Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 PM GMT

PDB ID	:	4J0A
Title	:	Crystal structure of hcv ns5b polymerase in complex with 2-{[(4-METHYLPHENYL)SULFONYL]AMINO}-4-PHENOXYBENZOIC ACID
Authors	:	Coulombe, R.
Deposited on	:	2013-01-30
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/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:

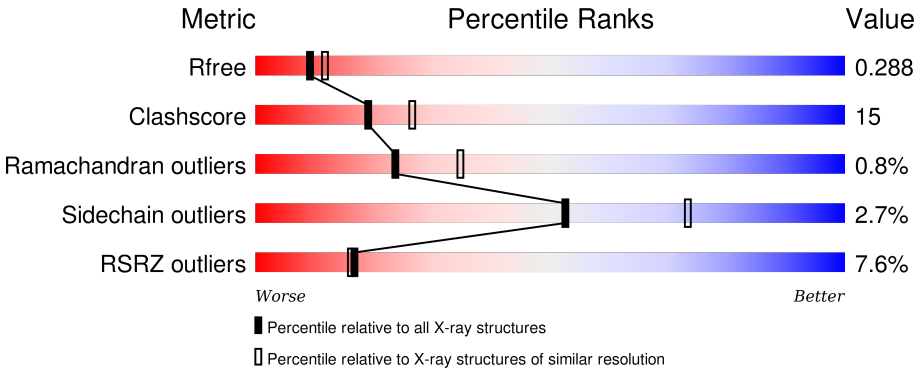
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	2% 73% 22%
1	B	576	13% 63% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1JL	A	601	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8976 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.

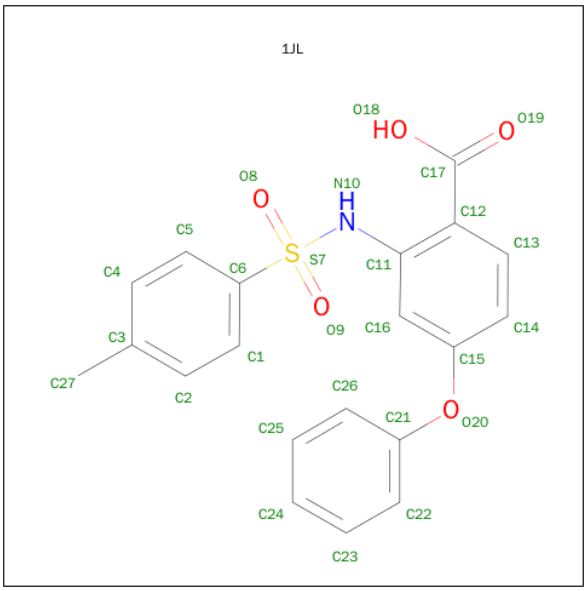
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	558	Total	C	N	O	S	0	0	0
			4346	2737	768	809	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is 2-{[(4-METHYLPHENYL)SULFONYL]AMINO}-4-PHENOXYBENZOIC ACID (three-letter code: 1JL) (formula: $C_{20}H_{17}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 3 is water.

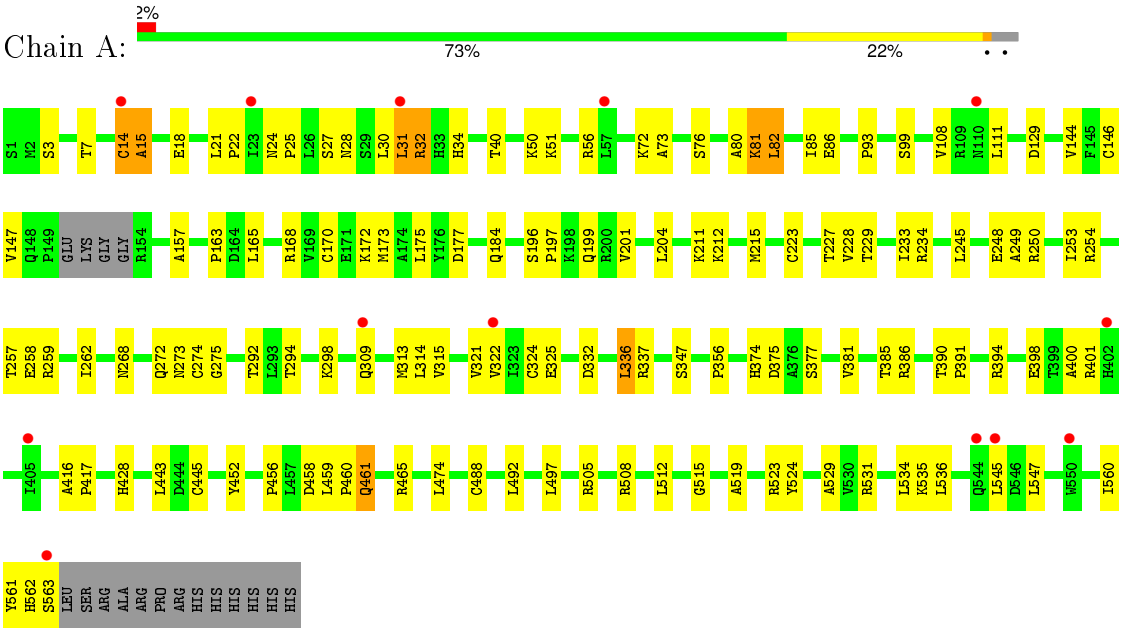
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total	O	0	0
			144	144		
3	B	101	Total	O	0	0
			101	101		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

