



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:13 PM UTC

PDB ID : 1VDE / pdb_00001vde
Title : PI-SCEI, A HOMING ENDONUCLEASE WITH PROTEIN SPLICING ACTIVITY
Authors : Duan, X.; Quiococho, F.A.
Deposited on : 1997-04-01
Resolution : 2.40 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

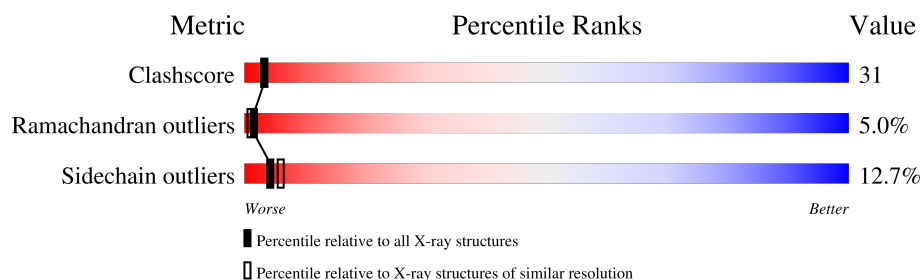
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	454	 51% 33% 8% • 6%
1	B	454	 41% 41% 11% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7116 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 PI-SCEI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3388	2141	587	647	13			
1	B	428	Total	C	N	O	S	0	0	0
			3381	2136	586	646	13			

- Molecule 2 is water.

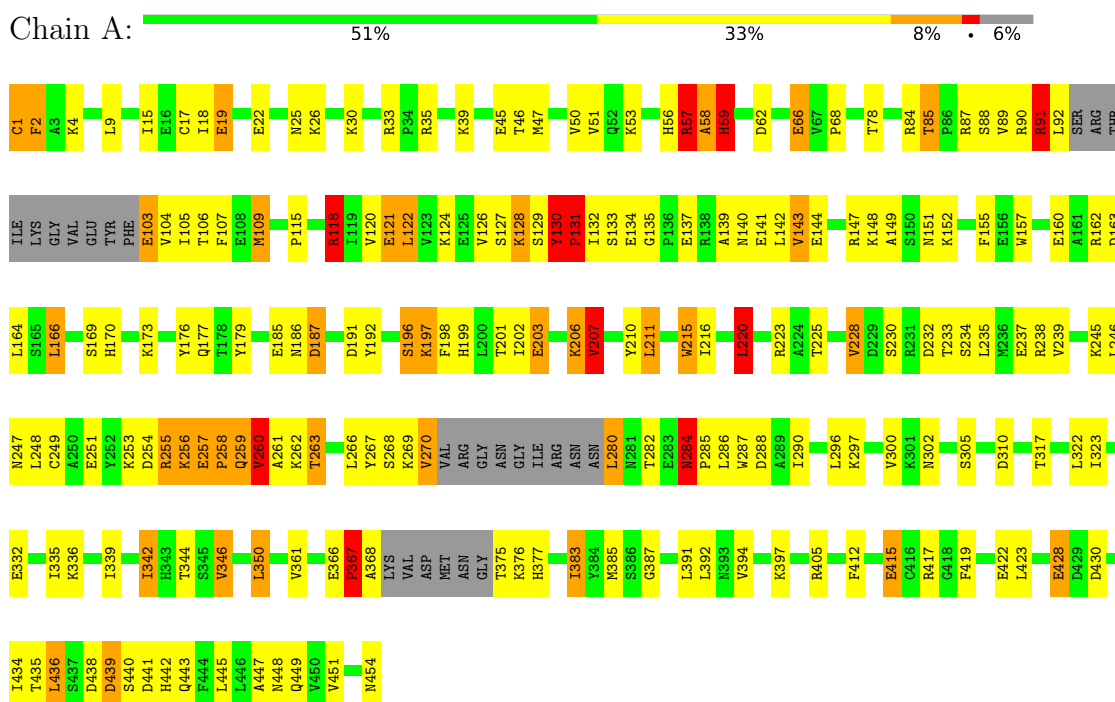
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	187	Total	O	0	0
			187	187		
2	B	160	Total	O	0	0
			160	160		

3 Residue-property plots

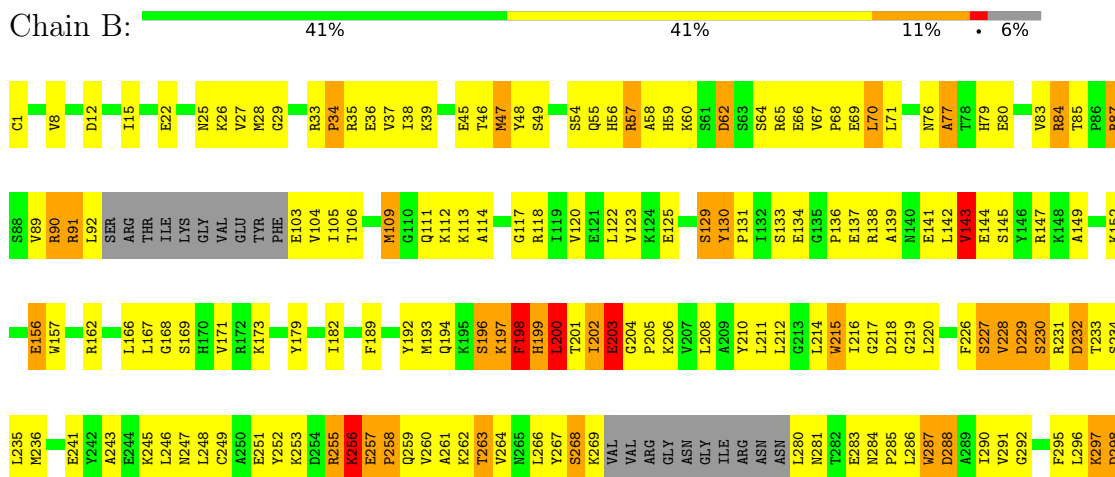
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

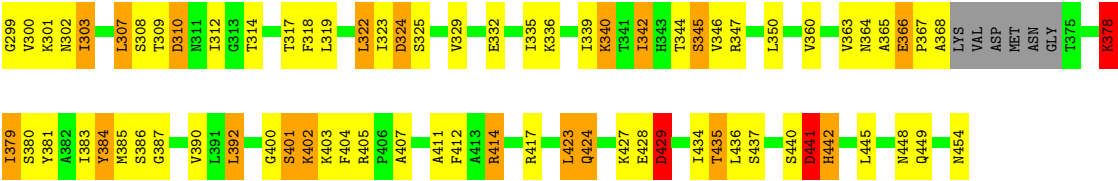
Note EDS was not executed.

