



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:22 PM UTC

PDB ID : 3D7U / pdb_00003d7u
Title : Structural basis for the recognition of c-Src by its inactivator Csk
Authors : Levinson, N.M.; Seeliger, M.A.; Cole, P.A.; Kuriyan, J.
Deposited on : 2008-05-21
Resolution : 4.11 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)	:	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

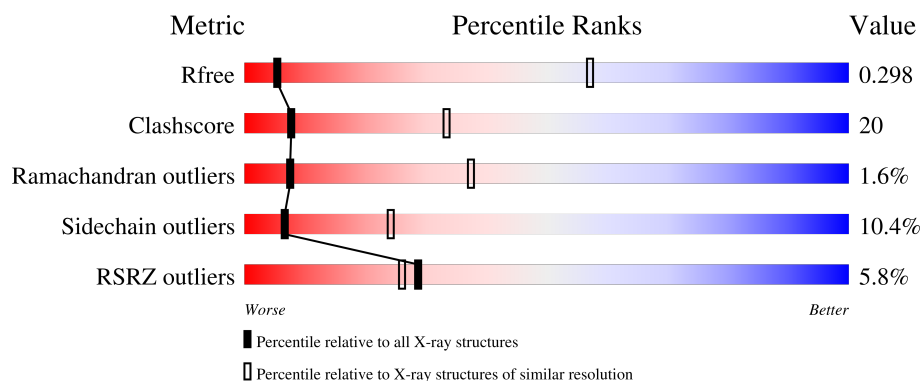
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.11 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	1249 (4.44-3.80)
Clashscore	190562	1031 (4.42-3.82)
Ramachandran outliers	187476	1211 (4.44-3.80)
Sidechain outliers	187428	1198 (4.44-3.80)
RSRZ outliers	180081	1246 (4.44-3.80)

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	263	8% 66% 26% 5%
1	C	263	5% 67% 25% 5%
2	B	277	3% 54% 35% 7%
2	D	277	6% 52% 34% 10%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8153 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 Tyrosine-protein kinase CSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2038	1306	349	370	13			
1	C	257	Total	C	N	O	S	0	0	0
			2038	1306	349	370	13			

- Molecule 2 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2080	1334	347	382	17			
2	D	248	Total	C	N	O	S	0	0	0
			1997	1283	334	363	17			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	257	LYS	-	expression tag	UNP P00523
B	258	ASP	-	expression tag	UNP P00523
B	259	ALA	-	expression tag	UNP P00523
B	524	GLU	-	expression tag	UNP P00523
B	525	PRO	-	expression tag	UNP P00523
B	526	GLN	-	expression tag	UNP P00523
B	527	TYR	-	expression tag	UNP P00523
B	528	GLN	-	expression tag	UNP P00523
B	529	PRO	-	expression tag	UNP P00523
B	530	GLY	-	expression tag	UNP P00523
B	531	GLU	-	expression tag	UNP P00523
B	532	ASN	-	expression tag	UNP P00523
B	533	LEU	-	expression tag	UNP P00523
D	257	LYS	-	expression tag	UNP P00523
D	258	ASP	-	expression tag	UNP P00523
D	259	ALA	-	expression tag	UNP P00523

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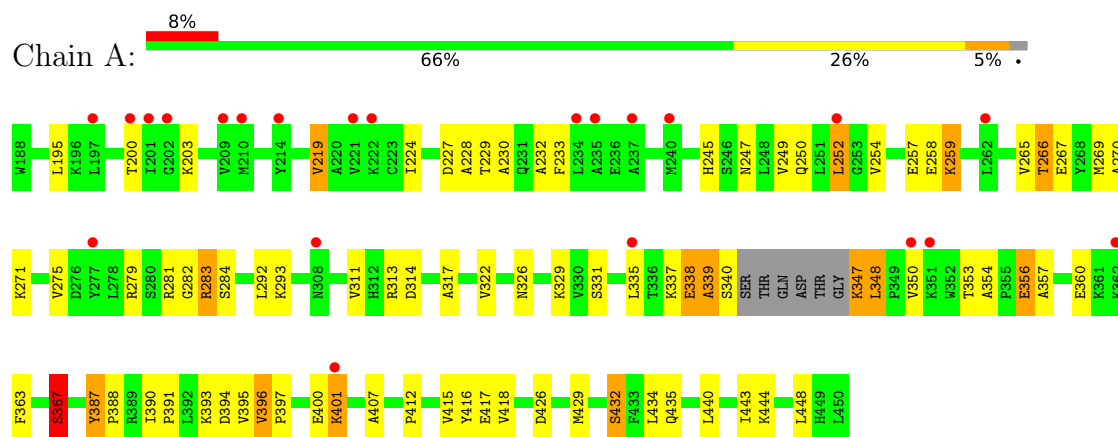
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Chain	Residue	Modelled	Actual	Comment	Reference
D	524	GLU	-	expression tag	UNP P00523
D	525	PRO	-	expression tag	UNP P00523
D	526	GLN	-	expression tag	UNP P00523
D	527	TYR	-	expression tag	UNP P00523
D	528	GLN	-	expression tag	UNP P00523
D	529	PRO	-	expression tag	UNP P00523
D	530	GLY	-	expression tag	UNP P00523
D	531	GLU	-	expression tag	UNP P00523
D	532	ASN	-	expression tag	UNP P00523
D	533	LEU	-	expression tag	UNP P00523

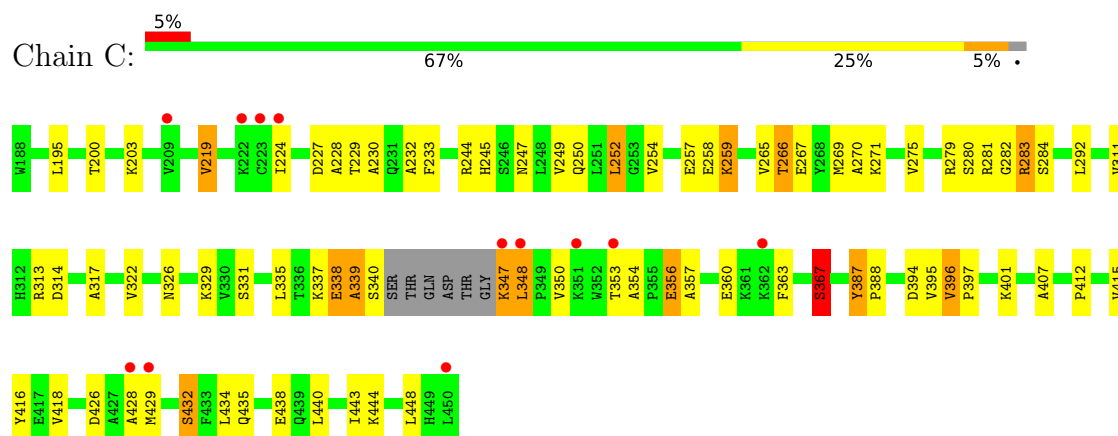
3 Residue-property plots [i](#)

