



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:59 PM UTC

PDB ID : 3P5B / pdb_00003p5b
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 : 3.30 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

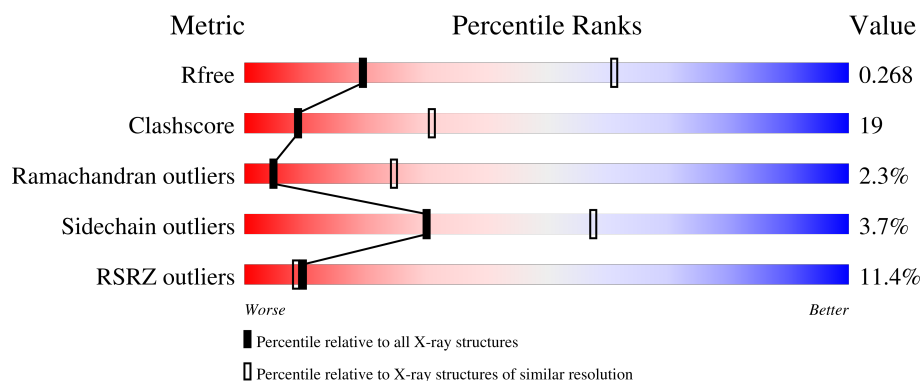
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	4% 92% 7%
2	A	540	15% 74% 15% 9%
3	L	400	7% 70% 22% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7464 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	493	Total	C	N	O	S	0	0	0
			3637	2243	668	694	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	394	Total	C	N	O	S	0	0	0
			3084	1931	535	593	25			

- 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	2	Total	Ca	0	0
			2	2		

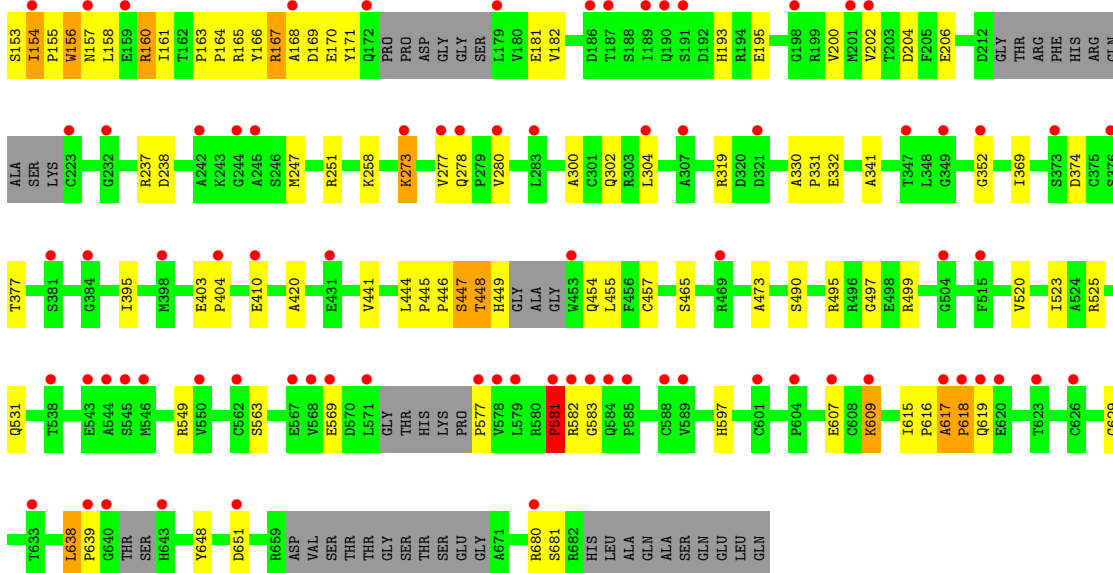
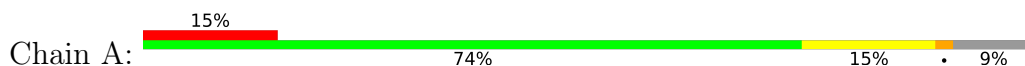
3 Residue-property plots [i](#)

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: Proprotein convertase subtilisin/kexin type 9