• Molecule 1: PI-SCEI



• Molecule 1: PI-SCEI





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.75 Å 102.40 Å 87.10 Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.6 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7116	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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	0.89	5/3450 (0.1%)	1.28	38/4654 (0.8%)
1	B	0.85	4/3443 (0.1%)	1.22	33/4644 (0.7%)
All	All	0.87	9/6893 (0.1%)	1.25	71/9298 (0.8%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	MET	SD-CE	-15.14	1.41	1.79
1	A	47	MET	SD-CE	-10.94	1.52	1.79
1	B	28	MET	SD-CE	-9.03	1.56	1.79
1	B	109	MET	SD-CE	-8.54	1.58	1.79
1	A	109	MET	SD-CE	-6.15	1.64	1.79
1	B	314	THR	CA-CB	6.15	1.63	1.53
1	A	207	VAL	CA-CB	5.73	1.61	1.54
1	A	290	ILE	CA-CB	5.59	1.60	1.54
1	A	451	VAL	CA-CB	5.10	1.60	1.54

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	HIS	N-CA-C	11.71	127.52	109.96
1	B	288	ASP	N-CA-C	-9.29	101.10	111.14
1	B	204	GLY	CA-C-N	9.21	129.41	119.28
1	B	204	GLY	C-N-CA	9.21	129.41	119.28
1	B	429	ASP	N-CA-C	8.87	129.70	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	SER	N-CA-C	8.71	123.24	109.65
1	A	151	ASN	N-CA-C	-8.66	101.56	112.90
1	A	440	SER	N-CA-C	-8.53	95.85	107.88
1	A	256	LYS	N-CA-C	-8.37	100.15	110.61
1	A	284	ASN	CA-C-N	8.26	128.74	119.32
1	A	284	ASN	C-N-CA	8.26	128.74	119.32
1	B	379	ILE	N-CA-C	8.01	121.04	108.87
1	B	303	ILE	CA-C-N	7.90	128.37	119.92
1	B	303	ILE	C-N-CA	7.90	128.37	119.92
1	B	199	HIS	N-CA-C	7.31	126.38	110.80
1	A	2	PHE	N-CA-C	7.17	120.27	109.95
1	B	324	ASP	N-CA-C	7.08	119.85	111.71
1	B	368	ALA	N-CA-C	-7.07	91.19	111.00
1	A	438	ASP	N-CA-C	-6.84	99.91	110.10
1	A	58	ALA	N-CA-C	6.81	125.31	110.80
1	A	203	GLU	N-CA-C	-6.71	104.66	114.39
1	A	186	ASN	N-CA-C	-6.63	99.58	109.86
1	A	305	SER	N-CA-C	6.62	118.50	111.28
1	A	131	PRO	N-CA-C	6.58	126.03	112.47
1	A	1	CYS	CB-CA-C	6.38	122.22	110.10
1	A	428	GLU	N-CA-C	-6.37	99.25	109.96
1	B	243	ALA	N-CA-C	-6.32	104.31	111.07
1	A	346	VAL	N-CA-C	-6.12	104.38	110.62
1	A	62	ASP	N-CA-C	6.07	115.47	108.49
1	A	394	VAL	N-CA-C	-5.99	105.01	110.82
1	B	77	ALA	N-CA-C	5.93	118.53	111.71
1	A	232	ASP	N-CA-C	5.92	118.42	107.99
1	B	200	LEU	N-CA-C	-5.90	98.24	110.80
1	A	342	ILE	N-CA-C	-5.88	105.98	113.22
1	B	414	ARG	N-CA-C	-5.87	99.57	108.67
1	B	401	SER	N-CA-C	5.86	118.14	111.11
1	B	71	LEU	N-CA-C	5.83	118.95	108.17
1	A	130	TYR	CA-C-N	5.78	127.07	119.84
1	A	130	TYR	C-N-CA	5.78	127.07	119.84
1	B	87	ARG	N-CA-C	-5.69	102.06	110.48
1	A	367	PRO	N-CA-C	5.68	124.16	112.47
1	B	283	GLU	N-CA-C	-5.66	101.92	110.70
1	A	284	ASN	CB-CA-C	5.65	117.05	109.42
1	B	312	ILE	N-CA-C	5.64	116.38	110.62
1	B	57	ARG	N-CA-C	5.59	118.19	109.52
1	B	441	ASP	N-CA-C	-5.56	98.21	107.99
1	A	201	THR	N-CA-C	5.53	122.58	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	TYR	CA-C-N	5.51	125.83	119.93
1	B	130	TYR	C-N-CA	5.51	125.83	119.93
1	A	85	THR	CA-C-N	-5.50	114.58	120.03
1	A	85	THR	C-N-CA	-5.50	114.58	120.03
1	A	135	GLY	CA-C-N	5.48	126.69	119.84
1	A	135	GLY	C-N-CA	5.48	126.69	119.84
1	B	143	VAL	N-CA-C	5.43	116.16	110.62
1	B	440	SER	N-CA-C	5.38	118.40	110.59
1	A	143	VAL	N-CA-C	5.38	115.48	110.42
1	A	118	ARG	N-CA-C	5.35	122.19	110.80
1	A	91	ARG	N-CA-C	5.28	122.05	110.80
1	B	308	SER	N-CA-C	5.25	118.78	112.38
1	B	445	LEU	N-CA-C	5.24	117.79	109.24
1	B	346	VAL	N-CA-C	-5.20	105.64	110.53
1	A	107	PHE	N-CA-C	-5.14	100.86	109.24
1	B	117	GLY	N-CA-C	5.14	120.93	114.25
1	B	34	PRO	N-CA-C	5.13	119.10	111.41
1	B	169	SER	N-CA-C	5.11	117.24	111.11
1	A	220	LEU	CB-CG-CD1	-5.06	95.51	110.70
1	A	155	PHE	N-CA-C	-5.06	102.58	110.42
1	B	168	GLY	N-CA-C	-5.04	106.08	112.54
1	A	263	THR	N-CA-C	-5.03	102.26	110.20
1	B	83	VAL	N-CA-C	5.02	116.82	108.99
1	A	185	GLU	N-CA-C	5.00	116.54	108.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	LEU	Mainchain

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	3388	0	3387	165	0
1	B	3381	0	3378	254	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	187	0	0	23	0
2	B	160	0	0	26	0
All	All	7116	0	6765	415	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 31.

