



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:20 am BST

PDB ID : 3P5B
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

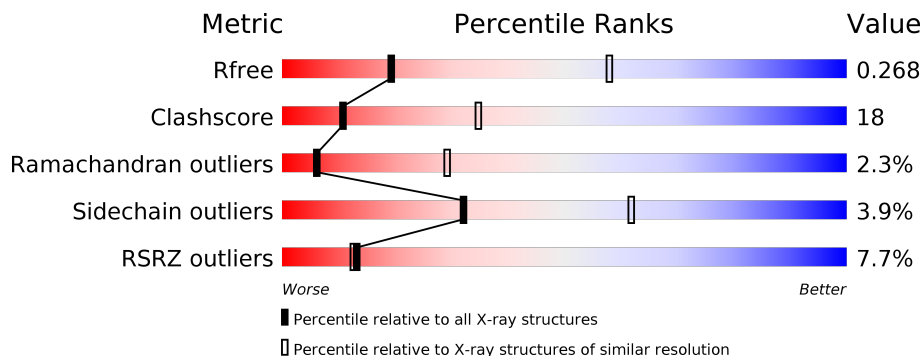
1 Overall quality at a glance i

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 92%, yellow 92%, yellow 97%, orange 97%, orange 99%, red 99%);"></div> <div style="margin-left: 10px;"> <p>92%</p> <p>7%</p> </div> </div>
2	A	540	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 5%, green 5%, green 74%, yellow 74%, yellow 89%, orange 89%, orange 94%, red 94%);"></div> <div style="margin-left: 10px;"> <p>5%</p> <p>74%</p> <p>15%</p> <p>9%</p> </div> </div>
3	L	400	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 12%, green 12%, green 70%, yellow 70%, yellow 93%, orange 93%, orange 98%, red 98%);"></div> <div style="margin-left: 10px;"> <p>12%</p> <p>70%</p> <p>23%</p> <p>5%</p> </div> </div>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	P	92	740	474	133	131	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	493	3637	2243	668	694	32	0	0	0

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

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

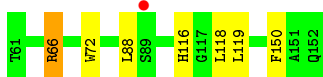
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	L	2	Total	Ca	0	0
			2	2		

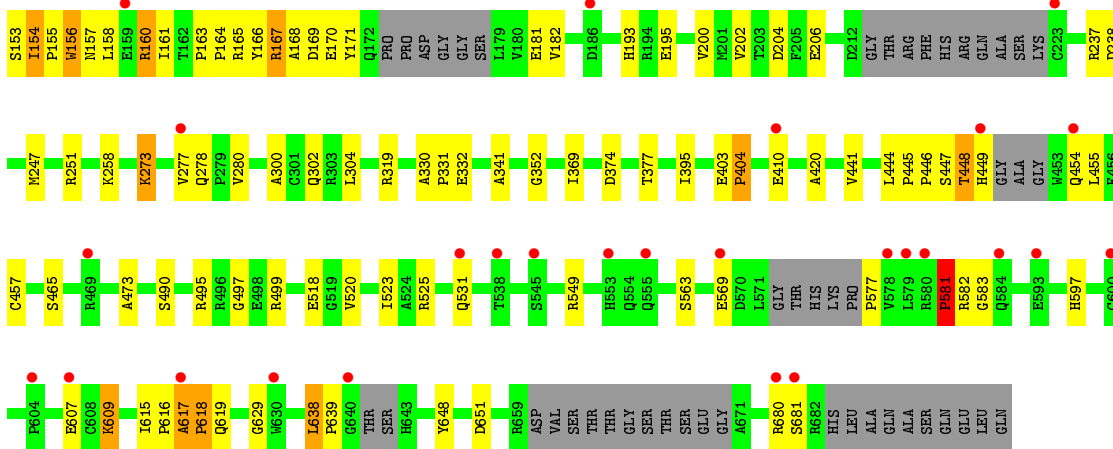
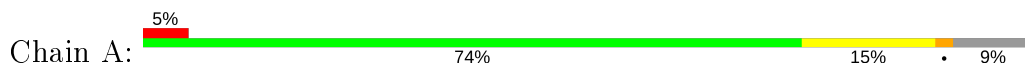
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

