



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:50 AM UTC

PDB ID : 3P5C / pdb_00003p5c
Title : The structure of the LDLR/PCSK9 complex reveals the receptor in an extended conformation
Authors : Lo Surdo, P.; Bottomley, M.J.; Calzetta, A.; Settembre, E.C.; Cirillo, A.; Pandit, S.; Ni, Y.; Hubbard, B.; Sitlani, A.; Carfi, A.
Deposited on : 2010-10-08
Resolution : 4.20 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

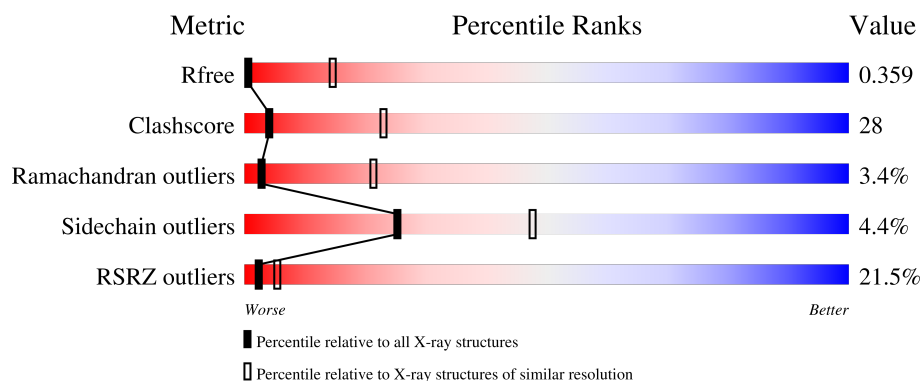
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	P	92	16% 88% 10% .
2	A	540	18% 72% 16% .. 8%
3	L	440	25% 63% 25% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7844 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	92	Total	C	N	O	S	0	0	0
			740	474	133	131	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	496	Total	C	N	O	S	0	0	0
			3659	2255	674	698	32			

- Molecule 3 is a protein called Low density lipoprotein receptor variant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	440	Total	C	N	O	S	0	0	0
			3441	2143	601	665	32			

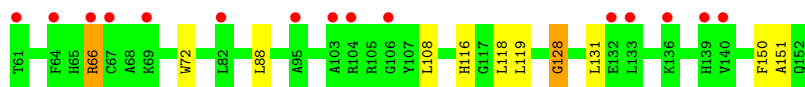
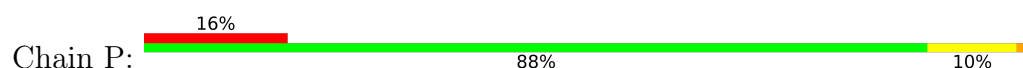
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	L	3	Total	Ca	0	0
			3	3		

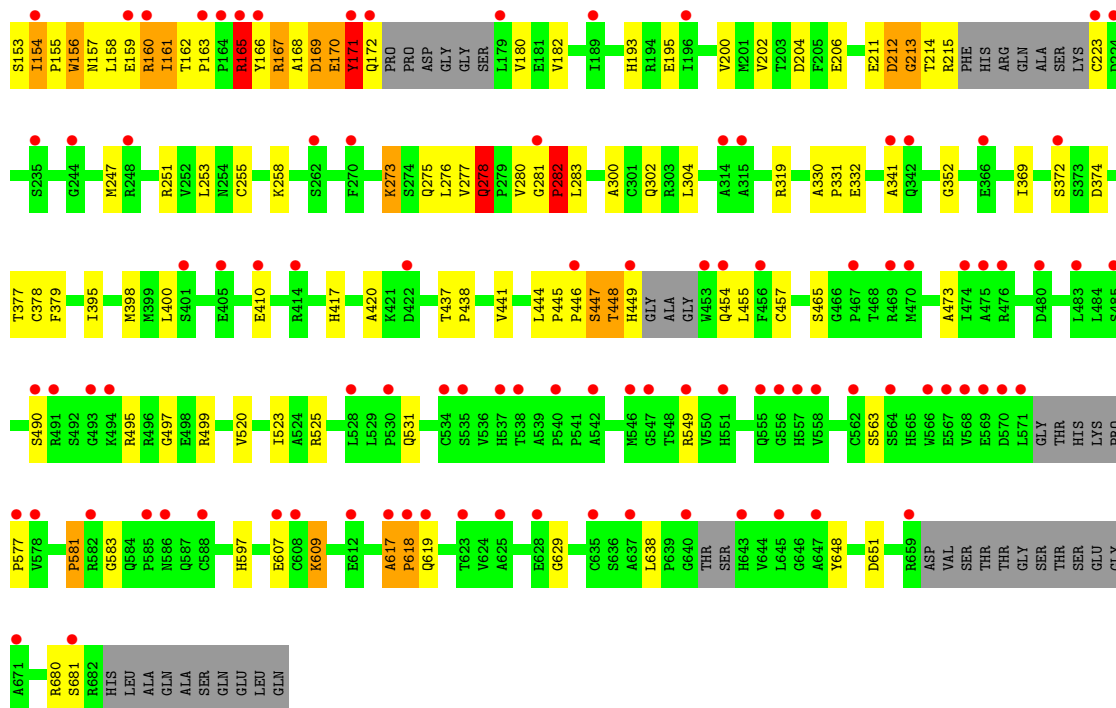
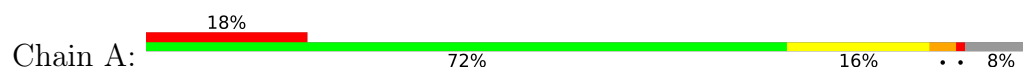
3 Residue-property plots

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: Proprotein convertase subtilisin/kexin type 9

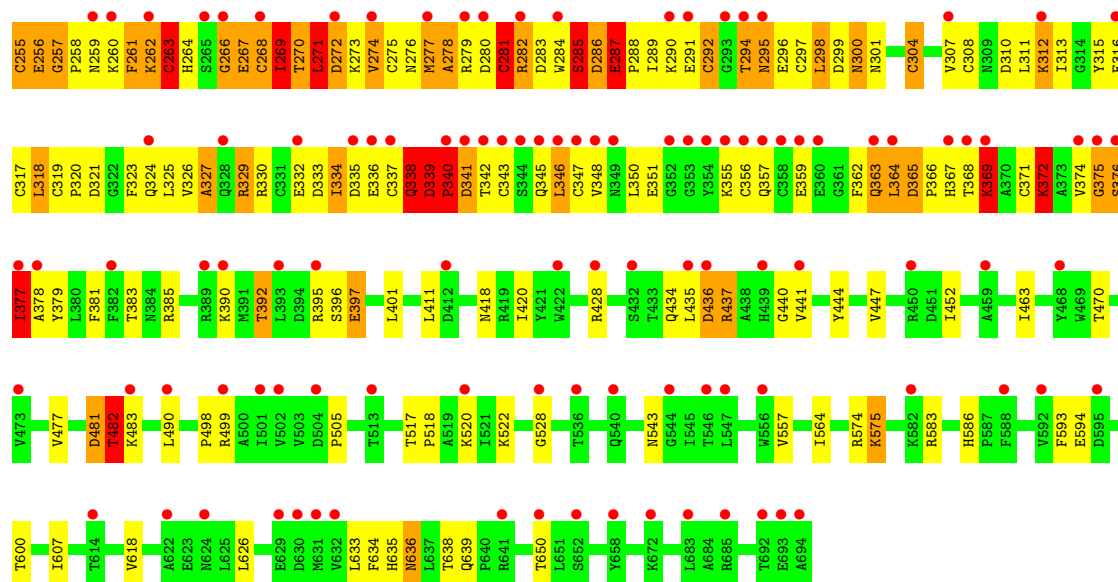


- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- Molecule 3: Low density lipoprotein receptor variant