All (415) 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:339:ILE:HD12	1:B:385:MET:HE1	1.35	1.07
1:B:257:GLU:HB2	1:B:261:ALA:HB3	1.41	1.03
1:A:130:TYR:HB3	1:A:131:PRO:CD	1.91	0.99
1:B:125:GLU:HB3	2:B:576:HOH:O	1.66	0.95
1:B:26:LYS:HD2	1:B:34:PRO:HB2	1.50	0.93
1:A:297:LYS:HG2	1:A:302:ASN:HB2	1.48	0.93
1:B:256:LYS:HD3	1:B:263:THR:HG23	1.49	0.93
2:A:525:HOH:O	1:B:386:SER:HB2	1.69	0.92
1:A:350:LEU:HD13	1:A:383:ILE:HG12	1.50	0.92
1:A:130:TYR:HB3	1:A:131:PRO:HD2	1.52	0.90
1:B:366:GLU:HB2	1:B:367:PRO:HD2	1.53	0.90
1:B:268:SER:H	1:B:280:LEU:HD13	1.37	0.89
1:B:92:LEU:HG	1:B:139:ALA:HB1	1.56	0.88
1:B:194:GLN:HA	1:B:198:PHE:HB2	1.58	0.86
1:B:46:THR:OG1	1:B:427:LYS:HG3	1.76	0.86
1:B:297:LYS:HE3	1:B:345:SER:HB3	1.57	0.85
1:A:442:HIS:HD2	1:A:454:ASN:HD21	1.24	0.85
1:B:114:ALA:HB3	2:B:541:HOH:O	1.76	0.85
1:A:187:ASP:HB2	2:A:551:HOH:O	1.75	0.85
1:B:46:THR:HG23	1:B:427:LYS:HA	1.59	0.85
1:B:91:ARG:HD3	2:B:494:HOH:O	1.76	0.84
1:A:233:THR:O	1:A:237:GLU:HG3	1.77	0.83
1:B:90:ARG:HH11	1:B:90:ARG:HG2	1.43	0.83
1:A:248:LEU:HD21	1:A:285:PRO:HD2	1.61	0.82
1:A:103:GLU:HA	1:A:129:SER:HB3	1.59	0.82
1:B:220:LEU:HD21	1:B:256:LYS:HE3	1.61	0.82
1:B:46:THR:HG23	1:B:427:LYS:CA	2.10	0.82
1:B:125:GLU:HG3	1:B:171:VAL:HG23	1.62	0.81
1:B:255:ARG:HD2	1:B:259:GLN:HA	1.61	0.81
1:B:217:GLY:HA3	1:B:325:SER:OG	1.81	0.80
1:B:247:ASN:ND2	1:B:269:LYS:HD3	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:O	1:B:323:ILE:HG12	1.81	0.80
1:B:229:ASP:HB2	1:B:261:ALA:C	2.06	0.80
1:B:428:GLU:HG3	1:B:429:ASP:N	1.99	0.78
1:A:269:LYS:HG2	1:A:270:VAL:N	1.99	0.77
1:B:227:SER:HA	1:B:262:LYS:O	1.84	0.77
1:B:227:SER:OG	1:B:261:ALA:HB1	1.84	0.76
1:B:232:ASP:HB3	1:B:402:LYS:NZ	2.00	0.76
1:B:85:THR:HG1	1:B:157:TRP:HH2	1.33	0.76
1:B:46:THR:HA	1:B:427:LYS:HA	1.67	0.76
1:A:199:HIS:NE2	1:A:246:LEU:HA	2.00	0.76
1:B:323:ILE:HD13	1:B:339:ILE:HD11	1.66	0.76
1:A:257:GLU:HB3	1:A:260:VAL:HG23	1.67	0.75
1:B:157:TRP:HZ2	2:B:588:HOH:O	1.68	0.75
1:A:297:LYS:HZ2	1:A:300:VAL:HB	1.52	0.75
1:A:197:LYS:HD3	1:A:288:ASP:HB2	1.68	0.74
1:B:45:GLU:O	1:B:47:MET:HE3	1.89	0.73
1:B:65:ARG:HG2	1:B:379:ILE:HG21	1.69	0.73
1:A:199:HIS:HE2	1:A:246:LEU:HA	1.53	0.73
1:B:268:SER:N	1:B:280:LEU:HD13	2.04	0.73
1:B:229:ASP:H	1:B:262:LYS:HB2	1.54	0.73
1:A:58:ALA:HB1	2:A:578:HOH:O	1.87	0.72
1:A:53:LYS:HG2	1:A:422:GLU:HG3	1.71	0.72
1:B:291:VAL:HG12	1:B:296:LEU:HB3	1.71	0.72
1:B:215:TRP:HE1	1:B:295:PHE:HB3	1.55	0.71
1:B:193:MET:HE3	1:B:208:LEU:HD22	1.70	0.71
1:B:194:GLN:HA	1:B:198:PHE:CB	2.21	0.71
1:B:194:GLN:NE2	1:B:198:PHE:HB3	2.06	0.70
1:A:147:ARG:HD3	1:B:411:ALA:N	2.06	0.70
1:A:220:LEU:HG	1:A:225:THR:OG1	1.91	0.70
1:A:256:LYS:HE2	2:A:608:HOH:O	1.90	0.70
1:B:92:LEU:HG	1:B:139:ALA:CB	2.22	0.70
1:B:267:TYR:HB3	1:B:280:LEU:HD12	1.73	0.70
1:A:255:ARG:HH11	1:A:259:GLN:HG2	1.57	0.70
1:B:47:MET:SD	2:B:611:HOH:O	2.50	0.69
1:B:280:LEU:HB3	1:B:284:ASN:OD1	1.92	0.69
1:A:144:GLU:O	1:A:148:LYS:HD2	1.93	0.69
1:A:33:ARG:HB3	1:A:33:ARG:CZ	2.23	0.69
1:B:29:GLY:HA3	1:B:35:ARG:HH11	1.58	0.69
1:B:255:ARG:HD2	1:B:259:GLN:H	1.58	0.69
1:B:203:GLU:CD	1:B:246:LEU:HD23	2.19	0.68
1:A:442:HIS:CD2	1:A:454:ASN:HD21	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:HB3	1:A:131:PRO:HD3	1.76	0.68
1:B:255:ARG:HD2	1:B:259:GLN:CA	2.24	0.68
1:A:207:VAL:HG11	1:A:245:LYS:HD2	1.75	0.67
1:A:207:VAL:HG23	1:A:246:LEU:HG	1.77	0.67
1:B:350:LEU:HD23	1:B:383:ILE:HD12	1.76	0.67
1:A:45:GLU:HG3	1:A:46:THR:N	2.10	0.66
2:A:638:HOH:O	1:B:404:PHE:HE2	1.77	0.66
1:B:256:LYS:HD3	1:B:263:THR:CG2	2.25	0.66
1:B:231:ARG:HH21	1:B:235:LEU:HD23	1.61	0.65
1:A:17:CYS:HB3	1:A:19:GLU:OE2	1.97	0.65