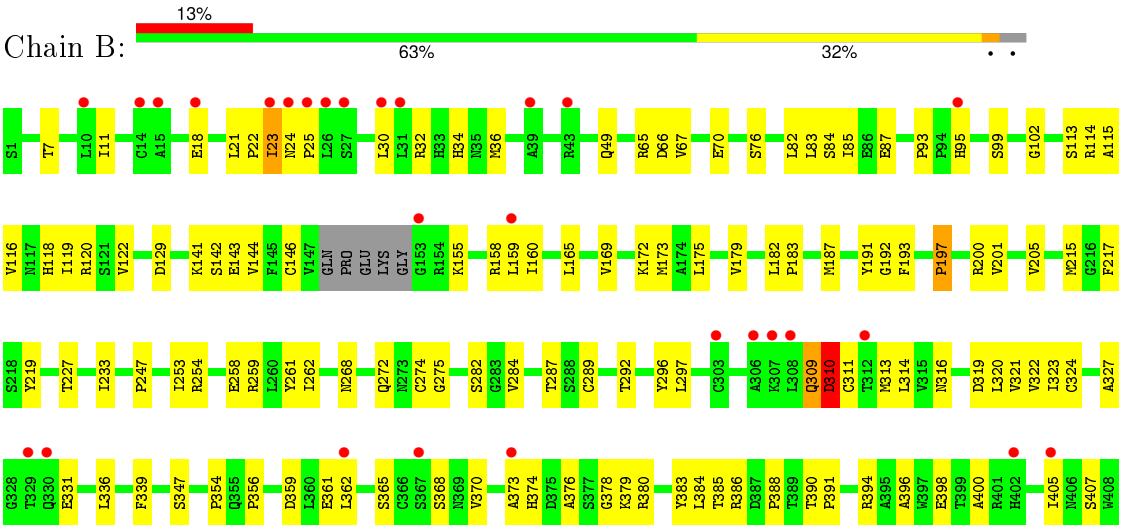
- Molecule 1: Genome polyprotein

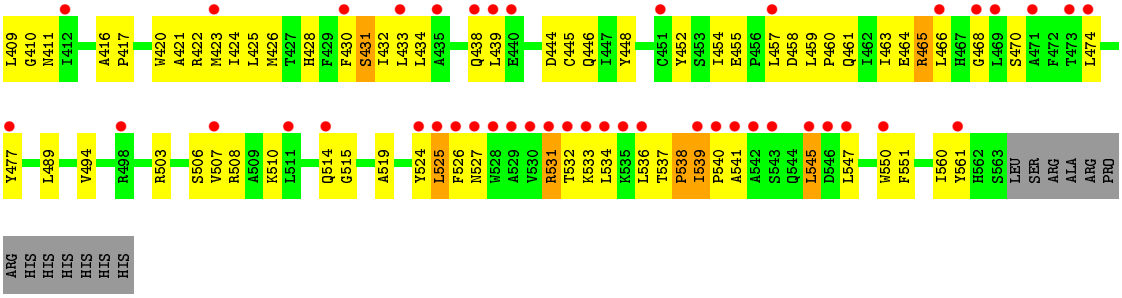
Chain A:



- Molecule 1: Genome polyprotein

Chain B:




L409 G410 N411 T412 A416 P417 W420 A421 R422 M423 I424 L425 M426 T427 H428 F429 F430 S431 I432 L433 L434 A435 Q438 L439 E440 D444 C445 Q446 T447 Y448 C451 Y452 S453 I454 E455 P456 L457 D458 L459 P460 Q461 I462 I463 E464 R465 L466 H467 G468 L469 S470 A471 F472 T473 L474
Y477 L489 V494 R498 R503 S506 V507 R508 A509 K510 L511 Q514 G515 A519 Y524 L525 F526 N527 W528 A529 V530 R531 T532 K533 L534 K535 L536 T537 P538 I539 P540 A541 A542 S543 Q544 L545 D546 L547 W550 F551 I560 Y561 H562 S563 LEU SER ARG ALA ARG PRO
ARG HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.63Å 107.91Å 135.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 99.2 (48.14-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.39Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.256 , 0.299 0.248 , 0.288	Depositor DCC
R_{free} test set	6193 reflections (11.31%)	DCC
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.4	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 60972 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 1JL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/4453	0.65	0/6044
1	B	0.40	0/4440	0.63	0/6025
All	All	0.40	0/8893	0.64	0/12069

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4358	0	4371	99	0
1	B	4346	0	4359	168	0
2	A	27	0	16	1	0
3	A	144	0	0	4	0
3	B	101	0	0	3	0
All	All	8976	0	8746	265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ARG:HH11	1:B:531:ARG:H	1.17	0.92
1:B:531:ARG:HH11	1:B:531:ARG:HG3	1.39	0.88
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.56	0.87
1:B:426:MET:HE1	1:B:525:LEU:HD22	1.58	0.85
1:A:81:LYS:O	1:A:82:LEU:HB3	1.77	0.82
1:B:506:SER:O	1:B:510:LYS:HG3	1.81	0.81
1:B:22:PRO:HD2	1:B:400:ALA:HB1	1.66	0.77
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.68	0.75
1:B:531:ARG:HD2	1:B:532:THR:N	2.02	0.75
1:B:143:GLU:OE1	1:B:158:ARG:NH1	2.20	0.75
1:B:65:ARG:HD2	3:B:619:HOH:O	1.87	0.73
1:B:531:ARG:NH1	1:B:531:ARG:HG3	2.02	0.73
1:B:84:SER:OG	1:B:87:GLU:HG3	1.90	0.71
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.72	0.70
1:B:309:GLN:O	1:B:324:CYS:HB2	1.92	0.70
1:A:456:PRO:O	1:A:459:LEU:HG	1.91	0.70
1:B:439:LEU:HB3	1:B:457:LEU:HD21	1.73	0.70
1:A:40:THR:HB	1:A:157:ALA:HB2	1.72	0.70
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.22	0.69
1:B:336:LEU:HD22	1:B:356:PRO:HD3	1.74	0.69
1:A:309:GLN:O	1:A:324:CYS:HB2	1.93	0.69
1:B:531:ARG:HD2	1:B:532:THR:H	1.59	0.68
1:B:233:ILE:HD12	1:B:262:ILE:HA	1.74	0.68
1:B:428:HIS:O	1:B:432:ILE:HG13	1.94	0.68
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.76	0.67
1:B:431:SER:HB2	1:B:507:VAL:HG21	1.77	0.66
1:B:201:VAL:O	1:B:205:VAL:HG23	1.96	0.66
1:A:531:ARG:HB2	1:A:531:ARG:NH1	2.11	0.66
1:A:81:LYS:O	1:A:82:LEU:CB	2.44	0.65
1:B:11:ILE:HD13	1:B:159:LEU:HD22	1.79	0.64
1:B:83:LEU:HB2	1:B:173:MET:HA	1.78	0.64
1:B:201:VAL:HG13	1:B:370:VAL:HG13	1.80	0.64
1:A:531:ARG:HB2	1:A:531:ARG:HH11	1.61	0.64
1:B:506:SER:OG	1:B:510:LYS:HE3	1.98	0.64
1:B:383:TYR:HH	1:B:477:TYR:HD2	1.47	0.63
1:A:257:THR:O	1:A:262:ILE:HG23	1.98	0.63