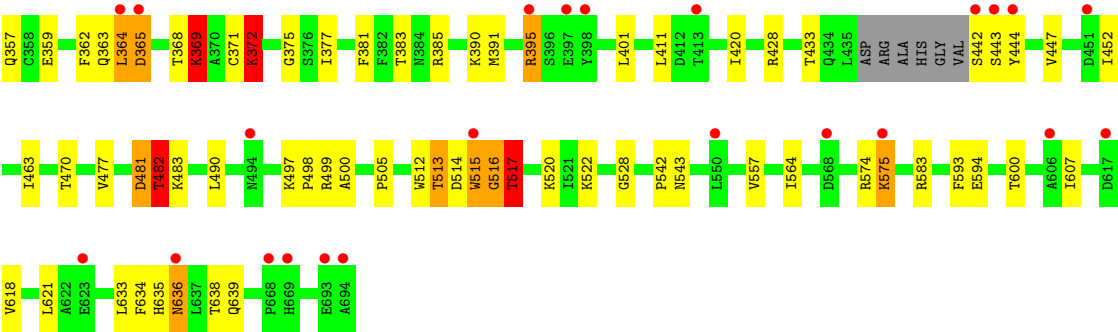


- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- Molecule 3: Low density lipoprotein receptor variant





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.00Å 109.70Å 178.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 98.2 (50.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.298 0.274 , 0.268	Depositor DCC
R_{free} test set	1158 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7464	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/757	0.69	0/1023
2	A	0.43	0/3702	0.75	4/5030 (0.1%)
3	L	0.59	4/3149 (0.1%)	1.16	16/4279 (0.4%)
All	All	0.50	4/7608 (0.1%)	0.93	20/10332 (0.2%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	516	GLY	N-CA	6.66	1.52	1.45
3	L	512	TRP	C-N	5.46	1.41	1.33
3	L	482	THR	N-CA	-5.28	1.39	1.46
3	L	481	ASP	C-N	-5.10	1.26	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	517	THR	CA-C-N	-33.88	77.48	119.84
3	L	517	THR	C-N-CA	-33.88	77.48	119.84
3	L	515	TRP	CA-C-N	9.47	131.64	122.27
3	L	515	TRP	C-N-CA	9.47	131.64	122.27
3	L	341	ASP	N-CA-C	-7.99	103.64	113.15
3	L	312	LYS	N-CA-C	-7.95	103.79	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	517	THR	C-N-CD	7.86	157.24	125.00
3	L	517	THR	O-C-N	-7.32	112.91	121.32
3	L	517	THR	CA-C-O	-7.22	110.26	120.16
3	L	339	ASP	N-CA-C	6.94	125.16	109.81
2	A	581	PRO	N-CA-CB	6.54	110.12	103.25
3	L	513	THR	N-CA-C	6.50	119.31	109.23
2	A	447	SER	N-CA-C	6.30	117.32	108.00
2	A	577	PRO	N-CA-CB	5.81	109.39	103.00
3	L	512	TRP	N-CA-C	5.66	115.75	108.34
3	L	350	LEU	N-CA-C	5.54	116.83	108.46
3	L	517	THR	CB-CA-C	5.49	120.98	110.17
2	A	447	SER	CB-CA-C	-5.32	108.90	116.34
3	L	516	GLY	CA-C-O	-5.19	117.09	122.28
3	L	338	GLN	N-CA-C	5.16	115.84	107.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	517	THR	Peptide

5.2 Too-close contacts [i](#)

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	7	0
2	A	3637	0	3512	80	3
3	L	3084	0	2990	193	0
4	A	1	0	0	0	0
4	L	2	0	0	0	0
All	All	7464	0	7252	273	3

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 19.