1:B:442:HIS:N	2:B:493:HOH:O	2.29	0.65
1:B:367:PRO:HA	2:B:613:HOH:O	1.97	0.65
1:B:109:MET:HG2	2:B:575:HOH:O	1.96	0.64
1:A:104:VAL:CG1	1:A:128:LYS:HB2	2.27	0.64
1:B:247:ASN:HD21	1:B:269:LYS:HD3	1.62	0.64
1:B:255:ARG:HD2	1:B:259:GLN:N	2.12	0.64
1:B:427:LYS:O	1:B:428:GLU:HG2	1.98	0.64
1:B:210:TYR:OH	1:B:235:LEU:HD11	1.98	0.63
1:B:48:TYR:HB3	1:B:423:LEU:HD22	1.80	0.63
1:A:230:SER:HB3	1:A:262:LYS:HG3	1.80	0.63
1:A:297:LYS:HG2	1:A:302:ASN:CB	2.27	0.63
1:B:90:ARG:HG2	1:B:90:ARG:NH1	2.12	0.63
1:A:33:ARG:HB3	1:A:33:ARG:NH1	2.14	0.63
1:A:87:ARG:NH2	1:A:149:ALA:HB3	2.14	0.62
1:B:257:GLU:HB3	1:B:260:VAL:HG23	1.82	0.62
1:B:258:PRO:O	1:B:260:VAL:HG22	1.98	0.62
1:B:303:ILE:HG23	1:B:307:LEU:HD23	1.81	0.62
1:A:122:LEU:HD11	1:A:124:LYS:HE3	1.80	0.62
1:A:258:PRO:O	1:A:260:VAL:HG22	1.99	0.62
1:A:130:TYR:CB	1:A:131:PRO:CD	2.76	0.62
1:B:85:THR:OG1	1:B:157:TRP:HH2	1.82	0.62
1:B:130:TYR:OH	1:B:136:PRO:HA	1.99	0.62
1:A:284:ASN:C	1:A:284:ASN:HD22	2.07	0.62
1:B:266:LEU:HD12	1:B:286:LEU:HD22	1.82	0.61
1:A:430:ASP:HB3	2:A:574:HOH:O	2.00	0.61
1:B:287:TRP:CD1	1:B:290:ILE:HD12	2.35	0.61
1:B:38:ILE:HG13	1:B:39:LYS:HG3	1.81	0.61
1:A:109:MET:HG3	1:A:121:GLU:OE1	2.00	0.61
1:A:51:VAL:HG12	2:A:577:HOH:O	1.99	0.61
1:B:365:ALA:HB1	1:B:379:ILE:HD11	1.82	0.60
1:B:322:LEU:HD13	1:B:339:ILE:HD13	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:NH2	1:B:235:LEU:HD23	2.15	0.60
1:B:46:THR:CA	1:B:427:LYS:HA	2.31	0.60
1:B:57:ARG:NH2	1:B:67:VAL:O	2.34	0.60
1:A:215:TRP:CZ3	1:A:220:LEU:O	2.55	0.60
1:B:366:GLU:HB2	1:B:367:PRO:CD	2.30	0.60
1:B:193:MET:HE3	1:B:208:LEU:CD2	2.31	0.60
1:B:206:LYS:N	1:B:206:LYS:HD2	2.16	0.60
1:B:297:LYS:O	1:B:299:GLY:N	2.35	0.59
1:B:84:ARG:HD3	1:B:156:GLU:HG2	1.82	0.59
1:B:125:GLU:CG	1:B:171:VAL:HG23	2.30	0.59
1:A:22:GLU:H	1:A:25:ASN:ND2	1.99	0.59
1:B:35:ARG:HB3	1:B:436:LEU:HD13	1.84	0.59
1:B:46:THR:CG2	1:B:427:LYS:HA	2.29	0.59
1:B:92:LEU:HD22	1:B:92:LEU:N	2.17	0.59
1:A:144:GLU:HB3	1:A:148:LYS:NZ	2.17	0.59
1:B:342:ILE:HG22	1:B:379:ILE:O	2.03	0.59
1:A:4:LYS:HG3	1:A:19:GLU:HG2	1.85	0.59
1:A:197:LYS:HD3	1:A:288:ASP:CB	2.31	0.58
1:B:232:ASP:HB2	1:B:400:GLY:HA2	1.86	0.58
1:A:215:TRP:HZ3	1:A:220:LEU:O	1.87	0.58
1:B:103:GLU:HG2	1:B:129:SER:HB3	1.85	0.58
1:B:112:LYS:HD3	1:B:166:LEU:HD12	1.86	0.58
1:B:230:SER:O	1:B:231:ARG:HB3	2.04	0.58
1:B:118:ARG:N	2:B:541:HOH:O	2.34	0.58
1:B:144:GLU:HB2	2:B:564:HOH:O	2.04	0.57
1:A:50:VAL:HG22	1:A:423:LEU:HD12	1.87	0.57
1:B:339:ILE:HD12	1:B:385:MET:CE	2.21	0.57
1:A:58:ALA:HB3	1:A:68:PRO:HB3	1.86	0.57
1:B:29:GLY:HA3	1:B:35:ARG:NH1	2.20	0.57
1:A:30:LYS:HE3	1:A:443:GLN:OE1	2.04	0.57
1:A:104:VAL:HG11	1:A:142:LEU:HD13	1.85	0.57
1:B:442:HIS:HB3	1:B:454:ASN:ND2	2.19	0.57
1:B:131:PRO:HB2	1:B:134:GLU:HG3	1.87	0.57
1:B:249:CYS:O	1:B:266:LEU:HA	2.05	0.57
1:B:253:LYS:HB2	1:B:263:THR:OG1	2.04	0.57
1:B:267:TYR:HD1	1:B:280:LEU:HB2	1.69	0.57
1:B:113:LYS:HD2	1:B:113:LYS:N	2.19	0.56
1:A:58:ALA:HB3	1:A:68:PRO:CA	2.34	0.56
2:A:640:HOH:O	1:B:173:LYS:HD2	2.04	0.56
1:A:436:LEU:HD23	2:A:572:HOH:O	2.05	0.56
1:A:442:HIS:HD2	1:A:454:ASN:ND2	1.98	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:NH2	1:B:378:LYS:HE3	2.20	0.56
1:B:123:VAL:HG22	2:B:575:HOH:O	2.05	0.56
1:B:232:ASP:HB2	1:B:401:SER:H	1.69	0.56
1:B:92:LEU:CG	1:B:139:ALA:HB1	2.33	0.56
1:B:202:ILE:HD12	1:B:202:ILE:H	1.71	0.56
1:B:287:TRP:O	1:B:291:VAL:HG22	2.04	0.56
1:A:15:ILE:HD13	1:A:447:ALA:HB1	1.89	0.55
1:B:56:HIS:HB3	2:B:599:HOH:O	2.05	0.55
1:B:231:ARG:HH21	1:B:235:LEU:CD2	2.19	0.55
1:A:211:LEU:HD23	1:A:246:LEU:HD12	1.88	0.55
1:A:249:CYS:SG	1:A:269:LYS:HA	2.47	0.55
1:A:269:LYS:HG2	1:A:270:VAL:H	1.66	0.55