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	320.89Å 320.89Å 77.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.20 30.00 – 4.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-4.20) 98.2 (30.00-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 4.13Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.325 , 0.348 0.331 , 0.359	Depositor DCC
R_{free} test set	1660 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	144.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 115.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.116 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	7844	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	P	0.46	0/757	0.76	1/1023 (0.1%)
2	A	0.55	6/3724 (0.2%)	0.86	20/5059 (0.4%)
3	L	0.74	12/3514 (0.3%)	1.14	39/4771 (0.8%)
All	All	0.63	18/7995 (0.2%)	0.99	60/10853 (0.6%)

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
3	L	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	257	GLY	C-O	10.92	1.38	1.24
3	L	376	SER	CA-C	9.65	1.63	1.53
2	A	171	TYR	N-CA	8.65	1.57	1.46
3	L	287	GLU	CA-C	8.15	1.63	1.52
3	L	287	GLU	C-N	-7.21	1.26	1.34
2	A	170	GLU	C-N	6.61	1.43	1.33
3	L	377	ILE	N-CA	6.53	1.54	1.46
3	L	287	GLU	N-CA	6.50	1.55	1.46
3	L	440	GLY	C-O	5.92	1.31	1.24
3	L	257	GLY	N-CA	5.50	1.52	1.44
2	A	171	TYR	C-N	5.47	1.41	1.33
3	L	482	THR	N-CA	-5.25	1.39	1.46
2	A	169	ASP	CA-C	5.22	1.59	1.52
2	A	278	GLN	N-CA	5.20	1.53	1.46
3	L	286	ASP	C-N	5.11	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	481	ASP	C-N	-5.11	1.26	1.33
3	L	258	PRO	N-CD	5.09	1.54	1.47
2	A	171	TYR	CA-C	5.01	1.59	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	287	GLU	CA-C-N	14.39	134.83	119.87
3	L	287	GLU	C-N-CA	14.39	134.83	119.87
3	L	272	ASP	N-CA-C	-12.55	94.79	111.74
3	L	257	GLY	O-C-N	-11.29	110.48	121.77
2	A	282	PRO	CA-N-CD	-11.18	96.34	112.00
3	L	436	ASP	CA-C-N	10.98	143.62	122.53
3	L	436	ASP	C-N-CA	10.98	143.62	122.53
3	L	257	GLY	CA-C-N	9.46	129.21	119.19
3	L	257	GLY	C-N-CA	9.46	129.21	119.19
2	A	214	THR	N-CA-C	-8.93	102.92	112.93
3	L	295	ASN	N-CA-C	-8.28	96.84	110.17
3	L	274	VAL	N-CA-C	7.98	125.94	109.34
3	L	270	THR	N-CA-C	7.98	120.27	108.14
3	L	341	ASP	N-CA-C	-7.94	103.70	113.15
3	L	376	SER	N-CA-C	7.76	120.65	109.71
3	L	281	CYS	N-CA-C	-7.76	94.28	110.80
3	L	436	ASP	CA-CB-CG	-7.52	105.08	112.60
3	L	285	SER	N-CA-C	-7.25	100.65	111.81
3	L	256	GLU	N-CA-C	6.99	121.98	113.17
3	L	263	CYS	N-CA-C	-6.96	95.97	110.80
3	L	339	ASP	N-CA-C	6.94	125.15	109.81
2	A	276	LEU	N-CA-C	-6.89	104.99	113.19
3	L	268	CYS	N-CA-C	-6.83	97.38	108.52
3	L	294	THR	CA-C-N	-6.59	111.43	122.64
3	L	294	THR	C-N-CA	-6.59	111.43	122.64
2	A	581	PRO	N-CA-CB	6.55	110.13	103.25
2	A	170	GLU	CA-C-N	6.44	133.84	121.54
2	A	170	GLU	C-N-CA	6.44	133.84	121.54
3	L	286	ASP	N-CA-C	-6.33	95.42	108.53
2	A	447	SER	N-CA-C	6.29	117.32	108.00
2	A	213	GLY	N-CA-C	6.28	121.55	110.80
3	L	287	GLU	N-CA-C	6.27	123.66	109.81
2	A	165	ARG	CA-C-N	-6.15	114.51	123.00
2	A	165	ARG	C-N-CA	-6.15	114.51	123.00
2	A	170	GLU	N-CA-C	6.11	120.19	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	267	GLU	N-CA-C	6.11	116.14	108.45
3	L	375	GLY	O-C-N	-5.99	114.92	122.70
2	A	281	GLY	CA-C-N	5.99	127.32	119.84
2	A	281	GLY	C-N-CA	5.99	127.32	119.84
3	L	261	PHE	N-CA-C	5.93	118.89	108.75
3	L	255	CYS	CA-C-N	-5.92	112.78	122.54
3	L	255	CYS	C-N-CA	-5.92	112.78	122.54
3	L	312	LYS	N-CA-C	-5.90	106.42	113.97
3	L	271	LEU	N-CA-C	-5.89	98.26	110.80
2	A	577	PRO	N-CA-CB	5.80	109.38	103.00
3	L	350	LEU	N-CA-C	5.57	116.87	108.46
3	L	397	GLU	N-CA-C	5.50	118.92	111.17
3	L	437	ARG	N-CA-C	-5.40	106.37	113.12
2	A	447	SER	CB-CA-C	-5.32	108.89	116.34
3	L	392	THR	N-CA-C	5.32	118.61	110.36
3	L	278	ALA	N-CA-C	5.30	116.46	108.46
2	A	171	TYR	N-CA-C	5.29	122.07	110.80
3	L	295	ASN	N-CA-CB	5.22	119.14	110.63
3	L	269	ILE	N-CA-C	5.20	115.21	108.35
2	A	211	GLU	CA-C-N	-5.17	115.86	122.79
2	A	211	GLU	C-N-CA	-5.17	115.86	122.79
1	P	128	GLY	N-CA-C	5.16	118.74	112.49
2	A	213	GLY	CA-C-N	5.16	131.22	122.65
2	A	213	GLY	C-N-CA	5.16	131.22	122.65
3	L	338	GLN	N-CA-C	5.15	115.81	107.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	257	GLY	Mainchain
3	L	375	GLY	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	P	740	0	750	11	0
2	A	3659	0	3537	113	19
3	L	3441	0	3321	311	20
4	A	1	0	0	0	0
4	L	3	0	0	0	0
All	All	7844	0	7608	425	20

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 28.