All (273) 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:A:447:SER:OG	2:A:449:HIS:HD2	1.23	1.20
3:L:339:ASP:HB3	3:L:340:PRO:HD2	1.19	1.14
3:L:299:ASP:O	3:L:300:ASN:ND2	1.81	1.14
3:L:339:ASP:HB3	3:L:340:PRO:CD	1.76	1.14
2:A:447:SER:OG	2:A:449:HIS:CD2	2.01	1.12
3:L:514:ASP:OD2	3:L:520:LYS:HE2	1.49	1.10
3:L:342:THR:HG22	3:L:343:CYS:H	1.21	1.06
3:L:395:ARG:NH2	3:L:395:ARG:HB2	1.72	1.04
3:L:339:ASP:CB	3:L:340:PRO:HD2	1.88	1.03
2:A:448:THR:HG22	2:A:448:THR:O	1.55	1.03
3:L:339:ASP:HA	3:L:342:THR:HB	1.42	0.99
3:L:304:CYS:HA	3:L:329:ARG:HG3	1.48	0.96
3:L:513:THR:HG21	3:L:542:PRO:O	1.65	0.95
2:A:167:ARG:HH11	2:A:167:ARG:HB3	1.29	0.95
3:L:311:LEU:HD21	3:L:316:GLU:HG2	1.50	0.93
3:L:326:VAL:HG21	3:L:332:GLU:HB2	1.55	0.87
2:A:455:LEU:H	2:A:680:ARG:NH2	1.72	0.87
3:L:365:ASP:HB2	3:L:372:LYS:HD3	1.56	0.86
3:L:395:ARG:HB2	3:L:395:ARG:HH21	1.36	0.86
3:L:342:THR:HG22	3:L:343:CYS:N	1.90	0.86
3:L:498:PRO:HA	3:L:513:THR:O	1.77	0.85
3:L:300:ASN:ND2	3:L:300:ASN:O	2.09	0.85
3:L:481:ASP:O	3:L:482:THR:C	2.19	0.85
3:L:300:ASN:C	3:L:300:ASN:HD22	1.82	0.84
3:L:311:LEU:HD23	3:L:315:TYR:HA	1.59	0.84
3:L:326:VAL:HG21	3:L:332:GLU:CB	2.08	0.84
3:L:395:ARG:CZ	3:L:621:LEU:HB3	2.08	0.83
3:L:514:ASP:C	3:L:516:GLY:H	1.84	0.83
3:L:513:THR:HG23	3:L:542:PRO:HG2	1.60	0.82
3:L:395:ARG:HD2	3:L:621:LEU:O	1.79	0.82
3:L:395:ARG:NH2	3:L:395:ARG:CB	2.43	0.81
3:L:513:THR:CG2	3:L:542:PRO:HG2	2.11	0.81
3:L:338:GLN:OE1	3:L:338:GLN:HA	1.81	0.80
3:L:395:ARG:CZ	3:L:395:ARG:HA	2.11	0.80
3:L:395:ARG:HA	3:L:395:ARG:NE	1.97	0.79
3:L:329:ARG:HA	3:L:329:ARG:NE	1.97	0.79
3:L:365:ASP:CB	3:L:372:LYS:HD3	2.12	0.78
3:L:342:THR:CG2	3:L:343:CYS:H	1.97	0.78
2:A:448:THR:O	2:A:448:THR:CG2	2.29	0.78
2:A:455:LEU:H	2:A:680:ARG:HH22	1.30	0.77
3:L:295:ASN:HD21	3:L:297:CYS:HB2	1.48	0.77
2:A:153:SER:C	2:A:155:PRO:HD3	2.11	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:156:TRP:CZ3	2:A:341:ALA:HA	2.21	0.76
3:L:395:ARG:NH1	3:L:621:LEU:HB3	2.01	0.76
3:L:481:ASP:O	3:L:483:LYS:N	2.18	0.75
3:L:482:THR:HG23	3:L:483:LYS:N	2.01	0.75
3:L:481:ASP:O	3:L:481:ASP:OD1	2.05	0.75
3:L:371:CYS:O	3:L:372:LYS:O	2.05	0.75
3:L:381:PHE:CE2	3:L:401:LEU:HD22	2.22	0.75
3:L:513:THR:CG2	3:L:542:PRO:O	2.35	0.75
2:A:680:ARG:HE	2:A:681:SER:H	1.33	0.74
3:L:334:ILE:N	3:L:334:ILE:HD12	2.02	0.74
2:A:181:GLU:OE2	2:A:280:VAL:HG11	1.88	0.73
3:L:359:GLU:HB2	3:L:362:PHE:HD2	1.53	0.73
2:A:447:SER:HG	2:A:449:HIS:CD2	2.06	0.73
3:L:319:CYS:HB3	3:L:323:PHE:HB2	1.70	0.73
3:L:381:PHE:CD2	3:L:401:LEU:HD22	2.25	0.72
2:A:618:PRO:HB2	2:A:619:GLN:HA	1.70	0.72
3:L:369:LYS:HG3	3:L:369:LYS:O	1.91	0.71
3:L:391:MET:SD	3:L:395:ARG:NH1	2.64	0.70
2:A:609:LYS:HE3	2:A:609:LYS:HA	1.74	0.69
3:L:575:LYS:NZ	3:L:575:LYS:HA	2.08	0.69
2:A:273:LYS:HE2	2:A:273:LYS:HA	1.74	0.69
3:L:334:ILE:HD12	3:L:334:ILE:H	1.54	0.69
3:L:348:VAL:HG13	3:L:355:LYS:HB3	1.75	0.68
3:L:447:VAL:HG13	3:L:482:THR:O	1.93	0.68
3:L:295:ASN:ND2	3:L:297:CYS:H	1.92	0.68