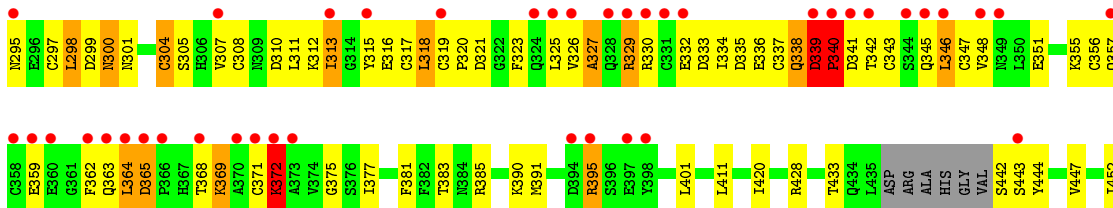
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

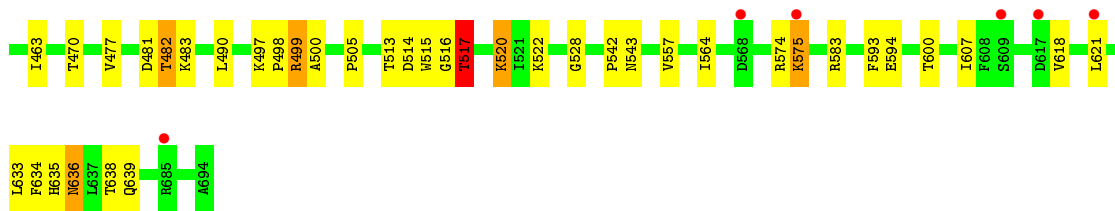


- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- 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 47.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 98.3 (47.07-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.33Å)	Xtrriage
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	Xtrriage
Anisotropy	0.254	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.31	0/757	0.46	0/1023
2	A	0.31	0/3702	0.47	2/5030 (0.0%)
3	L	0.44	0/3149	0.66	4/4279 (0.1%)
All	All	0.37	0/7608	0.56	6/10332 (0.1%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	517	THR	C-N-CD	13.73	157.24	128.40
3	L	517	THR	C-N-CA	-10.60	77.48	122.00
3	L	517	THR	CA-C-N	7.04	136.82	117.10
2	A	581	PRO	N-CA-CB	5.68	110.12	103.30
3	L	339	ASP	N-CA-C	5.24	125.16	111.00
2	A	577	PRO	N-CA-CB	5.08	109.39	103.30

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	78	3
3	L	3084	0	2990	191	0
4	A	1	0	0	0	0
4	L	2	0	0	0	0
All	All	7464	0	7252	269	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 18.