1:A:58:ALA:HB3	1:A:68:PRO:HA	1.88	0.55
1:A:170:HIS:HB3	2:A:638:HOH:O	2.05	0.55
1:B:196:SER:O	1:B:197:LYS:HB3	2.06	0.55
1:A:104:VAL:O	1:A:127:SER:HA	2.06	0.55
1:A:412:PHE:HD1	2:A:637:HOH:O	1.90	0.55
1:A:448:ASN:O	1:A:449:GLN:HB2	2.06	0.55
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.72	0.55
1:B:257:GLU:CB	1:B:261:ALA:HB3	2.26	0.55
1:A:361:VAL:HG13	1:A:383:ILE:CD1	2.37	0.55
1:A:104:VAL:HG13	1:A:128:LYS:HB2	1.89	0.54
1:A:441:ASP:O	1:A:443:GLN:HG3	2.07	0.54
1:B:229:ASP:HB2	1:B:261:ALA:CA	2.36	0.54
1:B:77:ALA:O	1:B:162:ARG:HG2	2.07	0.54
1:B:143:VAL:O	1:B:147:ARG:HG3	2.08	0.54
1:B:424:GLN:HB2	2:B:610:HOH:O	2.07	0.54
1:B:248:LEU:HD21	1:B:285:PRO:HG2	1.89	0.54
1:B:303:ILE:HD13	1:B:318:PHE:CE1	2.43	0.54
1:B:363:VAL:HG12	1:B:364:ASN:N	2.23	0.54
1:B:297:LYS:HE3	1:B:345:SER:CB	2.32	0.53
1:B:47:MET:HE1	1:B:76:ASN:HB3	1.90	0.53
1:B:197:LYS:HD3	1:B:197:LYS:C	2.33	0.53
1:B:256:LYS:O	1:B:257:GLU:HB2	2.08	0.53
1:B:347:ARG:HD2	1:B:363:VAL:HG11	1.91	0.53
1:A:361:VAL:HG13	1:A:383:ILE:HD12	1.89	0.53
1:B:130:TYR:CE2	1:B:138:ARG:HB2	2.43	0.53
1:B:340:LYS:HD2	1:B:340:LYS:H	1.71	0.53
1:A:336:LYS:HG3	1:A:385:MET:O	2.09	0.53
1:B:57:ARG:HH22	1:B:69:GLU:H	1.56	0.53
1:B:427:LYS:HG2	1:B:428:GLU:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:H	1:A:66:GLU:CD	2.17	0.53
1:A:266:LEU:O	1:A:280:LEU:HD22	2.08	0.53
1:B:194:GLN:CD	1:B:198:PHE:HD2	2.17	0.53
1:B:26:LYS:HE3	1:B:36:GLU:HB2	1.91	0.53
1:A:238:ARG:NH2	1:A:397:LYS:O	2.41	0.52
1:B:26:LYS:CE	1:B:36:GLU:HB2	2.40	0.52
1:A:88:SER:O	1:A:106:THR:HA	2.10	0.52
1:B:241:GLU:O	1:B:245:LYS:HG3	2.09	0.52
1:A:169:SER:O	1:A:173:LYS:HE2	2.09	0.52
1:B:1:CYS:SG	2:B:546:HOH:O	2.29	0.52
1:B:442:HIS:CD2	1:B:454:ASN:HD21	2.28	0.52
1:A:91:ARG:O	1:A:92:LEU:HB2	2.09	0.52
1:A:50:VAL:HG11	1:A:177:GLN:HE22	1.74	0.52
1:A:223:ARG:HG3	1:A:225:THR:HG23	1.92	0.52
1:B:109:MET:SD	2:B:575:HOH:O	2.59	0.52
1:A:366:GLU:HB3	1:A:367:PRO:HD2	1.92	0.51
1:B:229:ASP:HA	1:B:262:LYS:HD3	1.92	0.51
1:A:46:THR:HA	1:A:428:GLU:HA	1.92	0.51
1:A:234:SER:HB2	2:A:613:HOH:O	2.10	0.51
1:B:192:TYR:OH	1:B:292:GLY:HA3	2.10	0.51
1:A:85:THR:OG1	1:A:157:TRP:CH2	2.60	0.51
1:A:256:LYS:HB2	1:A:263:THR:CA	2.40	0.51
1:B:267:TYR:HB3	1:B:280:LEU:CD1	2.40	0.51
1:A:368:ALA:HA	1:A:377:HIS:O	2.10	0.51
1:A:339:ILE:HG13	1:A:385:MET:HE1	1.93	0.51
1:B:215:TRP:CH2	1:B:301:LYS:HG2	2.46	0.51
1:B:428:GLU:CG	1:B:429:ASP:N	2.68	0.51
1:B:137:GLU:HG3	1:B:138:ARG:HG3	1.93	0.51
1:B:251:GLU:O	1:B:264:VAL:HA	2.11	0.51
1:B:130:TYR:CD1	1:B:130:TYR:C	2.89	0.50
1:B:295:PHE:HA	1:B:302:ASN:O	2.11	0.50
1:A:143:VAL:O	1:A:147:ARG:HG3	2.11	0.50
1:B:69:GLU:HA	2:B:545:HOH:O	2.10	0.50
1:A:164:LEU:HD22	1:A:423:LEU:HD22	1.93	0.50
1:B:57:ARG:NH2	1:B:69:GLU:H	2.09	0.50
1:B:441:ASP:C	2:B:493:HOH:O	2.53	0.50
1:B:303:ILE:CG2	1:B:307:LEU:HD23	2.41	0.50
1:A:228:VAL:HG21	1:A:239:VAL:HG21	1.92	0.50
1:B:54:SER:OG	1:B:57:ARG:HB2	2.11	0.50
1:A:50:VAL:HG22	1:A:423:LEU:CD1	2.42	0.49
1:A:179:TYR:CZ	1:A:417:ARG:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ILE:CD1	1:B:385:MET:HE1	2.25	0.49
1:B:59:HIS:HA	1:B:66:GLU:HB3	1.94	0.49
1:A:147:ARG:HH11	1:B:411:ALA:HB2	1.77	0.49
1:A:257:GLU:HB3	1:A:260:VAL:CG2	2.38	0.49
1:B:157:TRP:NE1	2:B:587:HOH:O	2.27	0.49
1:A:163:ASP:O	1:A:166:LEU:HB2	2.11	0.49
1:B:87:ARG:NH2	1:B:149:ALA:HB3	2.28	0.49
1:B:428:GLU:HG3	1:B:429:ASP:HB2	1.95	0.49
1:B:54:SER:HB2	2:B:602:HOH:O	2.13	0.49
1:A:256:LYS:HB2	1:A:263:THR:N	2.27	0.49
1:B:206:LYS:HD2	1:B:206:LYS:H	1.77	0.49
1:A:58:ALA:HB3	1:A:68:PRO:CB	2.43	0.49
1:A:118:ARG:HH22	1:A:163:ASP:CG	2.21	0.49
1:A:176:TYR:HB2	1:A:419:PHE:O	2.13	0.49