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

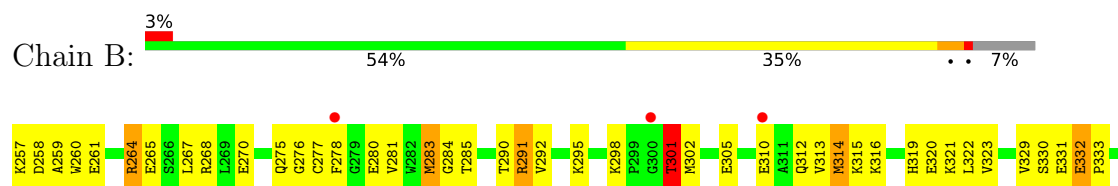
• Molecule 1: Tyrosine-protein kinase CSK

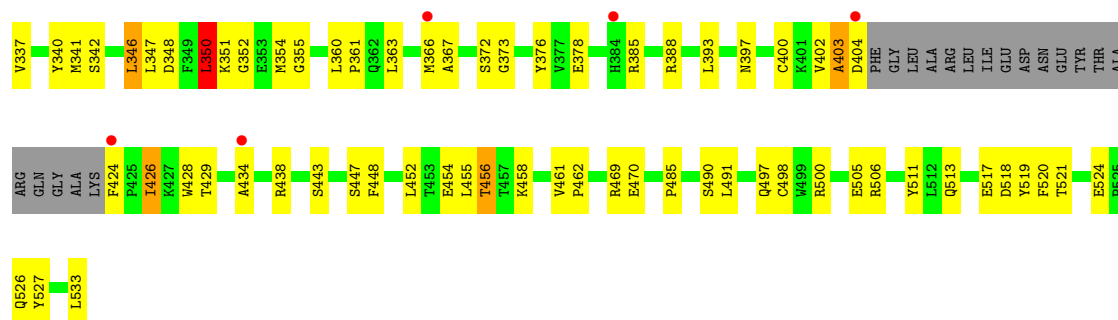


• Molecule 1: Tyrosine-protein kinase CSK

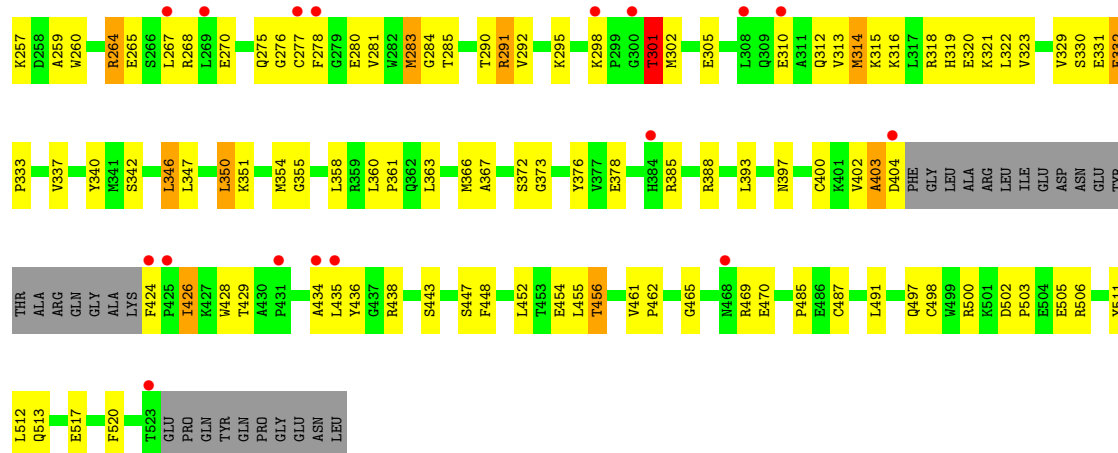


• Molecule 2: Proto-oncogene tyrosine-protein kinase Src





● Molecule 2: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	135.84Å 135.84Å 129.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.87 – 4.11 46.87 – 4.11	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.87-4.11) 98.5 (46.87-4.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.294 , 0.302 0.288 , 0.298	Depositor DCC
R_{free} test set	1053 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	162.2	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 133.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l 0.078 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8153	wwPDB-VP
Average B, all atoms (Å ²)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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	0.54	2/2080 (0.1%)	0.99	14/2806 (0.5%)
1	C	0.54	2/2080 (0.1%)	0.99	14/2806 (0.5%)
2	B	0.96	3/2130 (0.1%)	1.07	4/2882 (0.1%)
2	D	1.11	3/2044 (0.1%)	1.06	3/2765 (0.1%)
All	All	0.83	10/8334 (0.1%)	1.02	35/11259 (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
2	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	350	LEU	C-N	27.65	1.70	1.33
2	B	350	LEU	C-N	12.70	1.53	1.33
2	D	342	SER	C-O	7.76	1.34	1.24
2	B	342	SER	C-O	7.71	1.34	1.24
1	A	432	SER	C-O	7.67	1.34	1.23
1	C	432	SER	C-O	7.66	1.34	1.23
2	D	342	SER	C-N	-5.57	1.26	1.33
2	B	342	SER	C-N	-5.48	1.26	1.33
1	A	432	SER	C-N	-5.38	1.26	1.34
1	C	432	SER	C-N	-5.30	1.26	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	326	ASN	N-CA-C	9.32	124.17	112.24
1	A	326	ASN	N-CA-C	9.30	124.14	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	LEU	O-C-N	7.33	133.05	122.28
1	A	387	TYR	CA-C-N	7.21	126.74	119.24
1	A	387	TYR	C-N-CA	7.21	126.74	119.24
1	C	387	TYR	CA-C-N	7.18	126.71	119.24
1	C	387	TYR	C-N-CA	7.18	126.71	119.24
1	A	270	ALA	N-CA-C	6.37	119.90	111.75
1	C	270	ALA	N-CA-C	6.34	119.87	111.75
2	D	342	SER	CA-C-O	-6.24	112.59	119.95
1	A	350	VAL	N-CA-C	6.23	116.90	110.36
2	B	342	SER	CA-C-O	-6.18	112.66	119.95
1	C	350	VAL	N-CA-C	6.15	116.82	110.36
1	A	232	ALA	N-CA-C	-6.05	104.76	111.36
1	A	401	LYS	N-CA-C	-6.04	106.16	112.93
2	B	448	PHE	N-CA-C	-6.01	104.64	111.07
1	C	401	LYS	N-CA-C	-5.99	106.22	112.93
2	D	448	PHE	N-CA-C	-5.98	104.68	111.07
1	C	232	ALA	N-CA-C	-5.90	104.77	111.14
1	C	418	VAL	N-CA-C	-5.71	105.16	110.53
2	D	284	GLY	N-CA-C	5.61	118.43	110.74
1	A	418	VAL	N-CA-C	-5.61	105.26	110.53
2	B	284	GLY	N-CA-C	5.60	118.41	110.74
1	A	250	GLN	N-CA-C	5.49	118.58	109.46
1	C	250	GLN	N-CA-C	5.49	118.57	109.46
1	C	228	ALA	N-CA-C	5.28	117.72	111.33
1	A	228	ALA	N-CA-C	5.26	117.69	111.33
1	A	348	LEU	N-CA-C	5.23	116.26	109.72
1	C	348	LEU	N-CA-C	5.23	116.26	109.72
1	A	252	LEU	N-CA-C	-5.12	107.59	113.88
1	C	252	LEU	N-CA-C	-5.06	107.65	113.88
1	A	440	LEU	N-CA-C	-5.06	105.95	111.82
1	C	440	LEU	N-CA-C	-5.06	105.95	111.82
1	C	367	SER	N-CA-C	-5.03	105.89	112.23
1	A	367	SER	N-CA-C	-5.01	105.92	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	350	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	2038	0	2064	94	9
1	C	2038	0	2064	79	12
2	B	2080	0	2065	108	1
2	D	1997	0	1993	113	4
All	All	8153	0	8186	326	13

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 20.