All (425) 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)
3:L:274:VAL:CG2	3:L:312:LYS:HD3	1.25	1.67
2:A:166:TYR:CE2	2:A:168:ALA:HB2	1.27	1.62
2:A:166:TYR:HE2	2:A:168:ALA:CB	1.17	1.54
3:L:274:VAL:HG11	3:L:312:LYS:CG	1.32	1.50
3:L:374:VAL:HG11	3:L:418:ASN:CB	1.43	1.48
3:L:274:VAL:HG21	3:L:312:LYS:CD	1.45	1.47
2:A:159:GLU:O	2:A:162:THR:CG2	1.71	1.36
3:L:274:VAL:CG1	3:L:312:LYS:HG3	1.56	1.35
3:L:374:VAL:CG1	3:L:418:ASN:CG	2.01	1.33
3:L:255:CYS:SG	3:L:268:CYS:SG	1.46	1.30
3:L:274:VAL:CG1	3:L:312:LYS:CG	2.08	1.28
3:L:436:ASP:O	3:L:441:VAL:HG22	1.34	1.26
3:L:275:CYS:HA	3:L:287:GLU:CG	1.67	1.24
3:L:274:VAL:CB	3:L:312:LYS:HD3	1.68	1.24
3:L:374:VAL:CG1	3:L:418:ASN:CB	2.16	1.24
3:L:374:VAL:CG1	3:L:418:ASN:HB2	1.67	1.23
3:L:275:CYS:SG	3:L:292:CYS:SG	1.43	1.23
3:L:274:VAL:HG11	3:L:312:LYS:CD	1.68	1.22
2:A:159:GLU:O	2:A:162:THR:HG22	1.02	1.18
3:L:436:ASP:O	3:L:441:VAL:CG2	1.92	1.18
2:A:447:SER:OG	2:A:449:HIS:HD2	1.23	1.17
3:L:299:ASP:O	3:L:300:ASN:ND2	1.78	1.16
2:A:447:SER:OG	2:A:449:HIS:CD2	2.01	1.14
3:L:274:VAL:HB	3:L:312:LYS:CB	1.78	1.12
3:L:294:THR:HG22	3:L:295:ASN:O	1.48	1.12
3:L:339:ASP:HB3	3:L:340:PRO:CD	1.76	1.10
3:L:286:ASP:C	3:L:287:GLU:HG3	1.77	1.09
3:L:332:GLU:O	3:L:332:GLU:HG3	1.38	1.09
3:L:326:VAL:HG21	3:L:332:GLU:HB3	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:170:GLU:HG3	2:A:171:TYR:H	0.93	1.08
3:L:274:VAL:CB	3:L:312:LYS:HB3	1.83	1.08
3:L:275:CYS:HA	3:L:287:GLU:HG2	1.08	1.08
2:A:170:GLU:HG3	2:A:171:TYR:N	1.68	1.07
3:L:363:GLN:HG3	3:L:436:ASP:OD2	1.54	1.07
3:L:339:ASP:HB3	3:L:340:PRO:HD2	1.19	1.06
3:L:377:ILE:HD12	3:L:379:TYR:HE2	1.18	1.04
2:A:166:TYR:CE2	2:A:168:ALA:CA	2.41	1.04
2:A:166:TYR:CE2	2:A:168:ALA:CB	2.05	1.03
2:A:448:THR:HG22	2:A:448:THR:O	1.55	1.03
3:L:342:THR:HG22	3:L:343:CYS:H	1.21	1.03
3:L:374:VAL:HG11	3:L:418:ASN:HB2	1.04	1.03
3:L:376:SER:O	3:L:377:ILE:HG23	1.57	1.03
3:L:275:CYS:SG	3:L:292:CYS:CB	2.47	1.03
3:L:270:THR:HG22	3:L:272:ASP:H	1.25	1.02
3:L:377:ILE:HD12	3:L:379:TYR:CE2	1.92	1.02
3:L:270:THR:CG2	3:L:272:ASP:H	1.72	1.01
3:L:275:CYS:CA	3:L:287:GLU:HG2	1.91	1.01
3:L:339:ASP:HA	3:L:342:THR:HB	1.42	1.01
3:L:339:ASP:CB	3:L:340:PRO:HD2	1.88	1.00
3:L:304:CYS:HA	3:L:329:ARG:HG3	1.47	0.97
3:L:264:HIS:HB3	3:L:285:SER:HB3	1.46	0.96
3:L:363:GLN:CG	3:L:436:ASP:OD2	2.13	0.96
3:L:274:VAL:CG1	3:L:312:LYS:CD	2.35	0.95
2:A:180:VAL:HG22	2:A:282:PRO:HG2	1.48	0.95
3:L:379:TYR:CE1	3:L:392:THR:HG22	2.01	0.95
3:L:274:VAL:CB	3:L:312:LYS:CD	2.45	0.95
3:L:294:THR:HG22	3:L:295:ASN:C	1.91	0.94
3:L:376:SER:O	3:L:377:ILE:CG2	2.17	0.93
2:A:223:CYS:CB	2:A:255:CYS:SG	2.56	0.93
3:L:263:CYS:SG	3:L:266:GLY:HA3	2.09	0.93
3:L:274:VAL:HB	3:L:312:LYS:HB3	0.93	0.91
3:L:294:THR:CG2	3:L:295:ASN:O	2.18	0.91
3:L:374:VAL:HG13	3:L:418:ASN:CG	1.96	0.91
3:L:311:LEU:HD21	3:L:316:GLU:HG2	1.51	0.90
3:L:374:VAL:HG11	3:L:418:ASN:CG	1.79	0.90
2:A:455:LEU:H	2:A:680:ARG:NH2	1.72	0.88
2:A:170:GLU:CG	2:A:171:TYR:H	1.85	0.87
3:L:342:THR:HG22	3:L:343:CYS:N	1.90	0.87
3:L:378:ALA:O	3:L:379:TYR:CD2	2.27	0.87
3:L:255:CYS:SG	3:L:268:CYS:CB	2.62	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:269:ILE:HD13	3:L:280:ASP:O	1.75	0.86
2:A:166:TYR:CD2	2:A:168:ALA:HB2	2.09	0.86
3:L:274:VAL:CB	3:L:312:LYS:CB	2.50	0.86
3:L:481:ASP:O	3:L:482:THR:C	2.19	0.85
3:L:274:VAL:HG11	3:L:312:LYS:HG3	0.85	0.85
3:L:263:CYS:HB3	3:L:267:GLU:H	1.40	0.85
3:L:365:ASP:HB2	3:L:372:LYS:HD3	1.56	0.84
2:A:171:TYR:HE2	2:A:398:MET:HE2	1.40	0.84
3:L:374:VAL:HG13	3:L:418:ASN:ND2	1.92	0.84
3:L:374:VAL:HG12	3:L:418:ASN:CG	2.00	0.84
3:L:283:ASP:C	3:L:285:SER:H	1.86	0.83
3:L:300:ASN:ND2	3:L:300:ASN:O	2.11	0.83
3:L:311:LEU:HD23	3:L:315:TYR:HA	1.58	0.83
3:L:326:VAL:CG2	3:L:332:GLU:HB3	2.08	0.83
3:L:261:PHE:HD2	3:L:263:CYS:CA	1.92	0.83
2:A:159:GLU:O	2:A:162:THR:HG21	1.79	0.82
3:L:374:VAL:CG1	3:L:418:ASN:ND2	2.42	0.82
3:L:274:VAL:CG1	3:L:312:LYS:CB	2.58	0.82
2:A:161:ILE:HG13	2:A:161:ILE:O	1.77	0.81
3:L:338:GLN:OE1	3:L:338:GLN:HA	1.81	0.81
3:L:300:ASN:C	3:L:300:ASN:HD22	1.83	0.81
3:L:270:THR:HG22	3:L:271:LEU:N	1.96	0.81
2:A:171:TYR:HE2	2:A:398:MET:CE	1.92	0.81
3:L:262:LYS:O	3:L:264:HIS:N	2.15	0.80
3:L:261:PHE:CD2	3:L:263:CYS:CA	2.65	0.80
3:L:263:CYS:CB	3:L:267:GLU:H	1.93	0.80
2:A:455:LEU:H	2:A:680:ARG:HH22	1.30	0.80
3:L:261:PHE:HE2	3:L:264:HIS:H	1.29	0.80
3:L:280:ASP:N	3:L:286:ASP:OD2	2.13	0.80
3:L:332:GLU:O	3:L:332:GLU:CG	2.28	0.80
3:L:263:CYS:HB3	3:L:267:GLU:O	1.83	0.79
3:L:365:ASP:CB	3:L:372:LYS:HD3	2.12	0.78
2:A:180:VAL:HG22	2:A:282:PRO:CG	2.12	0.78
3:L:261:PHE:CD2	3:L:263:CYS:N	2.50	0.78
2:A:447:SER:HG	2:A:449:HIS:CD2	1.99	0.78
2:A:212:ASP:OD1	2:A:212:ASP:N	2.15	0.78
3:L:261:PHE:HD2	3:L:263:CYS:N	1.82	0.78
3:L:261:PHE:CD2	3:L:263:CYS:HA	2.17	0.78
3:L:329:ARG:HA	3:L:329:ARG:NE	1.97	0.78
2:A:180:VAL:CG2	2:A:282:PRO:HG2	2.14	0.78
2:A:280:VAL:HG23	2:A:282:PRO:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:264:HIS:HB3	3:L:285:SER:CB	2.12	0.78
3:L:378:ALA:HA	3:L:634:PHE:O	1.84	0.78
3:L:274:VAL:HG21	3:L:312:LYS:CE	2.14	0.77
3:L:274:VAL:CG1	3:L:312:LYS:HD3	2.07	0.77
2:A:282:PRO:O	2:A:282:PRO:HD2	1.85	0.76
2:A:680:ARG:HE	2:A:681:SER:H	1.33	0.76
3:L:481:ASP:O	3:L:483:LYS:N	2.18	0.76
3:L:255:CYS:CB	3:L:268:CYS:SG	2.74	0.76
2:A:153:SER:C	2:A:155:PRO:HD3	2.11	0.75
3:L:334:ILE:N	3:L:334:ILE:HD12	2.02	0.75
3:L:481:ASP:O	3:L:481:ASP:OD1	2.05	0.75
2:A:156:TRP:CZ3	2:A:341:ALA:HA	2.21	0.75
3:L:482:THR:HG23	3:L:483:LYS:N	2.01	0.75
3:L:342:THR:CG2	3:L:343:CYS:H	1.97	0.74
3:L:274:VAL:CB	3:L:312:LYS:CG	2.64	0.74
3:L:381:PHE:CE2	3:L:401:LEU:HD22	2.22	0.74
3:L:319:CYS:HB3	3:L:323:PHE:HB2	1.70	0.73
3:L:379:TYR:HE1	3:L:392:THR:HG22	1.54	0.73
3:L:371:CYS:O	3:L:372:LYS:O	2.05	0.73
2:A:171:TYR:CE2	2:A:398:MET:HE2	2.23	0.73
2:A:448:THR:O	2:A:448:THR:CG2	2.29	0.73
2:A:618:PRO:HB2	2:A:619:GLN:HA	1.70	0.73
3:L:270:THR:HG22	3:L:272:ASP:N	2.04	0.73
2:A:213:GLY:C	2:A:215:ARG:H	1.95	0.72
3:L:281:CYS:C	3:L:283:ASP:H	1.96	0.72
3:L:359:GLU:HB2	3:L:362:PHE:HD2	1.53	0.72
3:L:381:PHE:CD2	3:L:401:LEU:HD22	2.25	0.72
3:L:274:VAL:HG21	3:L:312:LYS:HD3	0.72	0.72
3:L:274:VAL:HG12	3:L:312:LYS:HG3	1.70	0.72
3:L:270:THR:CG2	3:L:271:LEU:H	2.03	0.72
