All	666/800 (83%)	568 (85%)	80 (12%)	18 (3%)	4	20

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LEU
1	A	316	ASN
1	A	317	CYS
1	A	373	THR
1	B	4	SER
1	B	102	LEU
1	B	316	ASN
1	B	317	CYS
1	B	373	THR
1	A	4	SER
1	A	70	SER
1	A	105	ASP
1	A	141	VAL
1	B	70	SER
1	B	105	ASP
1	B	141	VAL
1	A	398	PRO
1	B	398	PRO

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	294/357 (82%)	239 (81%)	55 (19%)	1	8
1	B	294/357 (82%)	240 (82%)	54 (18%)	1	8
All	All	588/714 (82%)	479 (82%)	109 (18%)	1	8

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	75	ASP
1	A	92	LEU
1	A	96	ILE
1	A	98	SER
1	A	102	LEU
1	A	103	ASP
1	A	106	LYS
1	A	110	THR
1	A	112	LEU
1	A	113	SER
1	A	116	GLU
1	A	118	ASN
1	A	122	SER
1	A	124	LEU
1	A	130	ASN
1	A	131	LEU
1	A	138	THR
1	A	153	GLU
1	A	155	ILE
1	A	159	ILE
1	A	169	ASP
1	A	170	ASP
1	A	176	ASP
1	A	177	THR
1	A	181	SER
1	A	186	ILE
1	A	191	ARG
1	A	198	THR
1	A	209	LEU
1	A	212	ILE
1	A	215	LEU
1	A	221	ILE
1	A	222	ASN
1	A	224	PHE
1	A	225	ILE
1	A	231	LEU
1	A	253	CYS
1	A	259	LEU
1	A	262	THR
1	A	281	SER
1	A	282	LEU
1	A	305	LEU

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Mol	Chain	Res	Type
1	A	315	ASN
1	A	317	CYS
1	A	327	VAL
1	A	340	ARG
1	A	345	SER
1	A	347	SER
1	A	358	VAL
1	A	360	ILE
1	A	365	THR
1	A	374	LEU
1	A	380	LEU
1	A	390	GLN
1	B	64	SER
1	B	75	ASP
1	B	92	LEU
1	B	96	ILE
1	B	98	SER
1	B	102	LEU
1	B	103	ASP
1	B	106	LYS
1	B	110	THR
1	B	112	LEU
1	B	113	SER
1	B	116	GLU
1	B	118	ASN
1	B	122	SER
1	B	124	LEU
1	B	130	ASN
1	B	131	LEU
1	B	138	THR
1	B	153	GLU
1	B	155	ILE
1	B	169	ASP
1	B	170	ASP
1	B	176	ASP
1	B	177	THR
1	B	181	SER
1	B	186	ILE
1	B	191	ARG
1	B	198	THR
1	B	209	LEU
1	B	212	ILE

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Mol	Chain	Res	Type
1	B	215	LEU
1	B	221	ILE
1	B	222	ASN
1	B	224	PHE
1	B	225	ILE
1	B	231	LEU
1	B	259	LEU
1	B	262	THR
1	B	281	SER
1	B	282	LEU
1	B	305	LEU
1	B	315	ASN
1	B	317	CYS
1	B	327	VAL
1	B	340	ARG
1	B	345	SER
1	B	347	SER
1	B	351	SER
1	B	358	VAL
1	B	360	ILE
1	B	365	THR
1	B	374	LEU
1	B	380	LEU
1	B	390	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	119	ASN
1	A	135	HIS
1	A	168	ASN
1	A	217	ASN
1	A	240	ASN
1	A	283	HIS
1	A	291	HIS
1	A	295	GLN
1	A	300	ASN
1	A	352	HIS
1	A	361	ASN
1	B	80	HIS
1	B	111	GLN

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Mol	Chain	Res	Type
1	B	119	ASN
1	B	135	HIS
1	B	168	ASN
1	B	217	ASN
1	B	283	HIS
1	B	291	HIS
1	B	295	GLN
1	B	300	ASN
1	B	306	ASN
1	B	352	HIS
1	B	361	ASN

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](#)

There are no ligands in this entry.

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	336/400 (84%)	-0.30	2 (0%) 85 69	68, 103, 171, 489	0
1	B	336/400 (84%)	-0.23	3 (0%) 81 61	71, 115, 212, 465	0
All	All	672/800 (84%)	-0.26	5 (0%) 84 66	68, 110, 192, 489	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	LEU	5.3
1	A	304	ARG	3.4
1	B	304	ARG	3.1
1	B	148	HIS	2.8
1	B	224	PHE	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.