3:L:329:ARG:HA	3:L:329:ARG:HE	1.58	0.68
2:A:377:THR:HB	3:L:310:ASP:HB3	1.75	0.67
3:L:395:ARG:NH2	3:L:621:LEU:HA	2.09	0.67
3:L:513:THR:HG23	3:L:542:PRO:CG	2.25	0.67
2:A:618:PRO:HB2	2:A:619:GLN:CA	2.24	0.67
3:L:326:VAL:CG1	3:L:330:ARG:HH21	2.08	0.67
3:L:339:ASP:O	3:L:341:ASP:N	2.28	0.67
2:A:629:GLY:O	2:A:680:ARG:HD2	1.94	0.67
3:L:514:ASP:O	3:L:516:GLY:N	2.26	0.66
3:L:482:THR:CG2	3:L:483:LYS:N	2.57	0.66
3:L:395:ARG:NH2	3:L:621:LEU:CA	2.58	0.66
3:L:593:PHE:CD1	3:L:633:LEU:HD21	2.30	0.66
3:L:326:VAL:HG12	3:L:330:ARG:HH21	1.61	0.66
2:A:374:ASP:OD2	3:L:307:VAL:HG21	1.96	0.66
2:A:454:GLN:HG3	2:A:680:ARG:HH12	1.61	0.65
3:L:463:ILE:HD12	3:L:505:PRO:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:395:ARG:HH21	3:L:395:ARG:CB	2.04	0.65
3:L:395:ARG:HH22	3:L:621:LEU:CD2	2.10	0.65
3:L:300:ASN:ND2	3:L:300:ASN:C	2.55	0.64
3:L:395:ARG:CZ	3:L:395:ARG:CA	2.75	0.64
3:L:304:CYS:HA	3:L:329:ARG:CG	2.26	0.64
3:L:301:ASN:HB3	3:L:304:CYS:HB2	1.80	0.64
3:L:395:ARG:HH12	3:L:621:LEU:HD22	1.62	0.64
3:L:339:ASP:CA	3:L:342:THR:HB	2.23	0.63
3:L:365:ASP:HB2	3:L:372:LYS:HZ3	1.63	0.63
2:A:618:PRO:CB	2:A:619:GLN:HA	2.28	0.62
2:A:167:ARG:HB3	2:A:167:ARG:NH1	2.08	0.62
3:L:359:GLU:HB2	3:L:362:PHE:CD2	2.34	0.62
3:L:364:LEU:HD23	3:L:364:LEU:H	1.62	0.62
2:A:680:ARG:HE	2:A:681:SER:N	1.97	0.62
3:L:317:CYS:HB3	3:L:329:ARG:NE	2.15	0.62
3:L:395:ARG:NH2	3:L:621:LEU:HB3	2.14	0.61
3:L:433:THR:HG1	3:L:442:SER:N	1.98	0.61
3:L:327:ALA:C	3:L:329:ARG:H	2.09	0.61
3:L:365:ASP:HB2	3:L:372:LYS:CD	2.31	0.61
3:L:514:ASP:C	3:L:516:GLY:N	2.53	0.61
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:317:CYS:SG	3:L:329:ARG:HG2	2.42	0.60
3:L:326:VAL:HG11	3:L:330:ARG:NH2	2.16	0.60
3:L:326:VAL:CG2	3:L:332:GLU:HB3	2.32	0.60
3:L:351:GLU:H	3:L:351:GLU:CD	2.10	0.59
3:L:593:PHE:HB2	3:L:633:LEU:CD2	2.33	0.59
3:L:317:CYS:C	3:L:318:LEU:HD23	2.27	0.59
3:L:575:LYS:HA	3:L:575:LYS:HZ3	1.66	0.59
3:L:348:VAL:CG1	3:L:355:LYS:HB3	2.33	0.59
3:L:364:LEU:HD23	3:L:364:LEU:N	2.18	0.59
3:L:326:VAL:O	3:L:327:ALA:HB3	2.02	0.58
2:A:154:ILE:HG12	2:A:154:ILE:O	2.03	0.58
3:L:325:LEU:CD1	3:L:329:ARG:HH11	2.17	0.58
3:L:395:ARG:NH2	3:L:621:LEU:CB	2.67	0.58
3:L:318:LEU:HD23	3:L:318:LEU:N	2.19	0.57
3:L:326:VAL:CG2	3:L:332:GLU:CB	2.80	0.57
3:L:326:VAL:HG21	3:L:332:GLU:HB3	1.87	0.57
3:L:375:GLY:O	3:L:635:HIS:ND1	2.38	0.57
3:L:297:CYS:C	3:L:299:ASP:H	2.11	0.57
3:L:329:ARG:HD3	3:L:330:ARG:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:395:ARG:CD	3:L:621:LEU:O	2.50	0.57
2:A:420:ALA:HB3	2:A:441:VAL:HB	1.87	0.57
3:L:557:VAL:HG12	3:L:564:ILE:HG12	1.87	0.56
3:L:334:ILE:H	3:L:334:ILE:CD1	2.19	0.56
2:A:457:CYS:HB3	2:A:525:ARG:HE	1.70	0.56
2:A:167:ARG:HH11	2:A:167:ARG:CB	2.11	0.56
3:L:320:PRO:HD2	3:L:323:PHE:CD2	2.41	0.55
2:A:454:GLN:CG	2:A:680:ARG:HH12	2.20	0.55
3:L:326:VAL:CG1	3:L:330:ARG:NH2	2.69	0.54
3:L:348:VAL:HG12	3:L:355:LYS:O	2.07	0.54
3:L:329:ARG:O	3:L:330:ARG:HB3	2.07	0.54