3:L:334:ILE:HD12	3:L:334:ILE:H	1.54	0.72
3:L:263:CYS:SG	3:L:267:GLU:N	2.63	0.71
3:L:369:LYS:HG3	3:L:369:LYS:O	1.90	0.71
3:L:376:SER:C	3:L:377:ILE:HG23	2.15	0.71
2:A:275:GLN:C	2:A:277:VAL:H	1.96	0.71
2:A:165:ARG:O	2:A:165:ARG:HG2	1.91	0.70
3:L:269:ILE:O	3:L:270:THR:OG1	2.10	0.69
3:L:270:THR:HG22	3:L:271:LEU:H	1.58	0.69
3:L:262:LYS:O	3:L:263:CYS:C	2.35	0.69
3:L:378:ALA:O	3:L:379:TYR:CG	2.46	0.69
2:A:609:LYS:HE3	2:A:609:LYS:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:273:LYS:HE2	2:A:273:LYS:HA	1.75	0.69
2:A:166:TYR:CE2	2:A:168:ALA:HA	2.26	0.69
3:L:273:LYS:HG2	3:L:273:LYS:O	1.93	0.68
3:L:575:LYS:NZ	3:L:575:LYS:HA	2.08	0.68
3:L:348:VAL:HG13	3:L:355:LYS:HB3	1.75	0.68
2:A:163:PRO:HD3	2:A:444:LEU:HB2	1.76	0.68
3:L:301:ASN:HB3	3:L:304:CYS:HB2	1.74	0.68
3:L:482:THR:CG2	3:L:483:LYS:N	2.57	0.68
3:L:447:VAL:HG13	3:L:482:THR:O	1.93	0.68
3:L:270:THR:CG2	3:L:271:LEU:N	2.56	0.68
2:A:374:ASP:OD2	3:L:307:VAL:HG21	1.93	0.67
3:L:363:GLN:NE2	3:L:436:ASP:CB	2.57	0.67
3:L:374:VAL:HG12	3:L:418:ASN:CB	2.20	0.67
3:L:339:ASP:CA	3:L:342:THR:HB	2.23	0.67
3:L:326:VAL:CG1	3:L:330:ARG:HH21	2.08	0.67
3:L:593:PHE:CD1	3:L:633:LEU:HD21	2.30	0.67
2:A:618:PRO:HB2	2:A:619:GLN:CA	2.24	0.67
3:L:270:THR:HG23	3:L:272:ASP:H	1.59	0.67
3:L:313:ILE:HG13	3:L:313:ILE:O	1.93	0.66
2:A:629:GLY:O	2:A:680:ARG:HD2	1.94	0.66
3:L:326:VAL:HG12	3:L:330:ARG:HH21	1.61	0.66
3:L:339:ASP:O	3:L:341:ASP:N	2.28	0.66
3:L:274:VAL:CG2	3:L:312:LYS:CD	2.20	0.66
2:A:454:GLN:HG3	2:A:680:ARG:HH12	1.61	0.66
3:L:575:LYS:HA	3:L:575:LYS:HZ3	1.62	0.65
3:L:329:ARG:HA	3:L:329:ARG:HE	1.58	0.65
3:L:294:THR:HG22	3:L:295:ASN:N	2.11	0.65
3:L:418:ASN:OD1	3:L:435:LEU:HD23	1.96	0.65
2:A:282:PRO:HB2	2:A:400:LEU:HD13	1.78	0.64
3:L:441:VAL:O	3:L:441:VAL:HG23	1.96	0.64
3:L:463:ILE:HD12	3:L:505:PRO:HB2	1.78	0.64
3:L:269:ILE:O	3:L:269:ILE:HG13	1.95	0.64
3:L:324:GLN:HB3	3:L:332:GLU:CD	2.22	0.64
3:L:364:LEU:HD23	3:L:364:LEU:H	1.62	0.64
3:L:271:LEU:HB2	3:L:273:LYS:HB2	1.79	0.64
3:L:304:CYS:HA	3:L:329:ARG:CG	2.26	0.64
2:A:618:PRO:CB	2:A:619:GLN:HA	2.28	0.63
3:L:263:CYS:HB3	3:L:267:GLU:N	2.13	0.63
3:L:286:ASP:O	3:L:287:GLU:HG3	1.98	0.63
3:L:365:ASP:HB2	3:L:372:LYS:HZ3	1.62	0.63
3:L:401:LEU:HD11	3:L:435:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:275:CYS:HA	3:L:287:GLU:CD	2.22	0.63
2:A:275:GLN:C	2:A:277:VAL:N	2.57	0.62
3:L:272:ASP:OD1	3:L:312:LYS:HD2	1.99	0.62
3:L:289:ILE:HG22	3:L:289:ILE:O	2.00	0.62
2:A:166:TYR:HE2	2:A:168:ALA:HB2	0.48	0.62
3:L:363:GLN:NE2	3:L:436:ASP:HB2	2.14	0.62
3:L:324:GLN:HB3	3:L:332:GLU:CG	2.30	0.61
2:A:680:ARG:HE	2:A:681:SER:N	1.97	0.61
3:L:297:CYS:C	3:L:299:ASP:H	2.08	0.61
3:L:261:PHE:CD2	3:L:262:LYS:C	2.78	0.61
3:L:317:CYS:HB3	3:L:329:ARG:NE	2.15	0.61
2:A:166:TYR:CE2	2:A:168:ALA:N	2.67	0.61
3:L:276:ASN:O	3:L:277:MET:C	2.42	0.61
3:L:359:GLU:HB2	3:L:362:PHE:CD2	2.34	0.61
3:L:365:ASP:HB2	3:L:372:LYS:CD	2.31	0.61
3:L:436:ASP:O	3:L:441:VAL:HG21	1.95	0.61
3:L:317:CYS:SG	3:L:329:ARG:HG2	2.42	0.60
1:P:66:ARG:HH11	1:P:66:ARG:HG2	1.65	0.60
2:A:523:ILE:HD13	2:A:648:TYR:HB3	1.83	0.60
3:L:326:VAL:HG11	3:L:330:ARG:NH2	2.16	0.60
3:L:327:ALA:C	3:L:329:ARG:H	2.09	0.60
2:A:277:VAL:O	2:A:278:GLN:HG3	2.02	0.59
3:L:374:VAL:HG12	3:L:418:ASN:HB2	1.74	0.59
3:L:317:CYS:C	3:L:318:LEU:HD23	2.28	0.59
2:A:162:THR:O	2:A:162:THR:HG23	2.02	0.59
2:A:280:VAL:CG2	2:A:282:PRO:O	2.49	0.59
2:A:167:ARG:HH11	2:A:167:ARG:HB3	1.68	0.59
3:L:274:VAL:O	3:L:274:VAL:HG23	2.02	0.59
3:L:348:VAL:CG1	3:L:355:LYS:HB3	2.32	0.59
3:L:275:CYS:HA	3:L:287:GLU:CB	2.32	0.59
3:L:326:VAL:O	3:L:327:ALA:HB3	2.02	0.59
3:L:593:PHE:HB2	3:L:633:LEU:CD2	2.32	0.59
3:L:281:CYS:C	3:L:283:ASP:N	2.61	0.59
3:L:278:ALA:O	3:L:286:ASP:OD2	2.20	0.59
3:L:351:GLU:H	3:L:351:GLU:CD	2.10	0.59
2:A:154:ILE:HG12	2:A:154:ILE:O	2.03	0.58
2:A:377:THR:HB	3:L:310:ASP:HB3	1.83	0.58
2:A:166:TYR:CD2	2:A:168:ALA:N	2.70	0.58
3:L:325:LEU:CD1	3:L:329:ARG:HH11	2.17	0.58
3:L:260:LYS:HA	3:L:270:THR:OG1	2.03	0.58
3:L:275:CYS:SG	3:L:292:CYS:HB2	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:364:LEU:HD23	3:L:364:LEU:N	2.18	0.58
3:L:283:ASP:C	3:L:285:SER:N	2.55	0.58
3:L:324:GLN:HB3	3:L:332:GLU:HG2	1.86	0.57
2:A:165:ARG:O	2:A:165:ARG:CG	2.51	0.57
3:L:289:ILE:HA	3:L:292:CYS:HB3	1.86	0.57
3:L:294:THR:CG2	3:L:295:ASN:N	2.68	0.57
2:A:457:CYS:HB3	2:A:525:ARG:HE	1.70	0.57
3:L:261:PHE:CE2	3:L:263:CYS:HA	2.39	0.57
3:L:418:ASN:ND2	3:L:435:LEU:HB3	2.20	0.57
3:L:329:ARG:HD3	3:L:330:ARG:H	1.70	0.56
2:A:420:ALA:HB3	2:A:441:VAL:HB	1.87	0.56
3:L:281:CYS:O	3:L:283:ASP:N	2.35	0.56
3:L:261:PHE:HE2	3:L:264:HIS:N	2.02	0.56
3:L:318:LEU:HD23	3:L:318:LEU:N	2.19	0.56
3:L:334:ILE:H	3:L:334:ILE:CD1	2.19	0.56
3:L:339:ASP:CB	3:L:340:PRO:CD	2.59	0.56
3:L:320:PRO:HD2	3:L:323:PHE:CD2	2.41	0.56
3:L:261:PHE:HD2	3:L:263:CYS:HA	1.61	0.55
3:L:291:GLU:O	3:L:292:CYS:C	2.49	0.55
3:L:366:PRO:HG3	3:L:397:GLU:OE2	2.06	0.55
3:L:348:VAL:HG12	3:L:355:LYS:O	2.07	0.55
3:L:557:VAL:HG12	3:L:564:ILE:HG12	1.87	0.54
3:L:329:ARG:O	3:L:330:ARG:HB3	2.07	0.54
2:A:454:GLN:CG	2:A:680:ARG:HH12	2.20	0.54
3:L:418:ASN:CG	3:L:435:LEU:HB3	2.34	0.53
3:L:286:ASP:C	3:L:287:GLU:CG	2.65	0.53
3:L:317:CYS:HB3	3:L:329:ARG:CZ	2.38	0.53
3:L:355:LYS:HD3	3:L:356:CYS:N	2.23	0.53
3:L:297:CYS:O	3:L:299:ASP:N	2.41	0.53
3:L:276:ASN:O	3:L:276:ASN:OD1	2.27	0.53
3:L:396:SER:OG	3:L:397:GLU:N	2.40	0.53
3:L:326:VAL:CG1	3:L:330:ARG:NH2	2.69	0.53
2:A:454:GLN:HG2	2:A:680:ARG:HH22	1.73	0.53
3:L:263:CYS:HB3	3:L:267:GLU:C	2.33	0.53
3:L:290:LYS:O	3:L:291:GLU:HB2	2.07	0.53
2:A:182:VAL:HB	2:A:247:MET:HG2	1.91	0.53
2:A:171:TYR:CE2	2:A:398:MET:CE	2.84	0.52
1:P:108:LEU:HD11	3:L:626:LEU:HD21	1.92	0.52
3:L:263:CYS:SG	3:L:266:GLY:CA	2.93	0.52
3:L:284:TRP:C	3:L:286:ASP:H	2.13	0.52
3:L:428:ARG:HD2	3:L:452:ILE:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:364:LEU:C	3:L:372:LYS:HZ1	2.17	0.52
3:L:317:CYS:CB	3:L:329:ARG:NE	2.72	0.52
3:L:378:ALA:C	3:L:379:TYR:CD2	2.88	0.52
3:L:574:ARG:O	3:L:575:LYS:HE2	2.09	0.52
3:L:355:LYS:HD3	3:L:355:LYS:C	2.35	0.52
3:L:376:SER:O	3:L:377:ILE:HG22	2.07	0.52
3:L:593:PHE:HB2	3:L:633:LEU:HD21	1.91	0.52
3:L:269:ILE:CD1	3:L:280:ASP:O	2.52	0.52