1:B:229:ASP:HA	1:B:262:LYS:CD	2.42	0.49
1:A:105:ILE:HA	1:A:126:VAL:O	2.12	0.48
1:B:297:LYS:HG3	1:B:298:ASP:N	2.27	0.48
1:A:210:TYR:HB2	1:A:317:THR:HG22	1.95	0.48
1:A:284:ASN:ND2	1:A:287:TRP:H	2.11	0.48
1:B:189:PHE:CD1	1:B:205:PRO:HB3	2.47	0.48
1:A:104:VAL:CG1	1:A:142:LEU:HD13	2.43	0.48
1:B:48:TYR:HB3	1:B:423:LEU:CD2	2.42	0.48
1:B:62:ASP:C	1:B:64:SER:H	2.22	0.48
1:B:268:SER:OG	1:B:280:LEU:HD22	2.14	0.48
1:B:211:LEU:HA	1:B:214:LEU:HD12	1.95	0.48
1:A:405:ARG:NH2	2:A:531:HOH:O	2.45	0.48
1:A:415:GLU:H	1:A:415:GLU:HG3	1.49	0.48
1:B:141:GLU:O	1:B:145:SER:HB2	2.13	0.48
1:A:256:LYS:HD3	1:A:263:THR:OG1	2.12	0.48
2:A:525:HOH:O	1:B:360:VAL:HB	2.13	0.48
1:B:137:GLU:HG3	1:B:138:ARG:N	2.29	0.48
1:B:67:VAL:HG12	1:B:347:ARG:NH1	2.29	0.48
1:B:211:LEU:HD12	1:B:246:LEU:HD12	1.94	0.48
1:B:232:ASP:HB3	1:B:402:LYS:HZ1	1.78	0.48
1:A:35:ARG:HB3	1:A:436:LEU:HG	1.95	0.47
1:A:215:TRP:CZ3	1:A:287:TRP:HZ3	2.31	0.47
1:B:85:THR:OG1	1:B:157:TRP:CH2	2.57	0.47
1:A:88:SER:HB2	1:B:407:ALA:O	2.14	0.47
1:B:57:ARG:HH22	1:B:69:GLU:HB2	1.80	0.47
1:B:286:LEU:O	1:B:290:ILE:HG13	2.15	0.47
1:B:57:ARG:HA	1:B:57:ARG:HD2	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HD12	1:B:235:LEU:HA	1.72	0.47
1:B:65:ARG:HH21	1:B:378:LYS:HE3	1.79	0.47
1:B:302:ASN:CB	1:B:345:SER:HB2	2.44	0.47
1:B:111:GLN:HA	1:B:120:VAL:O	2.15	0.47
1:A:284:ASN:HA	1:A:285:PRO:HD3	1.70	0.47
1:B:257:GLU:O	1:B:259:GLN:N	2.48	0.47
1:A:268:SER:OG	1:A:284:ASN:HB3	2.16	0.46
1:B:26:LYS:NZ	1:B:36:GLU:HB2	2.30	0.46
1:B:212:LEU:HD21	1:B:290:ILE:HG12	1.98	0.46
1:A:147:ARG:NH1	1:B:411:ALA:HB2	2.29	0.46
1:A:191:ASP:HA	2:A:601:HOH:O	2.15	0.46
1:B:384:TYR:CD1	1:B:384:TYR:N	2.83	0.46
1:A:78:THR:HG22	1:A:162:ARG:CZ	2.45	0.46
1:A:267:TYR:CD1	1:A:280:LEU:HD21	2.51	0.46
1:B:79:HIS:CE1	2:B:535:HOH:O	2.69	0.46
1:A:256:LYS:HD3	1:A:263:THR:HG23	1.97	0.46
1:B:89:VAL:HG23	1:B:106:THR:HG22	1.97	0.46
1:B:210:TYR:HB2	1:B:317:THR:HG22	1.98	0.46
1:B:329:VAL:HG12	1:B:405:ARG:NH1	2.31	0.46
1:A:199:HIS:HE2	1:A:246:LEU:CA	2.27	0.46
1:A:197:LYS:HD2	1:A:285:PRO:HA	1.98	0.46
1:B:37:VAL:HG13	1:B:434:ILE:HB	1.98	0.46
1:A:50:VAL:HG11	1:A:177:GLN:NE2	2.31	0.46
1:A:129:SER:O	1:A:130:TYR:CB	2.64	0.46
1:B:57:ARG:NH2	1:B:69:GLU:HB2	2.30	0.46
1:A:206:LYS:HB3	2:A:502:HOH:O	2.15	0.45
1:A:207:VAL:HG11	1:A:245:LYS:CD	2.44	0.45
1:A:160:GLU:OE1	1:A:162:ARG:NE	2.46	0.45
1:B:1:CYS:CB	1:B:79:HIS:CD2	2.99	0.45
1:B:288:ASP:O	1:B:292:GLY:N	2.48	0.45
1:A:255:ARG:HG3	1:A:259:GLN:NE2	2.31	0.45
1:A:256:LYS:HB2	1:A:263:THR:OG1	2.17	0.45
1:B:125:GLU:CD	1:B:171:VAL:HG23	2.41	0.45
1:B:200:LEU:O	1:B:200:LEU:HG	2.17	0.45
1:B:232:ASP:HB2	1:B:400:GLY:CA	2.46	0.45
1:A:192:TYR:HE2	1:A:197:LYS:NZ	2.14	0.45
1:A:246:LEU:O	1:A:247:ASN:HB2	2.17	0.45
1:B:189:PHE:HB2	1:B:310:ASP:OD2	2.16	0.45
1:A:56:HIS:O	1:A:57:ARG:NE	2.49	0.45
1:A:434:ILE:O	1:A:454:ASN:HB2	2.17	0.45
1:B:1:CYS:SG	1:B:454:ASN:O	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HD2	2:B:590:HOH:O	2.17	0.45
1:A:257:GLU:HB2	1:A:261:ALA:HB3	1.98	0.45
1:A:335:ILE:HG23	1:A:391:LEU:HD23	1.99	0.45
1:B:252:TYR:HB3	1:B:262:LYS:NZ	2.31	0.45
1:B:247:ASN:HD22	1:B:269:LYS:HD3	1.77	0.45
1:B:448:ASN:O	1:B:449:GLN:HB2	2.17	0.45
1:A:87:ARG:HD3	1:A:152:LYS:O	2.17	0.45
1:B:336:LYS:HB2	1:B:336:LYS:HE3	1.61	0.45
1:A:33:ARG:NH1	1:A:35:ARG:HH21	2.15	0.44
1:B:167:LEU:HD11	2:B:588:HOH:O	2.17	0.44
1:B:27:VAL:HG23	1:B:35:ARG:HB2	1.99	0.44
1:B:228:VAL:HG11	1:B:236:MET:CG	2.47	0.44
1:A:235:LEU:O	1:A:239:VAL:HG23	2.18	0.44
1:B:219:GLY:HA2	1:B:226:PHE:HA	1.99	0.44
1:B:79:HIS:HE1	2:B:535:HOH:O	2.01	0.44
1:B:232:ASP:HB2	1:B:401:SER:N	2.31	0.44
1:B:257:GLU:HB2	1:B:261:ALA:CB	2.30	0.44