All (269) 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:HB2	3:L:395:ARG:NH2	1.72	1.04
3:L:339:ASP:CB	3:L:340:PRO:HD2	1.88	1.03
2:A:448:THR:O	2:A:448:THR:HG22	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:HB3	2:A:167:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	3:L:338:GLN:OE1	1.81	0.80
3:L:481:ASP:O	3:L:482:THR:C	2.19	0.80
3:L:395:ARG:HA	3:L:395:ARG:CZ	2.11	0.80
3:L:300:ASN:C	3:L:300:ASN:HD22	1.82	0.80
3:L:395:ARG:NE	3:L:395:ARG:HA	1.97	0.79
3:L:329:ARG:NE	3:L:329:ARG:HA	1.97	0.79
3:L:514:ASP:C	3:L:516:GLY:H	1.84	0.78
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: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:OD1	3:L:481:ASP:O	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:HD12	3:L:334:ILE:N	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:O	3:L:369:LYS:HG3	1.91	0.71
2:A:153:SER:C	2:A:155:PRO:HD3	2.11	0.71
3:L:391:MET:SD	3:L:395:ARG:NH1	2.64	0.70
2:A:609:LYS:HA	2:A:609:LYS:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:334:ILE:H	3:L:334:ILE:HD12	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:HE	3:L:329:ARG:HA	1.58	0.68
2:A:377:THR:HB	3:L:310:ASP:HB3	1.75	0.67
3:L:482:THR:CG2	3:L:483:LYS:N	2.57	0.67
3:L:513:THR:HG23	3:L:542:PRO:CG	2.25	0.67
3:L:395:ARG:NH2	3:L:621:LEU:HA	2.09	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
3:L:433:THR:HG1	3:L:442:SER:N	1.93	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: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
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:395:ARG:CA	3:L:395:ARG:CZ	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:H	3:L:364:LEU:HD23	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:365:ASP:HB2	3:L:372:LYS:CD	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:326:VAL:CG2	3:L:332:GLU:HB3	2.32	0.60
3:L:593:PHE:HB2	3:L:633:LEU:CD2	2.33	0.59
3:L:348:VAL:CG1	3:L:355:LYS:HB3	2.33	0.59
3:L:364:LEU:N	3:L:364:LEU:HD23	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:575:LYS:HA	3:L:575:LYS:HZ3	1.67	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:329:ARG:HD3	3:L:330:ARG:H	1.70	0.57
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:327:ALA:C	3:L:329:ARG:H	2.09	0.57
3:L:514:ASP:C	3:L:516:GLY:N	2.53	0.56
3:L:557:VAL:HG12	3:L:564:ILE:HG12	1.87	0.56
3:L:334:ILE:CD1	3:L:334:ILE:H	2.19	0.56
2:A:457:CYS:HB3	2:A:525:ARG:HE	1.70	0.56
2:A:167:ARG:CB	2:A:167:ARG:HH11	2.11	0.56
3:L:320:PRO:HD2	3:L:323:PHE:CD2	2.41	0.55
3:L:351:GLU:CD	3:L:351:GLU:H	2.10	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:317:CYS:C	3:L:318:LEU:HD23	2.27	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
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:CD1	3:L:334:ILE:N	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:C	3:L:299:ASP:H	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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: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:364:LEU:C	3:L:372:LYS:HZ1	2.15	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:HA	2:A:531:GLN:HE21	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:O	3:L:313:ILE:HG12	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
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:HG3	2:A:165:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:499:ARG:HE	3:L:543:ASN:HD22	1.61	0.47
3:L:513:THR:HG21	3:L:542:PRO:C	2.33	0.47
3:L:317:CYS:SG	3:L:329:ARG:CG	3.03	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:340:PRO:C	3:L:342:THR:H	2.18	0.47
3:L:355:LYS:C	3:L:355:LYS:HD3	2.35	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
2:A:156:TRP:CE3	2:A:341:ALA:HA	2.51	0.46
3:L:295:ASN:HD21	3:L:297:CYS:CB	2.20	0.46
3:L:359:GLU:H	3:L:359:GLU:CD	2.17	0.46
3:L:326:VAL:O	3:L:327:ALA:CB	2.64	0.46
3:L:346:LEU:HD23	3:L:357:GLN:C	2.35	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:513:THR:CG2	3:L:542:PRO:CG	2.86	0.45
3:L:395:ARG:CG	3:L:395:ARG:HH21	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:318:LEU:C	3:L:329:ARG:HH12	2.18	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: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
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
1:P:66:ARG:HH11	1:P:66:ARG:CG	2.28	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:CA	3:L:395:ARG:NE	2.74	0.43
2:A:154:ILE:N	2:A:155:PRO:HD3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:167:ARG:O	2:A:168:ALA:C	2.56	0.43
2:A:273:LYS:HZ3	2:A:277:VAL:HG23	1.84	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:150:PHE:CE1	2:A:258:LYS:HG3	2.55	0.42
1:P:118:LEU:HD21	2:A:304:LEU:HD13	2.00	0.42
3:L:297:CYS:C	3:L:299:ASP:N	2.71	0.42
3:L:327:ALA:C	3:L:329:ARG:N	2.72	0.42
3:L:443:SER:HB2	3:L:444:TYR:C	2.40	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
3:L:635:HIS:O	3:L:638:THR:OG1	2.38	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:371:CYS:C	3:L:372:LYS:CE	2.88	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
3:L:339:ASP:C	3:L:342:THR:HB	2.41	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
3:L:365:ASP:CG	3:L:368:THR:H	2.24	0.41
3:L:371:CYS:C	3:L:372:LYS:HE2	2.41	0.41
2:A:200:VAL:HG22	2:A:247:MET:HB2	2.01	0.40
2:A:160:ARG:NH2	2:A:420:ALA:HB2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	P	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
2	A	479/540 (89%)	437 (91%)	34 (7%)	8 (2%)	9	35
3	L	390/400 (98%)	327 (84%)	49 (13%)	14 (4%)	3	20
All	All	959/1032 (93%)	850 (89%)	87 (9%)	22 (2%)	6	29