3:L:513:THR:CG2	3:L:542:PRO:HB2	2.37	0.54
3:L:364:LEU:C	3:L:372:LYS:HZ1	2.15	0.54
2:A:273:LYS:O	2:A:277:VAL:HG23	2.07	0.54
3:L:317:CYS:HB3	3:L:329:ARG:CZ	2.38	0.54
3:L:355:LYS:HD3	3:L:356:CYS:N	2.23	0.54
3:L:514:ASP:OD2	3:L:520:LYS:CE	2.40	0.54
3:L:334:ILE:N	3:L:334:ILE:CD1	2.71	0.53
3:L:312:LYS:HE2	3:L:312:LYS:HA	1.90	0.53
3:L:395:ARG:CZ	3:L:395:ARG:CB	2.86	0.53
3:L:395:ARG:HH22	3:L:621:LEU:HD23	1.73	0.53
3:L:428:ARG:HD2	3:L:452:ILE:O	2.08	0.53
3:L:317:CYS:CB	3:L:329:ARG:NE	2.72	0.53
3:L:297:CYS:O	3:L:299:ASP:N	2.43	0.52
3:L:339:ASP:CB	3:L:340:PRO:CD	2.59	0.52
2:A:157:ASN:O	2:A:161:ILE:HG23	2.10	0.52
3:L:574:ARG:O	3:L:575:LYS:HE2	2.09	0.52
2:A:499:ARG:HG2	2:A:597:HIS:CE1	2.45	0.52
3:L:513:THR:HG21	3:L:542:PRO:C	2.33	0.52
2:A:182:VAL:HB	2:A:247:MET:HG2	1.91	0.52
2:A:454:GLN:HG2	2:A:680:ARG:HH22	1.73	0.52
3:L:593:PHE:HB2	3:L:633:LEU:HD21	1.91	0.52
1:P:88:LEU:HD13	1:P:116:HIS:HB3	1.91	0.51
3:L:355:LYS:HD3	3:L:355:LYS:C	2.35	0.51
2:A:166:TYR:HE1	2:A:171:TYR:HE2	1.57	0.51
2:A:277:VAL:HB	2:A:278:GLN:NE2	2.25	0.51
3:L:340:PRO:C	3:L:342:THR:H	2.18	0.51
3:L:359:GLU:CD	3:L:359:GLU:H	2.17	0.51
3:L:346:LEU:HD23	3:L:357:GLN:C	2.35	0.51
3:L:520:LYS:HE3	3:L:522:LYS:HE3	1.92	0.51
3:L:636:ASN:ND2	3:L:639:GLN:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:600:THR:HG22	3:L:607:ILE:HG12	1.92	0.51
2:A:171:TYR:OH	2:A:445:PRO:O	2.28	0.50
3:L:347:CYS:SG	3:L:348:VAL:N	2.85	0.50
3:L:372:LYS:NZ	3:L:377:ILE:HD13	2.27	0.50
3:L:482:THR:CG2	3:L:483:LYS:H	2.24	0.50
2:A:454:GLN:HG3	2:A:680:ARG:NH1	2.27	0.50
3:L:304:CYS:SG	3:L:308:CYS:HB2	2.51	0.50
2:A:167:ARG:O	2:A:170:GLU:N	2.45	0.50
3:L:318:LEU:C	3:L:329:ARG:HH12	2.18	0.50
3:L:383:THR:HG23	3:L:411:LEU:HD22	1.94	0.50
3:L:365:ASP:OD2	3:L:368:THR:N	2.45	0.49
2:A:160:ARG:HH22	2:A:420:ALA:CB	2.25	0.49
3:L:313:ILE:N	3:L:313:ILE:HD13	2.27	0.49
3:L:497:LYS:O	3:L:514:ASP:HA	2.11	0.49
2:A:531:GLN:HE21	2:A:531:GLN:HA	1.77	0.49
3:L:346:LEU:CD2	3:L:357:GLN:HB2	2.42	0.49
3:L:372:LYS:HZ3	3:L:377:ILE:HD13	1.77	0.49
2:A:193:HIS:HD2	2:A:195:GLU:H	1.60	0.48
2:A:369:ILE:CD1	3:L:298:LEU:HD23	2.44	0.48
3:L:313:ILE:HG12	3:L:313:ILE:O	2.13	0.48
2:A:158:LEU:O	2:A:161:ILE:HG12	2.14	0.48
2:A:163:PRO:HD3	2:A:444:LEU:HB2	1.94	0.48
2:A:167:ARG:O	2:A:168:ALA:C	2.56	0.48
3:L:325:LEU:HD12	3:L:329:ARG:HH11	1.78	0.48
3:L:391:MET:SD	3:L:395:ARG:NE	2.86	0.48
3:L:513:THR:HG23	3:L:542:PRO:HB2	1.96	0.48
2:A:165:ARG:O	2:A:165:ARG:HG3	2.13	0.47
3:L:365:ASP:CB	3:L:372:LYS:HZ3	2.25	0.47
3:L:369:LYS:HE3	3:L:369:LYS:HA	1.95	0.47
3:L:499:ARG:HE	3:L:543:ASN:HD22	1.61	0.47
3:L:297:CYS:C	3:L:299:ASP:N	2.71	0.47
3:L:317:CYS:SG	3:L:329:ARG:CG	3.03	0.47
3:L:443:SER:HB2	3:L:444:TYR:C	2.40	0.47
3:L:327:ALA:C	3:L:329:ARG:N	2.72	0.47
3:L:355:LYS:HE3	3:L:357:GLN:HG2	1.95	0.47
2:A:202:VAL:HG12	2:A:204:ASP:H	1.80	0.47
2:A:490:SER:HB3	2:A:520:VAL:HG12	1.97	0.47
3:L:636:ASN:O	3:L:639:GLN:N	2.48	0.47
2:A:319:ARG:HB2	2:A:352:GLY:H	1.80	0.46