1:B:39:LYS:HB2	1:B:435:THR:HG23	1.98	0.44
1:B:281:ASN:N	1:B:284:ASN:ND2	2.65	0.44
1:A:144:GLU:HB3	1:A:148:LYS:HZ2	1.83	0.44
1:A:255:ARG:NH1	2:A:619:HOH:O	2.48	0.44
1:A:39:LYS:HB2	1:A:435:THR:HB	1.98	0.44
1:A:428:GLU:HG2	2:A:632:HOH:O	2.18	0.43
1:B:1:CYS:HB3	1:B:79:HIS:CD2	2.53	0.43
1:B:215:TRP:CZ2	1:B:301:LYS:HG2	2.54	0.43
1:A:103:GLU:CA	1:A:129:SER:HB3	2.37	0.43
1:A:297:LYS:NZ	1:A:300:VAL:CG1	2.81	0.43
1:B:347:ARG:HA	1:B:383:ILE:HD11	2.01	0.43
1:B:379:ILE:HD13	1:B:381:TYR:OH	2.18	0.43
1:B:412:PHE:CD1	1:B:412:PHE:C	2.97	0.43
1:A:342:ILE:HG12	2:A:473:HOH:O	2.19	0.43
1:B:90:ARG:NH2	2:B:485:HOH:O	2.52	0.43
1:B:201:THR:HG23	1:B:202:ILE:HD12	2.00	0.43
1:B:256:LYS:O	1:B:256:LYS:CG	2.67	0.43
1:A:89:VAL:HG21	1:A:143:VAL:HG22	2.00	0.43
1:B:392:LEU:HD12	1:B:392:LEU:HA	1.82	0.43
1:A:22:GLU:HG2	2:A:567:HOH:O	2.17	0.43
1:A:59:HIS:CG	2:A:578:HOH:O	2.72	0.43
1:B:210:TYR:CE2	1:B:214:LEU:HD11	2.53	0.43
1:B:232:ASP:O	1:B:234:SER:N	2.52	0.43
1:A:199:HIS:CE1	1:A:246:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLU:O	1:A:207:VAL:HG13	2.19	0.42
1:A:132:ILE:HG22	1:A:133:SER:N	2.35	0.42
1:A:253:LYS:HB3	1:A:263:THR:HB	2.01	0.42
1:A:284:ASN:C	1:A:284:ASN:ND2	2.74	0.42
1:B:46:THR:HG23	1:B:427:LYS:CB	2.49	0.42
1:B:89:VAL:HA	1:B:105:ILE:O	2.19	0.42
1:B:229:ASP:N	1:B:262:LYS:HB2	2.29	0.42
1:B:367:PRO:O	1:B:380:SER:HB3	2.19	0.42
1:A:215:TRP:CD1	1:A:216:ILE:N	2.88	0.42
1:B:68:PRO:HD2	1:B:347:ARG:NH2	2.34	0.42
1:B:211:LEU:HD23	1:B:214:LEU:HD12	1.99	0.42
1:A:85:THR:OG1	1:A:157:TRP:CZ3	2.66	0.42
1:B:324:ASP:HA	1:B:403:LYS:HD3	2.01	0.42
1:B:202:ILE:O	1:B:203:GLU:O	2.38	0.42
1:A:2:PHE:HD1	1:A:18:ILE:HD13	1.83	0.42
1:B:45:GLU:O	1:B:47:MET:CE	2.62	0.42
1:A:248:LEU:CD2	1:A:285:PRO:HD2	2.40	0.42
1:B:46:THR:HG23	1:B:427:LYS:N	2.35	0.42
1:A:322:LEU:HB3	1:A:339:ILE:HD13	2.01	0.41
1:A:361:VAL:CG1	1:A:383:ILE:CD1	2.98	0.41
1:B:87:ARG:HD3	1:B:152:LYS:O	2.20	0.41
1:B:303:ILE:HD13	1:B:318:PHE:HE1	1.82	0.41
1:B:57:ARG:HD3	2:B:602:HOH:O	2.18	0.41
1:B:80:GLU:HG2	2:B:593:HOH:O	2.19	0.41
1:A:256:LYS:NZ	1:A:263:THR:HG23	2.36	0.41
1:A:1:CYS:SG	1:A:454:ASN:OXT	2.78	0.41
1:B:266:LEU:HD12	1:B:286:LEU:CD2	2.48	0.41
1:A:39:LYS:HD3	1:A:435:THR:HG21	2.03	0.41
1:A:173:LYS:NZ	2:A:509:HOH:O	2.53	0.41
1:B:179:TYR:CE2	1:B:417:ARG:HB2	2.56	0.41
1:B:22:GLU:O	1:B:25:ASN:HB2	2.20	0.41
1:B:229:ASP:HA	1:B:262:LYS:HG3	2.03	0.41
1:B:84:ARG:CD	1:B:156:GLU:HG2	2.50	0.41
1:B:255:ARG:C	1:B:262:LYS:HA	2.46	0.41
1:A:2:PHE:CD1	1:A:2:PHE:N	2.89	0.41
1:A:346:VAL:O	1:A:350:LEU:HB2	2.21	0.41
1:B:65:ARG:NH2	1:B:378:LYS:HG3	2.36	0.41
1:B:92:LEU:HA	1:B:92:LEU:HD13	1.39	0.41
1:B:230:SER:O	1:B:232:ASP:N	2.54	0.41
1:B:87:ARG:HH22	1:B:149:ALA:HB3	1.86	0.41
1:B:229:ASP:HA	1:B:262:LYS:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LYS:HB3	1:B:262:LYS:O	2.21	0.41
1:B:390:VAL:HG13	1:B:414:ARG:NH1	2.36	0.41
1:A:141:GLU:O	1:A:142:LEU:C	2.63	0.40
1:A:220:LEU:HG	2:A:537:HOH:O	2.20	0.40
1:A:383:ILE:O	1:A:383:ILE:HG13	2.21	0.40
1:B:216:ILE:HA	1:B:301:LYS:HD2	2.04	0.40
1:B:319:LEU:HD23	1:B:319:LEU:HA	1.96	0.40
1:A:267:TYR:CD1	1:A:280:LEU:CD2	3.04	0.40
1:B:46:THR:CB	1:B:427:LYS:HA	2.52	0.40
1:B:182:ILE:HG21	1:B:309:THR:HG22	2.02	0.40
1:A:196:SER:HB3	1:A:197:LYS:H	1.75	0.40
1:B:228:VAL:H	1:B:262:LYS:H	1.69	0.40
1:A:230:SER:CB	1:A:262:LYS:HG3	2.50	0.40
1:A:323:ILE:HG13	1:A:339:ILE:HD11	2.03	0.40
1:A:436:LEU:H	1:A:454:ASN:HD22	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/454 (93%)	378 (90%)	25 (6%)	18 (4%)	2	1
1	B	420/454 (92%)	361 (86%)	35 (8%)	24 (6%)	1	0
All	All	841/908 (93%)	739 (88%)	60 (7%)	42 (5%)	1	1