3:L:346:LEU:HD23	3:L:357:GLN:C	2.35	0.52
3:L:365:ASP:CB	3:L:372:LYS:HZ3	2.23	0.51
1:P:88:LEU:HD13	1:P:116:HIS:HB3	1.91	0.51
3:L:359:GLU:CD	3:L:359:GLU:H	2.17	0.51
3:L:600:THR:HG22	3:L:607:ILE:HG12	1.92	0.51
2:A:277:VAL:O	2:A:278:GLN:CG	2.58	0.51
2:A:499:ARG:HG2	2:A:597:HIS:CE1	2.45	0.51
3:L:340:PRO:C	3:L:342:THR:H	2.18	0.51
3:L:374:VAL:HG11	3:L:418:ASN:ND2	2.20	0.51
3:L:520:LYS:HE3	3:L:522:LYS:HE3	1.92	0.51
3:L:262:LYS:NZ	3:L:262:LYS:HB3	2.26	0.51
2:A:157:ASN:O	2:A:161:ILE:HG23	2.11	0.51
3:L:593:PHE:CE1	3:L:635:HIS:HD2	2.28	0.51
3:L:636:ASN:ND2	3:L:639:GLN:O	2.44	0.51
3:L:326:VAL:CG2	3:L:332:GLU:CB	2.86	0.50
3:L:295:ASN:OD1	3:L:296:GLU:N	2.45	0.50
3:L:297:CYS:C	3:L:299:ASP:N	2.69	0.50
3:L:318:LEU:C	3:L:329:ARG:HH12	2.18	0.50
3:L:593:PHE:CZ	3:L:635:HIS:HD2	2.30	0.50
2:A:531:GLN:HE21	2:A:531:GLN:HA	1.77	0.50
3:L:261:PHE:CE2	3:L:263:CYS:CA	2.94	0.50
2:A:193:HIS:HD2	2:A:195:GLU:H	1.60	0.50
3:L:259:ASN:O	3:L:270:THR:HG21	2.12	0.50
3:L:482:THR:CG2	3:L:483:LYS:H	2.24	0.50
3:L:276:ASN:N	3:L:287:GLU:OE2	2.40	0.49
3:L:342:THR:CG2	3:L:343:CYS:N	2.60	0.49
3:L:377:ILE:CD1	3:L:379:TYR:HE2	2.07	0.49
3:L:346:LEU:CD2	3:L:357:GLN:HB2	2.42	0.49
2:A:160:ARG:HH22	2:A:420:ALA:CB	2.25	0.49
2:A:379:PHE:CE2	3:L:295:ASN:ND2	2.81	0.49
3:L:326:VAL:HG21	3:L:332:GLU:CB	2.25	0.49
3:L:325:LEU:HD12	3:L:329:ARG:HH11	1.78	0.48
3:L:355:LYS:HE3	3:L:357:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:383:THR:HG23	3:L:411:LEU:HD22	1.94	0.48
3:L:275:CYS:SG	3:L:287:GLU:HB3	2.54	0.48
3:L:347:CYS:SG	3:L:348:VAL:N	2.85	0.48
3:L:377:ILE:CD1	3:L:379:TYR:CE2	2.83	0.48
3:L:283:ASP:HB3	3:L:285:SER:HB2	1.96	0.48
3:L:374:VAL:HG11	3:L:418:ASN:HB3	1.74	0.48
2:A:454:GLN:HG3	2:A:680:ARG:NH1	2.26	0.48
3:L:369:LYS:HE3	3:L:369:LYS:HA	1.95	0.48
3:L:377:ILE:O	3:L:377:ILE:HG13	2.12	0.48
1:P:66:ARG:HH11	1:P:66:ARG:CG	2.28	0.47
3:L:317:CYS:SG	3:L:329:ARG:CG	3.03	0.47
3:L:499:ARG:HE	3:L:543:ASN:HD22	1.61	0.47
3:L:371:CYS:C	3:L:372:LYS:CE	2.88	0.47
2:A:277:VAL:O	2:A:277:VAL:HG12	2.15	0.46
2:A:319:ARG:HB2	2:A:352:GLY:H	1.80	0.46
1:P:128:GLY:O	1:P:131:LEU:HG	2.16	0.46
2:A:202:VAL:HG12	2:A:204:ASP:H	1.80	0.46
2:A:455:LEU:N	2:A:680:ARG:HH22	2.08	0.46
3:L:371:CYS:C	3:L:372:LYS:HE2	2.41	0.46
2:A:161:ILE:O	2:A:161:ILE:CG1	2.50	0.46
2:A:282:PRO:HB3	2:A:400:LEU:HD22	1.98	0.46
2:A:490:SER:HB3	2:A:520:VAL:HG12	1.96	0.46
3:L:583:ARG:HD3	3:L:618:VAL:HG11	1.98	0.46
2:A:273:LYS:O	2:A:277:VAL:HG23	2.16	0.46
3:L:327:ALA:C	3:L:329:ARG:N	2.72	0.45
3:L:418:ASN:OD1	3:L:435:LEU:CD2	2.64	0.45
2:A:167:ARG:O	2:A:168:ALA:C	2.59	0.45
2:A:206:GLU:HG3	2:A:251:ARG:HD3	1.98	0.45
3:L:365:ASP:CG	3:L:368:THR:H	2.24	0.45
3:L:365:ASP:OD2	3:L:368:THR:N	2.45	0.45
2:A:330:ALA:HA	2:A:331:PRO:HD3	1.86	0.45
2:A:395:ILE:HG23	2:A:444:LEU:HD23	1.98	0.45
3:L:339:ASP:C	3:L:342:THR:HB	2.41	0.45
3:L:374:VAL:HG12	3:L:418:ASN:OD1	2.15	0.45
3:L:279:ARG:NH2	3:L:282:ARG:HG3	2.31	0.45
2:A:563:SER:HB2	2:A:597:HIS:HB2	1.99	0.45
3:L:282:ARG:HB3	3:L:282:ARG:NH1	2.32	0.45
3:L:636:ASN:O	3:L:639:GLN:N	2.48	0.45
3:L:290:LYS:O	3:L:291:GLU:CB	2.65	0.45
3:L:345:GLN:HB3	3:L:359:GLU:CD	2.42	0.45
2:A:531:GLN:HA	2:A:531:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:617:ALA:HA	2:A:618:PRO:HA	1.89	0.45
3:L:268:CYS:C	3:L:269:ILE:HG23	2.42	0.45
2:A:156:TRP:CE3	2:A:341:ALA:HA	2.51	0.44
1:P:119:LEU:HD11	2:A:300:ALA:HB2	1.99	0.44
2:A:369:ILE:CD1	3:L:298:LEU:HD23	2.47	0.44
2:A:618:PRO:HD2	2:A:619:GLN:HG3	2.00	0.44
3:L:312:LYS:HE2	3:L:312:LYS:HA	1.99	0.44
3:L:326:VAL:O	3:L:327:ALA:CB	2.64	0.44
1:P:72:TRP:CD1	1:P:150:PHE:HE2	2.35	0.44
3:L:334:ILE:N	3:L:334:ILE:CD1	2.70	0.44
3:L:346:LEU:HB3	3:L:357:GLN:O	2.18	0.44
3:L:470:THR:HG22	3:L:477:VAL:HG22	1.98	0.44
3:L:273:LYS:NZ	3:L:280:ASP:CG	2.76	0.44
3:L:299:ASP:O	3:L:300:ASN:CG	2.54	0.44
3:L:273:LYS:O	3:L:273:LYS:CG	2.64	0.44
3:L:274:VAL:HG11	3:L:312:LYS:HD2	1.81	0.44
3:L:371:CYS:O	3:L:372:LYS:HE3	2.18	0.44
2:A:154:ILE:N	2:A:155:PRO:HD3	2.33	0.43
2:A:160:ARG:HH22	2:A:420:ALA:HB2	1.82	0.43
2:A:499:ARG:HD2	2:A:499:ARG:C	2.43	0.43
3:L:271:LEU:O	3:L:272:ASP:HB3	2.18	0.43
2:A:171:TYR:C	2:A:172:GLN:OE1	2.62	0.43
3:L:270:THR:CG2	3:L:272:ASP:N	2.57	0.43
3:L:276:ASN:N	3:L:287:GLU:CD	2.77	0.43
2:A:437:THR:HA	2:A:438:PRO:HD3	1.89	0.43
3:L:304:CYS:SG	3:L:308:CYS:HB2	2.58	0.43
3:L:271:LEU:C	3:L:273:LYS:N	2.70	0.43
3:L:273:LYS:CE	3:L:280:ASP:OD2	2.67	0.43
2:A:154:ILE:O	2:A:156:TRP:N	2.52	0.42
1:P:150:PHE:CE1	2:A:258:LYS:HG3	2.54	0.42
2:A:180:VAL:HG13	2:A:282:PRO:HG2	2.01	0.42
3:L:364:LEU:H	3:L:364:LEU:CD2	2.28	0.42
1:P:118:LEU:HD21	2:A:304:LEU:HD13	2.00	0.42
3:L:326:VAL:CG2	3:L:332:GLU:HG2	2.48	0.42
3:L:593:PHE:HB2	3:L:633:LEU:HD22	2.00	0.42
2:A:200:VAL:HG22	2:A:247:MET:HB2	2.01	0.42
3:L:390:LYS:HB2	3:L:401:LEU:HB2	2.01	0.42
3:L:272:ASP:C	3:L:274:VAL:HG13	2.43	0.42
3:L:633:LEU:HD23	3:L:638:THR:CG2	2.49	0.42
2:A:302:GLN:HA	2:A:332:GLU:HG3	2.01	0.42
3:L:272:ASP:C	3:L:274:VAL:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:108:LEU:HD11	3:L:626:LEU:CD2	2.49	0.42
2:A:332:GLU:CD	2:A:332:GLU:H	2.27	0.42
3:L:277:MET:O	3:L:278:ALA:HB2	2.20	0.42
2:A:161:ILE:O	2:A:444:LEU:HD12	2.19	0.42
2:A:495:ARG:HG2	2:A:497:GLY:H	1.84	0.42
3:L:517:THR:HA	3:L:518:PRO:HA	1.93	0.42
3:L:290:LYS:O	3:L:290:LYS:HG2	2.19	0.41
3:L:287:GLU:HA	3:L:288:PRO:HD2	1.87	0.41
3:L:490:LEU:HB3	3:L:528:GLY:HA3	2.01	0.41
2:A:158:LEU:O	2:A:161:ILE:HG12	2.19	0.41
2:A:445:PRO:HA	2:A:446:PRO:HD3	1.85	0.41
3:L:279:ARG:HH21	3:L:282:ARG:CG	2.34	0.41
3:L:345:GLN:HB3	3:L:359:GLU:OE2	2.20	0.41
3:L:635:HIS:O	3:L:638:THR:OG1	2.38	0.41
3:L:256:GLU:OE1	3:L:256:GLU:HA	2.20	0.41
2:A:465:SER:HB3	2:A:473:ALA:HB2	2.03	0.41
3:L:434:GLN:HB3	3:L:441:VAL:HB	2.03	0.41
3:L:411:LEU:HD12	3:L:420:ILE:HD11	2.03	0.41
1:P:151:ALA:HB2	2:A:253:LEU:HD13	2.03	0.41
2:A:372:SER:HB3	2:A:378:CYS:HB3	2.03	0.41
3:L:381:PHE:HE1	3:L:634:PHE:CB	2.33	0.40
3:L:327:ALA:O	3:L:329:ARG:N	2.54	0.40
3:L:470:THR:HB	3:L:498:PRO:HB2	2.02	0.40
3:L:371:CYS:C	3:L:372:LYS:HE3	2.46	0.40
3:L:636:ASN:HD22	3:L:636:ASN:HA	1.56	0.40
2:A:162:THR:CG2	2:A:162:THR:O	2.68	0.40
2:A:171:TYR:O	2:A:172:GLN:OE1	2.40	0.40