All (326) 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)
2:D:350:LEU:C	2:D:351:LYS:N	1.70	1.49
1:C:279:ARG:HD3	2:D:511:TYR:CE2	1.54	1.41
1:A:279:ARG:HD3	2:B:511:TYR:CE2	1.67	1.29
1:A:400:GLU:OE1	2:D:465:GLY:CA	1.79	1.27
1:C:279:ARG:CD	2:D:511:TYR:CE2	2.18	1.26
1:A:400:GLU:OE1	2:D:465:GLY:HA3	1.03	1.18
1:C:259:LYS:H	1:C:259:LYS:HD2	1.02	1.16
1:A:259:LYS:H	1:A:259:LYS:HD2	1.02	1.13
1:A:279:ARG:CD	2:B:511:TYR:CE2	2.32	1.12
1:A:283:ARG:HH21	2:B:378:GLU:HG2	0.97	1.12
1:A:393:LYS:NZ	2:B:526:GLN:HE22	1.53	1.04
1:A:393:LYS:NZ	2:B:526:GLN:NE2	2.05	1.04
2:B:275:GLN:HG3	2:B:276:GLY:H	1.22	1.04
2:D:350:LEU:O	2:D:355:GLY:HA3	1.59	1.02
1:A:283:ARG:NH2	2:B:378:GLU:HG2	1.73	1.01
1:A:279:ARG:NE	2:B:511:TYR:HE2	1.58	1.01
2:D:319:HIS:HB2	2:D:376:TYR:CD2	1.95	1.01
1:C:279:ARG:NE	2:D:511:TYR:HE2	1.60	0.97
2:B:259:ALA:C	2:B:260:TRP:N	2.23	0.97
2:D:319:HIS:CD2	2:D:373:GLY:HA2	2.01	0.95
1:C:279:ARG:NH1	2:D:511:TYR:OH	1.98	0.95
1:A:279:ARG:HD3	2:B:511:TYR:CD2	2.01	0.95
1:A:283:ARG:HH21	2:B:378:GLU:CG	1.79	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:321:LYS:O	2:D:402:VAL:N	2.00	0.94
1:A:393:LYS:HZ1	2:B:526:GLN:NE2	1.63	0.93
2:B:347:LEU:O	2:B:351:LYS:HB2	1.68	0.93
1:A:279:ARG:NE	2:B:511:TYR:CE2	2.36	0.92
1:A:396:VAL:HG13	1:A:397:PRO:HD3	1.52	0.92
1:C:279:ARG:NE	2:D:511:TYR:CE2	2.37	0.91
1:C:283:ARG:HH21	2:D:378:GLU:HG2	1.36	0.91
1:C:259:LYS:HD2	1:C:259:LYS:N	1.85	0.91
2:D:275:GLN:HG3	2:D:276:GLY:H	1.35	0.91
1:A:259:LYS:HD2	1:A:259:LYS:N	1.85	0.91
1:C:396:VAL:HG13	1:C:397:PRO:HD3	1.52	0.91
1:C:279:ARG:HD3	2:D:511:TYR:CZ	2.06	0.90
1:A:347:LYS:HD3	1:A:348:LEU:H	1.35	0.89
2:B:452:LEU:O	2:B:456:THR:OG1	1.91	0.89
1:A:279:ARG:CZ	2:B:511:TYR:HE2	1.86	0.89
1:C:347:LYS:HD3	1:C:348:LEU:H	1.35	0.87
2:D:452:LEU:O	2:D:456:THR:OG1	1.91	0.87
2:D:322:LEU:HD12	2:D:402:VAL:HB	1.54	0.87
1:A:283:ARG:NH2	2:B:378:GLU:CG	2.35	0.87
1:A:393:LYS:HZ1	2:B:526:GLN:HE22	1.12	0.87
1:C:363:PHE:CE2	1:C:367:SER:HB2	2.11	0.84
1:A:363:PHE:CE2	1:A:367:SER:HB2	2.11	0.84
1:C:280:SER:HB2	2:D:505:GLU:HA	1.59	0.84
2:D:275:GLN:CG	2:D:276:GLY:H	1.91	0.84
2:D:322:LEU:HA	2:D:402:VAL:O	1.78	0.83
1:C:347:LYS:HD3	1:C:348:LEU:N	1.93	0.83
2:D:323:VAL:H	2:D:403:ALA:HB2	1.44	0.82
1:A:347:LYS:HD3	1:A:348:LEU:N	1.93	0.82
2:B:275:GLN:CG	2:B:276:GLY:H	1.93	0.81
2:B:527:TYR:OH	2:B:533:LEU:OXT	1.99	0.80
1:A:279:ARG:CZ	2:B:511:TYR:CE2	2.66	0.79
2:D:319:HIS:HB2	2:D:376:TYR:CE2	2.17	0.79
1:A:259:LYS:H	1:A:259:LYS:CD	1.89	0.78
2:D:350:LEU:CA	2:D:351:LYS:N	2.46	0.78
2:B:347:LEU:O	2:B:351:LYS:CB	2.32	0.78
2:D:259:ALA:C	2:D:260:TRP:N	2.41	0.78
2:B:319:HIS:HB2	2:B:376:TYR:CD2	2.18	0.77
1:A:393:LYS:HZ2	2:B:526:GLN:NE2	1.81	0.77
2:B:319:HIS:CD2	2:B:373:GLY:HA2	2.20	0.76
2:D:275:GLN:HG3	2:D:276:GLY:N	1.99	0.75
2:B:322:LEU:HD12	2:B:402:VAL:HB	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:347:LEU:O	2:D:351:LYS:CB	2.35	0.74
2:B:323:VAL:HB	2:B:403:ALA:CB	2.18	0.74
1:C:396:VAL:HG13	1:C:397:PRO:CD	2.18	0.73
1:A:396:VAL:HG13	1:A:397:PRO:CD	2.18	0.73
1:A:279:ARG:CD	2:B:511:TYR:CD2	2.66	0.73
1:C:279:ARG:HG2	2:D:511:TYR:CD2	2.23	0.72
2:D:350:LEU:C	2:D:355:GLY:HA3	2.14	0.72
2:B:321:LYS:O	2:B:402:VAL:N	2.23	0.72
1:A:279:ARG:NH1	2:B:511:TYR:OH	2.23	0.71
1:C:259:LYS:H	1:C:259:LYS:CD	1.89	0.71
1:C:279:ARG:HD3	2:D:511:TYR:CD2	2.23	0.70
2:D:350:LEU:O	2:D:355:GLY:CA	2.38	0.69
1:C:283:ARG:NH2	2:D:378:GLU:HG2	2.06	0.69
1:A:390:ILE:O	2:B:521:THR:CG2	2.40	0.69
1:A:400:GLU:OE1	2:D:465:GLY:HA2	1.89	0.67
1:C:283:ARG:HD3	1:C:284:SER:H	1.60	0.67
2:D:347:LEU:O	2:D:351:LYS:HB2	1.95	0.67