3:L:371:CYS:C	3:L:372:LYS:CE	2.88	0.46
2:A:156:TRP:CE3	2:A:341:ALA:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:295:ASN:HD21	3:L:297:CYS:CB	2.20	0.46
3:L:326:VAL:O	3:L:327:ALA:CB	2.64	0.46
3:L:365:ASP:OD2	3:L:368:THR:OG1	2.28	0.46
3:L:583:ARG:HD3	3:L:618:VAL:HG11	1.97	0.46
2:A:206:GLU:HG3	2:A:251:ARG:HD3	1.98	0.46
3:L:339:ASP:C	3:L:342:THR:HB	2.41	0.46
3:L:371:CYS:C	3:L:372:LYS:HE2	2.41	0.45
3:L:513:THR:CG2	3:L:542:PRO:CG	2.86	0.45
3:L:365:ASP:CG	3:L:368:THR:H	2.24	0.45
3:L:395:ARG:HH21	3:L:395:ARG:CG	2.28	0.45
3:L:443:SER:HB2	3:L:444:TYR:CA	2.46	0.45
2:A:160:ARG:HH22	2:A:420:ALA:HB2	1.81	0.45
3:L:470:THR:HG22	3:L:477:VAL:HG22	1.98	0.45
2:A:563:SER:HB2	2:A:597:HIS:HB2	1.99	0.45
2:A:531:GLN:HA	2:A:531:GLN:NE2	2.32	0.45
1:P:119:LEU:HD11	2:A:300:ALA:HB2	1.99	0.44
3:L:345:GLN:HB3	3:L:359:GLU:CD	2.42	0.44
3:L:371:CYS:O	3:L:372:LYS:HE3	2.18	0.44
1:P:72:TRP:CD1	1:P:150:PHE:HE2	2.35	0.44
1:P:66:ARG:HH11	1:P:66:ARG:CG	2.28	0.44
3:L:346:LEU:HB3	3:L:357:GLN:O	2.18	0.44
3:L:513:THR:HG23	3:L:542:PRO:CB	2.47	0.44
3:L:636:ASN:HD22	3:L:636:ASN:HA	1.56	0.44
2:A:618:PRO:HD2	2:A:619:GLN:HG3	2.00	0.44
3:L:391:MET:CE	3:L:395:ARG:HH11	2.30	0.44
2:A:395:ILE:HG23	2:A:444:LEU:HD23	1.99	0.44
3:L:395:ARG:NE	3:L:395:ARG:CA	2.74	0.43
2:A:170:GLU:CD	2:A:447:SER:HA	2.43	0.43
2:A:154:ILE:N	2:A:155:PRO:HD3	2.33	0.43
2:A:499:ARG:HD2	2:A:499:ARG:C	2.44	0.43
2:A:615:ILE:HA	2:A:616:PRO:HD3	1.91	0.43
2:A:617:ALA:HA	2:A:618:PRO:HA	1.89	0.43
3:L:304:CYS:HB3	3:L:305:SER:H	1.70	0.43
3:L:513:THR:CG2	3:L:542:PRO:CB	2.96	0.43
3:L:295:ASN:ND2	3:L:297:CYS:N	2.63	0.43
2:A:581:PRO:HA	2:A:582:ARG:HA	1.85	0.43
2:A:154:ILE:O	2:A:156:TRP:N	2.52	0.43
2:A:495:ARG:HG2	2:A:497:GLY:H	1.84	0.43
3:L:342:THR:CG2	3:L:343:CYS:N	2.60	0.43
2:A:638:LEU:HA	2:A:639:PRO:HD3	1.92	0.43
1:P:118:LEU:HD21	2:A:304:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:150:PHE:CE1	2:A:258:LYS:HG3	2.55	0.42
2:A:332:GLU:CD	2:A:332:GLU:H	2.27	0.42
2:A:330:ALA:HA	2:A:331:PRO:HD3	1.86	0.42
3:L:593:PHE:HB2	3:L:633:LEU:HD22	2.01	0.42
3:L:513:THR:HG21	3:L:542:PRO:HB2	2.00	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
2:A:238:ASP:HB3	3:L:298:LEU:HD11	2.02	0.42
3:L:390:LYS:HB2	3:L:401:LEU:HB2	2.01	0.42
3:L:499:ARG:HB3	3:L:500:ALA:H	1.67	0.42
2:A:165:ARG:HG2	2:A:165:ARG:HH21	1.86	0.41
3:L:490:LEU:HB3	3:L:528:GLY:HA3	2.01	0.41
3:L:364:LEU:H	3:L:364:LEU:CD2	2.28	0.41
2:A:445:PRO:HA	2:A:446:PRO:HD3	1.85	0.41
2:A:444:LEU:HA	2:A:445:PRO:HD3	1.90	0.41
3:L:327:ALA:O	3:L:329:ARG:N	2.54	0.41
3:L:381:PHE:HE1	3:L:634:PHE:CB	2.33	0.41
2:A:160:ARG:NH2	2:A:420:ALA:HB2	2.36	0.40
2:A:200:VAL:HG22	2:A:247:MET:HB2	2.01	0.40
2:A:465:SER:HB3	2:A:473:ALA:HB2	2.03	0.40
3:L:391:MET:CE	3:L:395:ARG:NH1	2.85	0.40
3:L:443:SER:HB2	3:L:444:TYR:HA	2.03	0.40
3:L:345:GLN:HB3	3:L:359:GLU:OE2	2.20	0.40
3:L:411:LEU:HD12	3:L:420:ILE:HD11	2.03	0.40
2:A:403:GLU:HA	2:A:404:PRO:HD3	1.94	0.40
3:L:339:ASP:O	3:L:342:THR:N	2.54	0.40