All (20) 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)
2:A:160:ARG:NE	3:L:279:ARG:CZ[2_564]	1.19	1.01
2:A:159:GLU:OE2	3:L:284:TRP:CZ3[2_564]	1.27	0.93
2:A:160:ARG:CD	3:L:279:ARG:NH2[2_564]	1.50	0.70
2:A:160:ARG:NE	3:L:279:ARG:NE[2_564]	1.58	0.62
2:A:417:HIS:NE2	3:L:277:MET:CE[2_564]	1.58	0.62
2:A:165:ARG:NE	3:L:289:ILE:CD1[2_564]	1.63	0.57
2:A:160:ARG:NH2	3:L:279:ARG:CD[2_564]	1.69	0.51
2:A:159:GLU:OE2	3:L:284:TRP:CH2[2_564]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:ARG:NE	3:L:279:ARG:NH2[2_564]	1.82	0.38
2:A:160:ARG:CD	3:L:279:ARG:CZ[2_564]	1.91	0.29
2:A:160:ARG:NE	3:L:279:ARG:NH1[2_564]	1.94	0.26
2:A:160:ARG:O	3:L:279:ARG:NH1[2_564]	1.98	0.22
2:A:160:ARG:CG	3:L:279:ARG:NH2[2_564]	2.04	0.16
2:A:160:ARG:CG	3:L:279:ARG:NH1[2_564]	2.08	0.12
2:A:160:ARG:CA	3:L:279:ARG:NH2[2_564]	2.12	0.08
3:L:586:HIS:NE2	3:L:650:THR:OG1[4_454]	2.15	0.05
2:A:165:ARG:NH2	3:L:289:ILE:CD1[2_564]	2.17	0.03
2:A:159:GLU:OE2	3:L:284:TRP:CE3[2_564]	2.18	0.02
2:A:165:ARG:CZ	3:L:289:ILE:CD1[2_564]	2.18	0.02
2:A:160:ARG:CZ	3:L:279:ARG:NE[2_564]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
2	A	482/540 (89%)	435 (90%)	35 (7%)	12 (2%)	4	27
3	L	438/440 (100%)	351 (80%)	65 (15%)	22 (5%)	1	16
All	All	1010/1072 (94%)	872 (86%)	104 (10%)	34 (3%)	3	21