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.81	0.63
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.81	0.62
1:B:426:MET:CE	1:B:525:LEU:HD22	2.28	0.62
1:B:390:THR:HB	1:B:391:PRO:HD3	1.82	0.62
1:A:18:GLU:HB3	1:A:401:ARG:NH2	2.15	0.62
1:A:21:LEU:HD23	1:A:34:HIS:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LYS:HG2	1:B:380:ARG:N	2.16	0.61
1:B:23:ILE:O	1:B:24:ASN:HB2	2.00	0.61
1:B:531:ARG:HH11	1:B:531:ARG:N	1.95	0.61
1:B:85:ILE:HD13	1:B:116:VAL:HG13	1.83	0.61
1:B:368:SER:HB3	1:B:384:LEU:HD11	1.82	0.61
1:B:464:GLU:OE1	1:B:539:ILE:HB	2.00	0.60
1:B:503:ARG:O	1:B:507:VAL:HG23	2.01	0.60
1:A:228:VAL:HG12	1:A:233:ILE:CD1	2.32	0.60
1:B:434:LEU:HD12	1:B:507:VAL:HG13	1.83	0.60
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.84	0.59
1:A:497:LEU:HD22	2:A:601:1JL:O20	2.03	0.59
1:B:227:THR:HB	1:B:347:SER:O	2.02	0.59
1:B:434:LEU:HD21	1:B:439:LEU:HD11	1.84	0.58
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.32	0.58
1:A:129:ASP:HB3	1:A:259:ARG:NH1	2.18	0.58
1:B:422:ARG:HA	1:B:426:MET:SD	2.43	0.58
1:B:99:SER:HB2	1:B:165:LEU:HB3	1.85	0.57
1:B:421:ALA:O	1:B:426:MET:HG3	2.04	0.57
1:B:379:LYS:HG2	1:B:380:ARG:H	1.69	0.57
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.34	0.57
1:B:465:ARG:HG3	1:B:545:LEU:HB3	1.86	0.57
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.87	0.56
1:A:211:LYS:HE2	1:A:324:CYS:HA	1.86	0.56
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.70	0.56
1:B:405:ILE:HG21	1:B:446:GLN:HG3	1.88	0.56
1:B:531:ARG:CD	1:B:532:THR:HG23	2.35	0.56
1:B:144:VAL:HB	1:B:394:ARG:CG	2.32	0.56
1:A:227:THR:HB	1:A:347:SER:O	2.04	0.55
1:B:359:ASP:OD1	1:B:361:GLU:HB2	2.06	0.55
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.86	0.55
1:A:234:ARG:HD3	1:B:247:PRO:HG3	1.87	0.55
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.21	0.55
1:B:327:ALA:O	1:B:331:GLU:HB2	2.06	0.55
1:B:531:ARG:HD2	1:B:532:THR:HG23	1.89	0.55
1:A:228:VAL:HG12	1:A:233:ILE:HD11	1.87	0.55
1:B:531:ARG:NH1	1:B:531:ARG:H	1.98	0.55
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.89	0.55
1:A:465:ARG:NH1	1:A:545:LEU:O	2.22	0.55
1:B:310:ASP:O	1:B:324:CYS:HA	2.07	0.54
1:B:336:LEU:O	1:B:339:PHE:HB3	2.08	0.54
1:A:229:THR:O	1:A:233:ILE:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ASN:HD21	1:B:534:LEU:H	1.55	0.54
1:A:394:ARG:O	1:A:398:GLU:HG3	2.08	0.54
1:B:531:ARG:HH11	1:B:531:ARG:CG	2.13	0.53
1:A:170:CYS:HA	1:A:173:MET:CE	2.38	0.53
1:B:115:ALA:O	1:B:119:ILE:HG13	2.08	0.53
1:A:512:LEU:HD21	1:A:523:ARG:HG2	1.90	0.53
1:A:21:LEU:HD23	1:A:34:HIS:CB	2.39	0.53
1:A:175:LEU:HD21	1:A:253:ILE:HG12	1.89	0.53
1:A:14:CYS:O	1:A:15:ALA:HB2	2.09	0.53
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.23	0.53
1:A:108:VAL:CG2	1:A:165:LEU:HD21	2.37	0.53
1:A:314:LEU:HB3	1:A:321:VAL:HG12	1.91	0.52
1:B:22:PRO:CD	1:B:400:ALA:HB1	2.37	0.52
1:B:85:ILE:CD1	1:B:116:VAL:HG13	2.39	0.52
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.90	0.52
1:A:14:CYS:O	1:A:14:CYS:SG	2.67	0.52
1:A:80:ALA:HB3	1:A:245:LEU:HD23	1.92	0.52
1:B:538:PRO:O	1:B:539:ILE:C	2.48	0.52