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.60	0.67
1:A:283:ARG:HD3	1:A:284:SER:H	1.60	0.66
1:C:281:ARG:HH11	1:C:281:ARG:HG3	1.60	0.66
2:B:319:HIS:HD2	2:B:373:GLY:HA2	1.59	0.65
2:D:319:HIS:CB	2:D:376:TYR:CD2	2.77	0.65
2:B:323:VAL:H	2:B:403:ALA:HB2	1.61	0.65
2:D:275:GLN:NE2	2:D:280:GLU:HG2	2.12	0.64
1:A:224:ILE:HD12	1:A:233:PHE:HA	1.79	0.64
1:C:356:GLU:HB3	1:C:360:GLU:OE2	1.98	0.64
1:C:224:ILE:HD12	1:C:233:PHE:HA	1.80	0.64
1:A:356:GLU:HB3	1:A:360:GLU:OE2	1.98	0.63
1:A:257:GLU:HB3	1:A:259:LYS:HD3	1.81	0.63
1:C:257:GLU:HB3	1:C:259:LYS:HD3	1.81	0.63
1:C:280:SER:HB2	2:D:505:GLU:CA	2.29	0.63
2:B:490:SER:OG	2:B:524:GLU:OE1	2.12	0.63
2:B:346:LEU:HD11	2:B:455:LEU:HD21	1.78	0.62
2:B:275:GLN:NE2	2:B:280:GLU:HG2	2.15	0.62
1:C:245:HIS:CD2	1:C:247:ASN:H	2.18	0.62
1:A:245:HIS:CD2	1:A:247:ASN:H	2.18	0.62
2:D:319:HIS:NE2	2:D:373:GLY:HA2	2.14	0.62
1:C:314:ASP:HB2	1:C:335:LEU:HD12	1.82	0.61
1:C:279:ARG:CG	2:D:511:TYR:CD2	2.84	0.61
2:D:319:HIS:HD2	2:D:373:GLY:HA2	1.59	0.61
2:D:363:LEU:HD23	2:D:366:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:GLN:HG3	2:B:276:GLY:N	2.06	0.61
1:A:314:ASP:HB2	1:A:335:LEU:HD12	1.82	0.61
2:B:363:LEU:HD23	2:B:366:MET:HE2	1.82	0.61
2:B:275:GLN:CG	2:B:276:GLY:N	2.64	0.60
2:B:275:GLN:CD	2:B:280:GLU:HG2	2.26	0.59
1:C:283:ARG:HH21	2:D:378:GLU:CG	2.12	0.59
1:A:219:VAL:HG22	1:A:252:LEU:HD12	1.85	0.59
1:A:388:PRO:HB3	2:B:518:ASP:OD2	2.03	0.59
1:C:279:ARG:CD	2:D:511:TYR:CD2	2.82	0.59
2:D:319:HIS:CD2	2:D:376:TYR:HB3	2.38	0.59
2:D:323:VAL:N	2:D:403:ALA:HB2	2.16	0.59
2:B:258:ASP:CG	2:B:260:TRP:HB2	2.28	0.58
1:C:219:VAL:HG22	1:C:252:LEU:HD12	1.85	0.58
2:D:402:VAL:O	2:D:403:ALA:HB2	2.03	0.58
2:D:424:PHE:CE1	2:D:426:ILE:HG12	2.37	0.58
2:B:367:ALA:HB2	2:B:455:LEU:HD13	1.85	0.58
2:D:367:ALA:HB2	2:D:455:LEU:HD13	1.85	0.58
1:A:283:ARG:NH2	2:B:378:GLU:OE1	2.37	0.58
1:C:283:ARG:NH2	2:D:378:GLU:OE1	2.37	0.58
1:C:280:SER:CB	2:D:505:GLU:HA	2.34	0.58
1:A:391:PRO:HA	2:B:521:THR:HG23	1.86	0.57
1:A:258:GLU:HA	1:A:258:GLU:OE1	2.03	0.57
1:C:258:GLU:HA	1:C:258:GLU:OE1	2.03	0.57
2:B:402:VAL:O	2:B:403:ALA:HB2	2.03	0.57
2:D:283:MET:HG3	2:D:340:TYR:CZ	2.40	0.57
2:D:323:VAL:HB	2:D:403:ALA:CB	2.35	0.57
1:A:279:ARG:HG2	2:B:511:TYR:CD2	2.40	0.56
1:A:390:ILE:C	2:B:521:THR:CG2	2.79	0.56
2:B:428:TRP:HE1	2:B:454:GLU:CD	2.13	0.56
1:C:249:VAL:HG21	1:C:331:SER:HB3	1.86	0.56
2:D:424:PHE:CD1	2:D:426:ILE:HG12	2.40	0.56
2:B:258:ASP:HB2	2:B:260:TRP:N	2.20	0.56
1:A:390:ILE:C	2:B:521:THR:HG21	2.30	0.56
2:D:350:LEU:HD12	2:D:358:LEU:HD12	1.87	0.56
1:A:249:VAL:HG21	1:A:331:SER:HB3	1.86	0.56
2:B:281:VAL:HG22	2:B:295:LYS:HG3	1.88	0.56
2:D:281:VAL:HG22	2:D:295:LYS:HG3	1.88	0.56
2:D:350:LEU:C	2:D:351:LYS:CA	2.73	0.56
2:B:283:MET:HG3	2:B:340:TYR:CZ	2.40	0.56
2:B:426:ILE:CD1	2:B:434:ALA:HB1	2.36	0.55
2:D:322:LEU:HD12	2:D:402:VAL:CB	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLU:HB3	2:D:465:GLY:HA2	1.89	0.55
2:D:426:ILE:CD1	2:D:434:ALA:HB1	2.36	0.55
2:D:428:TRP:HE1	2:D:454:GLU:CD	2.13	0.55
1:C:279:ARG:CZ	2:D:511:TYR:CE2	2.89	0.55
2:B:319:HIS:HB2	2:B:376:TYR:CE2	2.41	0.55
2:D:347:LEU:O	2:D:351:LYS:HB3	2.05	0.55
1:A:283:ARG:NH2	2:B:378:GLU:CD	2.64	0.55
1:A:390:ILE:O	2:B:521:THR:HG22	2.06	0.55
2:B:322:LEU:HA	2:B:402:VAL:O	2.06	0.54
2:B:275:GLN:OE1	2:B:280:GLU:HG2	2.07	0.54
2:B:367:ALA:HB2	2:B:455:LEU:CD1	2.38	0.54
1:C:283:ARG:NH2	2:D:378:GLU:CG	2.70	0.54
2:B:323:VAL:HB	2:B:403:ALA:HB3	1.89	0.54
1:A:271:LYS:HB2	1:A:322:VAL:HB	1.89	0.54
1:A:434:LEU:C	1:A:434:LEU:HD23	2.33	0.54
1:A:311:VAL:HG11	1:A:363:PHE:CD2	2.43	0.54