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	282	PRO
2	A	448	THR
2	A	581	PRO
2	A	618	PRO
3	L	271	LEU
3	L	327	ALA
3	L	339	ASP

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Mol	Chain	Res	Type
3	L	340	PRO
3	L	346	LEU
3	L	369	LYS
3	L	372	LYS
3	L	482	THR
2	A	171	TYR
3	L	298	LEU
2	A	278	GLN
3	L	263	CYS
3	L	281	CYS
3	L	282	ARG
3	L	304	CYS
2	A	154	ILE
2	A	617	ALA
2	A	651	ASP
3	L	277	MET
3	L	336	GLU
3	L	444	TYR
3	L	287	GLU
3	L	321	ASP
3	L	385	ARG
3	L	594	GLU
2	A	156	TRP
3	L	377	ILE
2	A	161	ILE
2	A	583	GLY
3	L	266	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	P	79/79 (100%)	78 (99%)	1 (1%)	61	71
2	A	388/430 (90%)	376 (97%)	12 (3%)	35	56
3	L	388/388 (100%)	363 (94%)	25 (6%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	855/897 (95%)	817 (96%)	38 (4%)	25	48

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	66	ARG
2	A	160	ARG
2	A	165	ARG
2	A	167	ARG
2	A	169	ASP
2	A	212	ASP
2	A	273	LYS
2	A	283	LEU
2	A	410	GLU
2	A	549	ARG
2	A	607	GLU
2	A	609	LYS
2	A	638	LEU
3	L	262	LYS
3	L	263	CYS
3	L	269	ILE
3	L	285	SER
3	L	287	GLU
3	L	292	CYS
3	L	300	ASN
3	L	318	LEU
3	L	329	ARG
3	L	333	ASP
3	L	334	ILE
3	L	335	ASP
3	L	337	CYS
3	L	338	GLN
3	L	340	PRO
3	L	363	GLN
3	L	364	LEU
3	L	365	ASP
3	L	367	HIS
3	L	369	LYS
3	L	372	LYS
3	L	395	ARG
3	L	437	ARG
3	L	575	LYS