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	130	TYR
1	A	131	PRO

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Mol	Chain	Res	Type
1	A	137	GLU
1	A	197	LYS
1	A	257	GLU
1	B	60	LYS
1	B	196	SER
1	B	199	HIS
1	B	202	ILE
1	B	203	GLU
1	B	229	ASP
1	B	233	THR
1	B	256	LYS
1	B	298	ASP
1	B	378	LYS
1	B	442	HIS
1	A	57	ARG
1	A	260	VAL
1	A	332	GLU
1	A	367	PRO
1	A	439	ASP
1	A	139	ALA
1	A	259	GLN
1	B	58	ALA
1	B	257	GLU
1	B	258	PRO
1	B	429	ASP
1	A	91	ARG
1	B	70	LEU
1	B	230	SER
1	B	255	ARG
1	A	255	ARG
1	B	91	ARG
1	B	228	VAL
1	B	332	GLU
1	A	202	ILE
1	B	198	PHE
1	B	218	ASP
1	A	258	PRO
1	A	387	GLY
1	B	387	GLY

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	371/392 (95%)	325 (88%)	46 (12%)	4	6
1	B	370/392 (94%)	322 (87%)	48 (13%)	4	5
All	All	741/784 (94%)	647 (87%)	94 (13%)	4	6

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	GLU
1	A	26	LYS
1	A	57	ARG
1	A	59	HIS
1	A	66	GLU
1	A	84	ARG
1	A	90	ARG
1	A	103	GLU
1	A	115	PRO
1	A	120	VAL
1	A	121	GLU
1	A	122	LEU
1	A	128	LYS
1	A	130	TYR
1	A	134	GLU
1	A	140	ASN
1	A	166	LEU
1	A	187	ASP
1	A	198	PHE
1	A	206	LYS
1	A	207	VAL
1	A	211	LEU
1	A	215	TRP
1	A	220	LEU
1	A	228	VAL
1	A	251	GLU

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Mol	Chain	Res	Type
1	A	254	ASP
1	A	260	VAL
1	A	270	VAL
1	A	280	LEU
1	A	282	THR
1	A	284	ASN
1	A	286	LEU
1	A	296	LEU
1	A	310	ASP
1	A	344	THR
1	A	350	LEU
1	A	375	THR
1	A	376	LYS
1	A	383	ILE
1	A	392	LEU
1	A	415	GLU
1	A	436	LEU
1	A	439	ASP
1	A	445	LEU
1	B	8	VAL
1	B	12	ASP
1	B	15	ILE
1	B	49	SER
1	B	55	GLN
1	B	62	ASP
1	B	70	LEU
1	B	84	ARG
1	B	90	ARG
1	B	104	VAL
1	B	122	LEU
1	B	129	SER
1	B	133	SER
1	B	142	LEU
1	B	143	VAL
1	B	156	GLU
1	B	197	LYS
1	B	198	PHE
1	B	200	LEU
1	B	203	GLU
1	B	215	TRP
1	B	227	SER
1	B	232	ASP

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Mol	Chain	Res	Type
1	B	256	LYS
1	B	263	THR
1	B	268	SER
1	B	287	TRP
1	B	297	LYS
1	B	300	VAL
1	B	307	LEU
1	B	310	ASP
1	B	322	LEU
1	B	335	ILE
1	B	340	LYS
1	B	342	ILE
1	B	344	THR
1	B	345	SER
1	B	366	GLU
1	B	378	LYS
1	B	384	TYR
1	B	392	LEU
1	B	402	LYS
1	B	423	LEU
1	B	424	GLN
1	B	429	ASP
1	B	435	THR
1	B	437	SER
1	B	441	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	20	ASN
1	A	25	ASN
1	A	56	HIS
1	A	79	HIS
1	A	186	ASN
1	A	284	ASN
1	A	442	HIS
1	A	454	ASN
1	B	79	HIS
1	B	170	HIS
1	B	199	HIS
1	B	247	ASN

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Mol	Chain	Res	Type
1	B	284	ASN
1	B	377	HIS
1	B	449	GLN
1	B	454	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.