1:A:279:ARG:HG2	2:B:511:TYR:HD2	1.72	0.54
2:D:350:LEU:CD1	2:D:358:LEU:CD1	2.86	0.54
1:A:275:VAL:HG23	1:A:317:ALA:C	2.33	0.54
1:C:275:VAL:HG23	1:C:317:ALA:C	2.33	0.54
2:D:319:HIS:CE1	2:D:376:TYR:HB2	2.42	0.54
1:A:354:ALA:HB1	1:A:356:GLU:OE2	2.08	0.53
1:C:434:LEU:HD23	1:C:434:LEU:C	2.33	0.53
2:D:367:ALA:HB2	2:D:455:LEU:CD1	2.38	0.53
1:A:279:ARG:CG	2:B:511:TYR:CD2	2.91	0.53
1:C:271:LYS:HB2	1:C:322:VAL:HB	1.90	0.53
1:C:280:SER:CB	2:D:505:GLU:O	2.56	0.53
1:C:311:VAL:HG11	1:C:363:PHE:CD2	2.43	0.53
1:C:354:ALA:HB1	1:C:356:GLU:OE2	2.08	0.53
2:B:332:GLU:HA	2:B:333:PRO:C	2.34	0.53
1:C:313:ARG:NH2	1:C:337:LYS:HD2	2.24	0.53
2:D:332:GLU:HA	2:D:333:PRO:C	2.34	0.53
2:D:363:LEU:HA	2:D:366:MET:HG3	1.91	0.53
2:B:350:LEU:O	2:B:355:GLY:HA3	2.09	0.52
1:A:393:LYS:HZ2	2:B:526:GLN:HE22	1.40	0.52
2:D:275:GLN:CG	2:D:276:GLY:N	2.62	0.52
1:A:313:ARG:NH2	1:A:337:LYS:HD2	2.24	0.52
2:B:363:LEU:HA	2:B:366:MET:HG3	1.91	0.52
1:A:219:VAL:HG11	1:A:265:VAL:HG13	1.92	0.52
1:C:279:ARG:CG	2:D:511:TYR:CE2	2.90	0.52
1:A:348:LEU:HD13	1:A:363:PHE:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:ARG:O	2:D:376:TYR:CZ	2.63	0.51
1:C:257:GLU:HB3	1:C:259:LYS:CD	2.40	0.51
1:A:257:GLU:HB3	1:A:259:LYS:CD	2.40	0.51
1:A:313:ARG:NH2	1:A:340:SER:OG	2.44	0.51
1:A:394:ASP:O	1:A:397:PRO:HG2	2.10	0.51
2:B:323:VAL:N	2:B:402:VAL:O	2.43	0.51
2:D:264:ARG:NH1	2:D:329:VAL:HG11	2.26	0.51
1:C:313:ARG:NH2	1:C:340:SER:OG	2.44	0.51
1:C:394:ASP:O	1:C:397:PRO:HG2	2.11	0.50
1:C:219:VAL:CG1	1:C:265:VAL:HG13	2.41	0.50
1:C:283:ARG:HD3	1:C:283:ARG:N	2.25	0.50
1:A:279:ARG:NH1	2:B:511:TYR:CZ	2.79	0.50
1:A:283:ARG:HD3	1:A:283:ARG:N	2.25	0.50
1:C:432:SER:OG	1:C:435:GLN:HG3	2.11	0.50
2:D:363:LEU:HD13	2:D:455:LEU:O	2.11	0.50
1:C:348:LEU:HD13	1:C:363:PHE:HE1	1.75	0.50
2:B:363:LEU:HD13	2:B:455:LEU:O	2.11	0.50
1:A:219:VAL:CG1	1:A:265:VAL:HG13	2.42	0.50
1:C:219:VAL:HG11	1:C:265:VAL:HG13	1.92	0.50
2:B:264:ARG:NH1	2:B:329:VAL:HG11	2.26	0.50
1:A:432:SER:OG	1:A:435:GLN:HG3	2.12	0.49
2:B:259:ALA:C	2:B:260:TRP:CA	2.85	0.49
2:D:350:LEU:CB	2:D:351:LYS:N	2.76	0.49
2:D:346:LEU:HD22	2:D:350:LEU:HD22	1.95	0.49
2:B:323:VAL:CG2	2:B:403:ALA:HB3	2.43	0.49
2:B:259:ALA:N	2:B:260:TRP:N	2.60	0.48
2:B:291:ARG:HG2	2:B:340:TYR:CD2	2.48	0.48
1:A:387:TYR:N	1:A:388:PRO:HD3	2.28	0.48
2:B:346:LEU:HD22	2:B:350:LEU:HD22	1.95	0.48
2:D:323:VAL:N	2:D:402:VAL:O	2.46	0.48
2:D:350:LEU:HB3	2:D:351:LYS:N	2.28	0.48
2:D:291:ARG:HG2	2:D:340:TYR:CD2	2.49	0.48
2:D:350:LEU:C	2:D:355:GLY:CA	2.86	0.48
1:C:281:ARG:HG3	1:C:281:ARG:NH1	2.28	0.48
2:D:402:VAL:O	2:D:403:ALA:CB	2.62	0.48
1:C:245:HIS:CD2	1:C:247:ASN:HB2	2.49	0.48
2:D:350:LEU:HD12	2:D:358:LEU:CD1	2.44	0.48
2:B:270:GLU:OE1	2:B:285:THR:OG1	2.32	0.47
2:B:372:SER:HA	2:B:513:GLN:OE1	2.15	0.47
1:A:245:HIS:CD2	1:A:247:ASN:HB2	2.49	0.47
1:C:387:TYR:N	1:C:388:PRO:HD3	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:SER:HA	2:D:513:GLN:OE1	2.15	0.47
1:A:281:ARG:HG3	1:A:281:ARG:NH1	2.28	0.47
1:A:266:THR:HG22	1:A:267:GLU:O	2.15	0.47
2:B:258:ASP:O	2:B:261:GLU:CB	2.63	0.47
2:B:341:MET:HG3	2:B:393:LEU:HB3	1.97	0.47
2:B:402:VAL:O	2:B:403:ALA:CB	2.62	0.46
2:D:270:GLU:OE1	2:D:285:THR:OG1	2.32	0.46
1:C:283:ARG:NH2	2:D:378:GLU:CD	2.74	0.46
2:B:313:VAL:HG23	2:B:314:MET:N	2.31	0.45
1:C:266:THR:HG22	1:C:267:GLU:O	2.15	0.45
1:C:279:ARG:HG2	2:D:511:TYR:HD2	1.74	0.45
1:C:292:LEU:HD21	1:C:444:LYS:HB2	1.98	0.45
2:B:361:PRO:HA	2:B:520:PHE:CE2	2.51	0.45
2:D:313:VAL:HG23	2:D:314:MET:N	2.32	0.45
2:D:361:PRO:HA	2:D:520:PHE:CE2	2.52	0.45
1:A:269:MET:HE1	1:A:329:LYS:HG3	1.98	0.45