All (3) 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:237:ARG:CZ	2:A:569:GLU:OE1[3_644]	1.85	0.35
2:A:237:ARG:NH1	2:A:569:GLU:OE1[3_644]	1.96	0.24
2:A:237:ARG:NH2	2:A:569:GLU:CD[3_644]	2.09	0.11

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	479/540 (89%)	437 (91%)	34 (7%)	8 (2%)	7	30
3	L	390/400 (98%)	327 (84%)	49 (13%)	14 (4%)	2	17
All	All	959/1032 (93%)	850 (89%)	87 (9%)	22 (2%)	5	25

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	448	THR
2	A	581	PRO
2	A	618	PRO
3	L	327	ALA
3	L	339	ASP
3	L	340	PRO
3	L	346	LEU
3	L	369	LYS
3	L	372	LYS
3	L	482	THR
3	L	298	LEU
3	L	304	CYS
3	L	515	TRP
2	A	154	ILE
2	A	617	ALA
2	A	651	ASP
3	L	336	GLU
3	L	321	ASP
3	L	385	ARG
3	L	594	GLU
2	A	156	TRP
2	A	583	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	74
2	A	386/430 (90%)	376 (97%)	10 (3%)	40	64
3	L	347/352 (99%)	328 (94%)	19 (6%)	19	48
All	All	812/861 (94%)	782 (96%)	30 (4%)	30	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	66	ARG
2	A	160	ARG
2	A	164	PRO
2	A	167	ARG
2	A	169	ASP
2	A	273	LYS
2	A	410	GLU
2	A	549	ARG
2	A	607	GLU
2	A	609	LYS
2	A	638	LEU
3	L	300	ASN
3	L	313	ILE
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	369	LYS
3	L	372	LYS