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

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Mol	Chain	Res	Type
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 [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	P	79/79 (100%)	78 (99%)	1 (1%)	69 82
2	A	386/430 (90%)	374 (97%)	12 (3%)	40 67
3	L	347/352 (99%)	328 (94%)	19 (6%)	21 52
All	All	812/861 (94%)	780 (96%)	32 (4%)	32 62

All (32) 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	404	PRO
2	A	410	GLU
2	A	518	GLU

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Mol	Chain	Res	Type
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	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	372	LYS
3	L	395	ARG
3	L	499	ARG
3	L	517	THR
3	L	520	LYS
3	L	575	LYS
3	L	636	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	193	HIS
2	A	449	HIS
2	A	464	HIS
2	A	531	GLN
3	L	295	ASN
3	L	300	ASN
3	L	309	ASN
3	L	586	HIS
3	L	636	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	0.33	1 (1%) 80 81	37, 56, 81, 86	0
2	A	493/540 (91%)	0.49	27 (5%) 25 23	34, 68, 96, 110	0
3	L	394/400 (98%)	0.67	47 (11%) 4 4	25, 63, 98, 116	0
All	All	979/1032 (94%)	0.55	75 (7%) 13 12	25, 65, 97, 116	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	341	ASP	5.7
3	L	364	LEU	4.3
3	L	357	GLN	3.9
3	L	358	CYS	3.9
3	L	360	GLU	3.9
3	L	346	LEU	3.8
3	L	340	PRO	3.8
3	L	617	ASP	3.6
2	A	604	PRO	3.6
3	L	372	LYS	3.5
2	A	277	VAL	3.5
3	L	324	GLN	3.5
3	L	325	LEU	3.4
3	L	313	ILE	3.3
3	L	365	ASP	3.2
3	L	397	GLU	3.2
3	L	331	CYS	3.1
3	L	368	THR	3.1
3	L	359	GLU	3.0
3	L	370	ALA	3.0
2	A	578	VAL	3.0
3	L	349	ASN	2.9
2	A	469	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	569	GLU	2.9
3	L	366	PRO	2.9
3	L	373	ALA	2.9
3	L	363	GLN	2.9
2	A	531	GLN	2.8
3	L	326	VAL	2.8
2	A	545	SER	2.7
3	L	609	SER	2.7
3	L	342	THR	2.7
2	A	223	CYS	2.6
2	A	640	GLY	2.6
2	A	607	GLU	2.6
3	L	315	TYR	2.6
2	A	617	ALA	2.6
3	L	443	SER	2.6
2	A	579	LEU	2.6
3	L	329	ARG	2.5
3	L	328	GLN	2.5
3	L	319	CYS	2.5
2	A	555	GLN	2.5
2	A	410	GLU	2.5
3	L	332	GLU	2.5
3	L	345	GLN	2.5
3	L	395	ARG	2.4
2	A	186	ASP	2.4
3	L	295	ASN	2.3
3	L	307	VAL	2.3
2	A	580	ARG	2.3
3	L	348	VAL	2.3
2	A	553	HIS	2.3
1	P	89	SER	2.3
2	A	584	GLN	2.2
3	L	575	LYS	2.2
3	L	330	ARG	2.2
2	A	593	GLU	2.2
2	A	680	ARG	2.2
2	A	449	HIS	2.2
3	L	339	ASP	2.2
3	L	568	ASP	2.2
2	A	630	TRP	2.1
3	L	398	TYR	2.1
2	A	600	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	362	PHE	2.1
3	L	344	SER	2.1
3	L	394	ASP	2.1
2	A	454	GLN	2.0
2	A	681	SER	2.0
3	L	685	ARG	2.0
3	L	621	LEU	2.0
2	A	159	GLU	2.0
2	A	538	THR	2.0
3	L	371	CYS	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 carbohydrates 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	0.81	0.07	64,64,64,64	0
4	CA	L	3	1/1	0.83	0.15	117,117,117,117	0
4	CA	A	2	1/1	0.92	0.17	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.