1:A:390:ILE:O	2:B:521:THR:HG21	2.15	0.45
2:B:498:CYS:O	2:B:506:ARG:HG2	2.17	0.45
1:A:292:LEU:HD21	1:A:444:LYS:HB2	1.98	0.45
2:D:502:ASP:HA	2:D:503:PRO:HD3	1.87	0.45
1:C:269:MET:HE1	1:C:329:LYS:HG3	1.98	0.44
1:C:279:ARG:NH1	2:D:511:TYR:CZ	2.85	0.44
2:B:505:GLU:O	2:B:506:ARG:C	2.61	0.44
1:A:279:ARG:NH1	2:B:511:TYR:CE2	2.84	0.44
2:D:505:GLU:O	2:D:506:ARG:C	2.61	0.44
2:B:275:GLN:HE22	2:B:280:GLU:HG2	1.80	0.44
2:D:323:VAL:HB	2:D:403:ALA:HB3	2.00	0.44
2:D:498:CYS:O	2:D:506:ARG:HG2	2.17	0.44
1:C:200:THR:HG21	1:C:203:LYS:HG3	2.00	0.44
1:A:412:PRO:HB2	1:A:415:VAL:HG23	1.99	0.43
2:B:366:MET:HB3	2:B:400:CYS:SG	2.58	0.43
2:D:360:LEU:O	2:D:361:PRO:C	2.61	0.43
1:A:393:LYS:NZ	2:B:526:GLN:HE21	2.05	0.43
1:C:279:ARG:CZ	2:D:511:TYR:HE2	2.21	0.43
2:D:322:LEU:CA	2:D:402:VAL:O	2.60	0.43
2:D:323:VAL:HG21	2:D:393:LEU:HD12	2.00	0.43
1:C:412:PRO:HB2	1:C:415:VAL:HG23	1.99	0.43
1:A:200:THR:HG21	1:A:203:LYS:HG3	2.00	0.43
2:B:360:LEU:O	2:B:361:PRO:C	2.61	0.43
1:A:353:THR:HG22	1:A:357:ALA:HB3	2.01	0.43
1:C:280:SER:HB2	2:D:505:GLU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:THR:HG22	1:C:357:ALA:HB3	2.01	0.43
1:A:227:ASP:OD2	1:A:230:ALA:HA	2.19	0.43
1:C:229:THR:O	1:C:230:ALA:HB3	2.19	0.43
1:A:388:PRO:CA	2:B:518:ASP:OD2	2.66	0.43
1:A:443:ILE:HG23	1:A:448:LEU:HB2	2.00	0.43
1:C:443:ILE:HG23	1:C:448:LEU:HB2	2.00	0.43
2:D:347:LEU:O	2:D:351:LYS:N	2.52	0.43
2:D:366:MET:HB3	2:D:400:CYS:SG	2.58	0.43
1:C:426:ASP:OD2	1:C:429:MET:HG2	2.19	0.42
1:C:227:ASP:OD2	1:C:230:ALA:HA	2.19	0.42
1:C:280:SER:HB3	2:D:505:GLU:O	2.19	0.42
1:C:283:ARG:N	1:C:283:ARG:CD	2.83	0.42
1:A:348:LEU:HD13	1:A:363:PHE:CE1	2.55	0.42
2:D:260:TRP:NE1	2:D:315:LYS:HG2	2.34	0.42
2:D:388:ARG:HB3	2:D:428:TRP:CD1	2.54	0.42
2:B:260:TRP:NE1	2:B:315:LYS:HG2	2.34	0.42
2:B:323:VAL:CB	2:B:403:ALA:CB	2.95	0.42
2:B:323:VAL:N	2:B:403:ALA:HB2	2.32	0.42
2:D:322:LEU:CD1	2:D:402:VAL:CG1	2.98	0.42
1:A:283:ARG:HD3	1:A:284:SER:N	2.30	0.42
2:D:461:VAL:HG12	2:D:462:PRO:O	2.20	0.42
2:B:461:VAL:HG12	2:B:462:PRO:O	2.20	0.42
2:B:388:ARG:HB3	2:B:428:TRP:CD1	2.54	0.42
1:C:338:GLU:O	1:C:339:ALA:C	2.63	0.42
1:C:338:GLU:O	1:C:340:SER:N	2.52	0.42
1:A:229:THR:O	1:A:230:ALA:HB3	2.19	0.42
2:B:354:MET:O	2:B:355:GLY:C	2.62	0.41
1:A:245:HIS:HD2	1:A:247:ASN:HB2	1.86	0.41
1:A:407:ALA:HB2	1:A:416:TYR:CG	2.55	0.41
1:A:426:ASP:OD2	1:A:429:MET:HG2	2.19	0.41
1:C:348:LEU:HD13	1:C:363:PHE:CE1	2.55	0.41
1:A:283:ARG:N	1:A:283:ARG:CD	2.82	0.41
1:A:338:GLU:O	1:A:340:SER:N	2.52	0.41
1:C:219:VAL:CG2	1:C:252:LEU:HD12	2.49	0.41
1:C:407:ALA:HB2	1:C:416:TYR:CG	2.55	0.41
2:D:319:HIS:CD2	2:D:376:TYR:CB	3.04	0.41
2:B:267:LEU:HD21	2:B:337:VAL:HG21	2.03	0.41
2:B:278:PHE:HA	2:B:301:THR:HG21	2.03	0.41
2:D:319:HIS:CG	2:D:376:TYR:CD2	3.08	0.41
2:B:350:LEU:HG	2:B:458:LYS:HA	2.00	0.41
2:D:267:LEU:HD21	2:D:337:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:LEU:HD21	2:B:366:MET:HE3	2.03	0.41
1:A:283:ARG:HH22	2:B:378:GLU:HB3	1.85	0.41
1:C:245:HIS:HD2	1:C:247:ASN:HB2	1.86	0.41
2:D:354:MET:O	2:D:355:GLY:C	2.62	0.41
1:A:338:GLU:O	1:A:339:ALA:C	2.63	0.41
2:D:275:GLN:NE2	2:D:280:GLU:OE1	2.54	0.41
2:B:319:HIS:CB	2:B:376:TYR:CD2	2.98	0.41
2:B:519:TYR:CZ	2:B:524:GLU:HG3	2.57	0.41
2:D:278:PHE:HA	2:D:301:THR:HG21	2.03	0.40
2:D:456:THR:HG21	2:D:487:CYS:SG	2.61	0.40
2:D:511:TYR:O	2:D:512:LEU:C	2.64	0.40
1:A:388:PRO:CB	2:B:518:ASP:OD2	2.67	0.40
2:B:348:ASP:O	2:B:352:GLY:N	2.54	0.40
2:D:323:VAL:CG2	2:D:403:ALA:HB3	2.51	0.40
1:A:259:LYS:N	1:A:259:LYS:CD	2.63	0.40
2:B:350:LEU:C	2:B:355:GLY:HA3	2.47	0.40