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Mol	Chain	Res	Type
3	L	636	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	99	GLN
1	P	113	HIS
2	A	193	HIS
2	A	298	ASN
2	A	317	ASN
2	A	449	HIS
2	A	464	HIS
2	A	513	ASN
2	A	531	GLN
3	L	264	HIS
3	L	300	ASN
3	L	309	ASN
3	L	357	GLN
3	L	427	GLN
3	L	439	HIS
3	L	464	HIS
3	L	635	HIS
3	L	636	ASN
3	L	639	GLN
3	L	644	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	P	92/92 (100%)	1.23	15 (16%) 4 8	80, 150, 197, 200	0
2	A	496/540 (91%)	1.21	97 (19%) 3 6	77, 171, 200, 200	0
3	L	440/440 (100%)	1.43	109 (24%) 2 5	67, 164, 200, 200	0
All	All	1028/1072 (95%)	1.31	221 (21%) 2 5	67, 166, 200, 200	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	359	GLU	8.4
3	L	284	TRP	8.1
3	L	346	LEU	7.9
2	A	164	PRO	7.7
2	A	154	ILE	6.8
3	L	357	GLN	6.7
3	L	347	CYS	6.4
3	L	282	ARG	6.1
3	L	412	ASP	6.1
3	L	358	CYS	5.7
3	L	291	GLU	5.4
2	A	165	ARG	5.4
3	L	277	MET	5.2
3	L	368	THR	5.1
2	A	179	LEU	5.0
1	P	104	ARG	4.8
3	L	502	VAL	4.7
3	L	363	GLN	4.7
3	L	348	VAL	4.7
3	L	312	LYS	4.7
2	A	485	SER	4.5
3	L	272	ASP	4.4
3	L	345	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
2	A	659	ARG	4.2
2	A	453	TRP	4.2
3	L	335	ASP	4.2
2	A	570	ASP	4.2
3	L	369	LYS	4.1
2	A	643	HIS	4.1
3	L	694	ALA	4.1
2	A	538	THR	4.1
2	A	617	ALA	4.1
2	A	618	PRO	4.1
3	L	355	LYS	4.1
3	L	630	ASP	4.0
3	L	588	PHE	3.9
3	L	274	VAL	3.8
2	A	244	GLY	3.8
3	L	375	GLY	3.8
3	L	614	THR	3.7
2	A	628	GLU	3.7
2	A	612	GLU	3.7
2	A	530	PRO	3.7
3	L	629	GLU	3.7
3	L	349	ASN	3.6
3	L	377	ILE	3.6
3	L	540	GLN	3.6
2	A	635	CYS	3.6
2	A	159	GLU	3.6
3	L	356	CYS	3.5
3	L	389	ARG	3.5
3	L	344	SER	3.5
2	A	571	LEU	3.5
3	L	378	ALA	3.5
3	L	364	LEU	3.5
2	A	568	VAL	3.5
3	L	473	VAL	3.5
3	L	268	CYS	3.5
3	L	262	LYS	3.5
3	L	367	HIS	3.4
2	A	546	MET	3.3
3	L	295	ASN	3.3
3	L	499	ARG	3.3
2	A	281	GLY	3.3
3	L	354	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
3	L	395	ARG	3.2
3	L	428	ARG	3.2
2	A	558	VAL	3.2
3	L	342	THR	3.2
2	A	469	ARG	3.2
2	A	577	PRO	3.1
2	A	585	PRO	3.1
3	L	546	THR	3.1
1	P	64	PHE	3.1
3	L	693	GLU	3.1
3	L	641	ARG	3.1
1	P	140	VAL	3.1
1	P	66	ARG	3.1
3	L	360	GLU	3.1
3	L	376	SER	3.0
2	A	562	CYS	3.0
3	L	459	ALA	3.0
3	L	336	GLU	3.0
3	L	279	ARG	3.0
3	L	328	GLN	3.0
3	L	631	MET	2.9
3	L	528	GLY	2.9
3	L	353	GLY	2.9
1	P	132	GLU	2.9
3	L	439	HIS	2.9
2	A	401	SER	2.9
2	A	607	GLU	2.9
2	A	535	SER	2.8
2	A	569	GLU	2.8
2	A	172	GLN	2.8
2	A	549	ARG	2.8
3	L	501	ILE	2.8
2	A	567	GLU	2.8
3	L	441	VAL	2.8
3	L	337	CYS	2.8
3	L	436	ASP	2.8
2	A	248	ARG	2.8
3	L	685	ARG	2.7
2	A	640	GLY	2.7
3	L	390	LYS	2.7
2	A	405	GLU	2.7
2	A	262	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	374	VAL	2.7
3	L	683	LEU	2.7
2	A	224	ASP	2.7
2	A	556	GLY	2.7
2	A	671	ALA	2.7
2	A	235	SER	2.7
1	P	103	ALA	2.7
2	A	456	PHE	2.7
3	L	290	LYS	2.7
3	L	468	TYR	2.7
3	L	260	LYS	2.7
2	A	160	ARG	2.7
2	A	608	CYS	2.7
1	P	136	LYS	2.6
2	A	270	PHE	2.6
2	A	542	ALA	2.6
1	P	106	GLY	2.6
2	A	493	GLY	2.6
3	L	450	ARG	2.6
2	A	534	CYS	2.6
3	L	340	PRO	2.6
2	A	449	HIS	2.6
2	A	537	HIS	2.6
3	L	352	GLY	2.6
2	A	623	THR	2.6
3	L	265	SER	2.6
2	A	410	GLU	2.6
2	A	454	GLN	2.6
2	A	586	ASN	2.5
2	A	467	PRO	2.5
1	P	133	LEU	2.5
3	L	435	LEU	2.5
2	A	163	PRO	2.5
2	A	491	ARG	2.5
2	A	578	VAL	2.5
3	L	556	TRP	2.5
2	A	647	ALA	2.5
2	A	494	LYS	2.5
3	L	547	LEU	2.5
2	A	474	ILE	2.5
2	A	414	ARG	2.5
3	L	341	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	637	ALA	2.5
3	L	592	VAL	2.5
1	P	139	HIS	2.4
2	A	342	GLN	2.4
2	A	223	CYS	2.4
2	A	470	MET	2.4
2	A	476	ARG	2.4
2	A	645	LEU	2.4
2	A	540	PRO	2.4
3	L	692	THR	2.4
3	L	490	LEU	2.4
1	P	67	CYS	2.4
1	P	69	LYS	2.3
3	L	280	ASP	2.3
1	P	95	ALA	2.3
2	A	625	ALA	2.3
2	A	366	GLU	2.3
3	L	393	LEU	2.3
3	L	504	ASP	2.3
3	L	343	CYS	2.3
3	L	622	ALA	2.3
2	A	557	HIS	2.3
2	A	314	ALA	2.3
3	L	483	LYS	2.3
3	L	259	ASN	2.2
2	A	566	TRP	2.2
1	P	61	THR	2.2
2	A	681	SER	2.2
2	A	166	TYR	2.2
2	A	582	ARG	2.2
3	L	294	THR	2.2
3	L	316	GLU	2.2
2	A	475	ALA	2.2
2	A	551	HIS	2.2
3	L	266	GLY	2.2
2	A	564	SER	2.2
2	A	480	ASP	2.2
3	L	595	ASP	2.2
3	L	536	THR	2.2
2	A	446	PRO	2.1
3	L	293	GLY	2.1
3	L	422	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	483	LEU	2.1
3	L	432	SER	2.1
2	A	555	GLN	2.1
3	L	544	GLY	2.1
3	L	652	SER	2.1
3	L	332	GLU	2.1
2	A	189	ILE	2.1
2	A	196	ILE	2.1
2	A	528	LEU	2.1
3	L	658	TYR	2.1
2	A	490	SER	2.1
3	L	672	LYS	2.1
3	L	582	LYS	2.1
3	L	624	ASN	2.1
2	A	341	ALA	2.1
3	L	382	PHE	2.1
3	L	307	VAL	2.1
2	A	547	GLY	2.0
3	L	324	GLN	2.0
3	L	650	THR	2.0
1	P	82	LEU	2.0
2	A	171	TYR	2.0
2	A	315	ALA	2.0
2	A	372	SER	2.0
3	L	520	LYS	2.0
2	A	422	ASP	2.0
2	A	619	GLN	2.0
3	L	632	VAL	2.0
3	L	513	THR	2.0
2	A	588	CYS	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	L	1	1/1	0.71	0.24	155,155,155,155	0
4	CA	L	3	1/1	0.71	0.17	155,155,155,155	0
4	CA	A	4	1/1	0.81	0.08	155,155,155,155	0
4	CA	L	2	1/1	0.93	0.09	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.