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Mol	Chain	Res	Type
3	L	395	ARG
3	L	517	THR
3	L	575	LYS
3	L	636	ASN

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

Mol	Chain	Res	Type
1	P	99	GLN
1	P	113	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
2	A	557	HIS
3	L	295	ASN
3	L	300	ASN
3	L	309	ASN
3	L	427	GLN
3	L	464	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 3 ligands modelled in this entry, 3 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%)	0.57	4 (4%) 40 25	37, 56, 81, 86	0
2	A	493/540 (91%)	1.10	79 (16%) 5 4	34, 68, 96, 110	0
3	L	394/400 (98%)	0.86	29 (7%) 20 15	25, 63, 98, 116	0
All	All	979/1032 (94%)	0.95	112 (11%) 10 8	25, 65, 97, 116	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	410	GLU	5.0
2	A	186	ASP	4.7
2	A	569	GLU	4.3
2	A	640	GLY	4.3
2	A	179	LEU	4.1
2	A	623	THR	4.1
2	A	578	VAL	4.1
2	A	562	CYS	4.1
2	A	639	PRO	4.0
2	A	546	MET	4.0
3	L	364	LEU	3.9
2	A	469	ARG	3.9
2	A	584	GLN	3.9
2	A	223	CYS	3.8
3	L	395	ARG	3.7
3	L	694	ALA	3.5
2	A	617	ALA	3.4
2	A	577	PRO	3.4
2	A	607	GLU	3.3
3	L	575	LYS	3.3
2	A	453	TRP	3.2
2	A	582	ARG	3.1
2	A	571	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	201	MET	3.1
2	A	504	GLY	3.1
2	A	589	VAL	3.1
3	L	451	ASP	3.0
2	A	244	GLY	3.0
2	A	198	GLY	3.0
3	L	669	HIS	2.9
3	L	340	PRO	2.9
2	A	245	ALA	2.9
3	L	443	SER	2.8
2	A	568	VAL	2.8
2	A	191	SER	2.8
2	A	567	GLU	2.8
2	A	604	PRO	2.8
2	A	643	HIS	2.8
2	A	515	PHE	2.7
2	A	242	ALA	2.7
2	A	588	CYS	2.7
2	A	273	LYS	2.7
3	L	397	GLU	2.7
3	L	413	THR	2.7
2	A	545	SER	2.6
3	L	617	ASP	2.6
2	A	154	ILE	2.6
2	A	609	LYS	2.6
2	A	172	GLN	2.6
2	A	544	ALA	2.6
2	A	585	PRO	2.6
2	A	278	GLN	2.6
3	L	568	ASP	2.6
2	A	232	GLY	2.6
1	P	118	LEU	2.6
2	A	579	LEU	2.6
2	A	373	SER	2.5
1	P	119	LEU	2.5
3	L	494	ASN	2.4
2	A	349	GLY	2.4
3	L	398	TYR	2.4
1	P	132	GLU	2.4
2	A	601	CYS	2.4
3	L	550	LEU	2.4
3	L	351	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	538	THR	2.3
2	A	626	CYS	2.4
3	L	668	PRO	2.4
2	A	619	GLN	2.3
2	A	189	ILE	2.3
2	A	651	ASP	2.3
2	A	159	GLU	2.3
1	P	70	ASP	2.3
2	A	157	ASN	2.2
3	L	444	TYR	2.2
2	A	376	SER	2.2
2	A	398	MET	2.2
3	L	352	GLY	2.2
3	L	515	TRP	2.2
3	L	442	SER	2.2
2	A	583	GLY	2.2
3	L	341	ASP	2.2
2	A	202	VAL	2.2
2	A	307	ALA	2.2
2	A	431	GLU	2.2
3	L	331	CYS	2.2
2	A	543	GLU	2.1
2	A	280	VAL	2.1
2	A	168	ALA	2.1
2	A	384	GLY	2.1
2	A	277	VAL	2.1
3	L	606	ALA	2.1
2	A	618	PRO	2.1
2	A	304	LEU	2.1
2	A	321	ASP	2.1
3	L	319	CYS	2.1
2	A	680	ARG	2.1
2	A	404	PRO	2.1
3	L	623	GLU	2.1
2	A	550	VAL	2.1
2	A	347	THR	2.1
2	A	283	LEU	2.0
3	L	365	ASP	2.0
2	A	352	GLY	2.0
2	A	581	PRO	2.0
2	A	620	GLU	2.0
2	A	381	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	636	ASN	2.0
2	A	187	THR	2.0
2	A	633	THR	2.0
2	A	190	GLN	2.0
3	L	693	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	3	1/1	0.61	0.13	117,117,117,117	0
4	CA	L	1	1/1	0.85	0.09	64,64,64,64	0
4	CA	A	2	1/1	0.95	0.06	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.