All (13) 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:401:LYS:O	1:C:438:GLU:CD[3_664]	0.35	1.85
1:A:401:LYS:O	1:C:438:GLU:OE2[3_664]	1.08	1.12
1:A:401:LYS:O	1:C:438:GLU:OE1[3_664]	1.30	0.90
1:A:401:LYS:C	1:C:438:GLU:OE1[3_664]	1.52	0.68
1:A:401:LYS:C	1:C:438:GLU:CD[3_664]	1.54	0.66
1:A:401:LYS:C	1:C:438:GLU:OE2[3_664]	1.70	0.50
1:C:244:ARG:CD	2:D:435:LEU:O[2_655]	1.74	0.46
1:A:401:LYS:O	1:C:438:GLU:CG[3_664]	1.75	0.45
1:A:293:LYS:NZ	2:B:424:PHE:CE1[2_665]	1.86	0.34
1:A:417:GLU:OE2	1:C:428:ALA:CB[3_664]	1.94	0.26
1:C:244:ARG:NH1	2:D:436:TYR:CD1[2_655]	2.00	0.20
1:C:244:ARG:NE	2:D:435:LEU:O[2_655]	2.13	0.07
1:C:244:ARG:NH2	2:D:435:LEU:CD2[2_655]	2.18	0.02

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	253/263 (96%)	237 (94%)	13 (5%)	3 (1%)	10	42
1	C	253/263 (96%)	237 (94%)	13 (5%)	3 (1%)	10	42
2	B	252/277 (91%)	219 (87%)	28 (11%)	5 (2%)	6	33
2	D	242/277 (87%)	209 (86%)	28 (12%)	5 (2%)	5	32
All	All	1000/1080 (93%)	902 (90%)	82 (8%)	16 (2%)	7	37

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ALA
1	A	395	VAL
2	B	403	ALA
1	C	339	ALA
1	C	395	VAL
2	D	403	ALA
2	B	290	THR
2	B	310	GLU
2	D	290	THR
2	D	310	GLU
1	A	282	GLY
1	C	282	GLY
2	B	301	THR
2	D	301	THR
2	B	485	PRO
2	D	485	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/225 (98%)	209 (95%)	11 (5%)	22	45
1	C	220/225 (98%)	209 (95%)	11 (5%)	22	45
2	B	225/239 (94%)	190 (84%)	35 (16%)	2	14
2	D	216/239 (90%)	181 (84%)	35 (16%)	2	13
All	All	881/928 (95%)	789 (90%)	92 (10%)	7	24

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
1	A	219	VAL
1	A	254	VAL
1	A	259	LYS
1	A	266	THR
1	A	283	ARG
1	A	338	GLU
1	A	347	LYS
1	A	356	GLU
1	A	367	SER
1	A	396	VAL
2	B	257	LYS
2	B	264	ARG
2	B	265	GLU
2	B	268	ARG
2	B	277	CYS
2	B	283	MET
2	B	291	ARG
2	B	292	VAL
2	B	298	LYS
2	B	301	THR
2	B	302	MET
2	B	305	GLU
2	B	312	GLN
2	B	314	MET
2	B	316	LYS
2	B	320	GLU
2	B	330	SER
2	B	331	GLU
2	B	332	GLU

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Mol	Chain	Res	Type
2	B	346	LEU
2	B	385	ARG
2	B	397	ASN
2	B	404	ASP
2	B	426	ILE
2	B	429	THR
2	B	438	ARG
2	B	443	SER
2	B	447	SER
2	B	456	THR
2	B	469	ARG
2	B	470	GLU
2	B	491	LEU
2	B	497	GLN
2	B	500	ARG
2	B	517	GLU
1	C	195	LEU
1	C	219	VAL
1	C	254	VAL
1	C	259	LYS
1	C	266	THR
1	C	283	ARG
1	C	338	GLU
1	C	347	LYS
1	C	356	GLU
1	C	367	SER
1	C	396	VAL
2	D	257	LYS
2	D	264	ARG
2	D	265	GLU
2	D	268	ARG
2	D	277	CYS
2	D	283	MET
2	D	291	ARG
2	D	292	VAL
2	D	298	LYS
2	D	301	THR
2	D	302	MET
2	D	305	GLU
2	D	312	GLN
2	D	314	MET
2	D	316	LYS

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Mol	Chain	Res	Type
2	D	320	GLU
2	D	330	SER
2	D	331	GLU
2	D	332	GLU
2	D	346	LEU
2	D	385	ARG
2	D	397	ASN
2	D	404	ASP
2	D	426	ILE
2	D	429	THR
2	D	438	ARG
2	D	443	SER
2	D	447	SER
2	D	456	THR
2	D	469	ARG
2	D	470	GLU
2	D	491	LEU
2	D	497	GLN
2	D	500	ARG
2	D	517	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	245	HIS
1	A	247	ASN
1	A	326	ASN
1	A	442	HIS
2	B	287	ASN
2	B	526	GLN
1	C	226	ASN
1	C	245	HIS
1	C	247	ASN
1	C	326	ASN
1	C	442	HIS
2	D	324	GLN

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	2
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	259:ALA	C	260:TRP	N	2.41
1	B	259:ALA	C	260:TRP	N	2.23
1	D	350:LEU	C	351:LYS	N	1.70

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	257/263 (97%)	0.61	22 (8%) 16 18	143, 178, 256, 262	0
1	C	257/263 (97%)	0.42	12 (4%) 36 30	149, 189, 243, 252	0
2	B	258/277 (93%)	0.30	8 (3%) 51 38	140, 182, 212, 232	0
2	D	248/277 (89%)	0.49	17 (6%) 23 21	143, 198, 221, 229	0
All	All	1020/1080 (94%)	0.46	59 (5%) 29 26	140, 186, 244, 262	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	434	ALA	5.4
1	A	209	VAL	5.0
2	D	424	PHE	4.1
2	B	310	GLU	3.8
2	D	404	ASP	3.7
2	D	310	GLU	3.5
1	C	428	ALA	3.5
1	A	252	LEU	3.4
2	B	424	PHE	3.4
2	B	434	ALA	3.3
2	B	278	PHE	3.2
2	B	404	ASP	3.1
1	C	348	LEU	3.1
1	A	201	ILE	3.1
1	A	237	ALA	3.1
2	D	384	HIS	3.1
1	A	240	MET	3.1
2	D	523	THR	3.0
1	C	224	ILE	3.0
2	D	278	PHE	2.9
2	B	300	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	350	VAL	2.6
1	A	335	LEU	2.6
2	D	269	LEU	2.5
1	A	222	LYS	2.5
1	A	277	TYR	2.5
2	D	267	LEU	2.5
1	C	351	LYS	2.5
2	D	308	LEU	2.4
1	A	234	LEU	2.4
1	A	197	LEU	2.4
2	B	384	HIS	2.4
1	A	202	GLY	2.3
1	C	353	THR	2.3
1	C	209	VAL	2.3
1	C	347	LYS	2.3
2	D	425	PRO	2.3
1	A	210	MET	2.3
1	C	362	LYS	2.3
1	A	308	ASN	2.3
1	A	200	THR	2.2
1	A	262	LEU	2.2
2	B	366	MET	2.2
2	D	435	LEU	2.2
1	A	214	TYR	2.2
2	D	431	PRO	2.2
2	D	298	LYS	2.2
1	A	221	VAL	2.2
1	A	362	LYS	2.2
1	C	223	CYS	2.2
1	C	450	LEU	2.2
2	D	468	ASN	2.1
1	C	429	MET	2.1
2	D	300	GLY	2.1
1	C	222	LYS	2.0
1	A	235	ALA	2.0
2	D	277	CYS	2.0
1	A	351	LYS	2.0
1	A	401	LYS	2.0

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

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.