1:B:102:GLY:O	1:B:114:ARG:HD3	2.09	0.52
1:A:505:ARG:HG3	1:A:529:ALA:HB1	1.92	0.52
1:B:431:SER:HB2	1:B:507:VAL:CG2	2.40	0.52
1:A:390:THR:HB	1:A:391:PRO:HD3	1.91	0.51
1:A:85:ILE:HG12	1:A:173:MET:SD	2.51	0.51
1:B:537:THR:O	1:B:539:ILE:N	2.43	0.51
1:B:192:GLY:HA3	1:B:316:ASN:OD1	2.09	0.51
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.76	0.51
1:B:120:ARG:NH1	1:B:120:ARG:HG3	2.25	0.51
1:B:66:ASP:O	1:B:70:GLU:HG3	2.10	0.51
1:A:374:HIS:O	1:A:474:LEU:HA	2.11	0.51
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.41	0.51
1:B:93:PRO:HB3	1:B:95:HIS:CE1	2.46	0.51
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.51	0.51
1:A:170:CYS:HA	1:A:173:MET:HE3	1.91	0.51
1:B:313:MET:SD	1:B:322:VAL:HG22	2.51	0.51
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.93	0.51
1:B:82:LEU:HD12	1:B:173:MET:O	2.11	0.50
1:B:215:MET:SD	1:B:215:MET:O	2.69	0.50
1:B:524:TYR:CE2	1:B:536:LEU:HB3	2.46	0.50
1:A:27:SER:OG	1:A:400:ALA:HB2	2.11	0.50
1:B:18:GLU:HA	1:B:18:GLU:OE2	2.11	0.50
1:A:458:ASP:HA	1:A:461:GLN:HE22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:HG2	1:B:142:SER:N	2.27	0.49
1:B:434:LEU:CD2	1:B:439:LEU:HD11	2.42	0.49
1:B:489:LEU:HD22	1:B:494:VAL:HB	1.94	0.49
1:A:512:LEU:CD2	1:A:523:ARG:HG2	2.43	0.49
1:B:7:THR:HG23	1:B:275:GLY:HA2	1.95	0.49
1:B:423:MET:HG2	1:B:424:ILE:HG13	1.94	0.49
1:B:359:ASP:HB3	1:B:362:LEU:HG	1.94	0.49
1:B:416:ALA:CB	1:B:463:ILE:HG23	2.42	0.49
1:A:18:GLU:HG3	1:A:401:ARG:NH1	2.28	0.48
1:B:444:ASP:HA	1:B:452:TYR:O	2.13	0.48
1:B:118:HIS:O	1:B:122:VAL:HG23	2.14	0.48
1:B:433:LEU:HB3	1:B:439:LEU:HD23	1.96	0.48
1:A:56:ARG:HD3	1:A:56:ARG:N	2.28	0.48
1:A:443:LEU:HD21	3:A:786:HOH:O	2.14	0.48
1:B:233:ILE:HD13	1:B:261:TYR:O	2.13	0.48
1:B:201:VAL:CG2	1:B:384:LEU:HB2	2.44	0.47
1:B:426:MET:O	1:B:430:PHE:HB2	2.14	0.47
1:B:175:LEU:O	1:B:179:VAL:HG22	2.14	0.47
1:B:187:MET:HE1	1:B:292:THR:CG2	2.44	0.47
1:A:294:THR:CG2	1:A:298:LYS:HE3	2.44	0.47
1:A:228:VAL:CG1	1:A:233:ILE:HD11	2.45	0.47
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.96	0.47
1:B:439:LEU:O	1:B:457:LEU:HG	2.14	0.47
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.49	0.47
1:B:454:ILE:HG22	1:B:455:GLU:N	2.30	0.47
1:B:383:TYR:OH	1:B:477:TYR:HD2	1.97	0.47
1:A:163:PRO:O	1:A:168:ARG:NH1	2.48	0.47
1:B:120:ARG:HG3	1:B:120:ARG:HH11	1.80	0.46
1:B:141:LYS:HD2	1:B:143:GLU:CD	2.36	0.46
1:B:215:MET:SD	1:B:215:MET:C	2.94	0.46
1:B:461:GLN:HG2	1:B:541:ALA:CB	2.45	0.46
1:B:374:HIS:HA	1:B:379:LYS:O	2.16	0.46
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.97	0.46
1:A:445:CYS:HB2	3:A:742:HOH:O	2.15	0.46
1:B:284:VAL:HG22	1:B:287:THR:OG1	2.16	0.46
1:B:311:CYS:HB3	1:B:313:MET:CE	2.45	0.46
1:B:160:ILE:HA	1:B:282:SER:OG	2.16	0.46
1:B:376:ALA:C	1:B:378:GLY:H	2.19	0.46
1:A:534:LEU:O	1:A:535:LYS:C	2.53	0.46
1:B:187:MET:HG2	1:B:296:TYR:CG	2.50	0.45
1:B:365:SER:HB2	3:B:697:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ARG:HH11	1:B:158:ARG:HG3	1.81	0.45
1:A:40:THR:HB	1:A:157:ALA:CB	2.45	0.45
1:B:448:TYR:CE2	1:B:551:PHE:HD1	2.35	0.45
1:A:28:ASN:O	1:A:32:ARG:HD2	2.17	0.45
1:B:309:GLN:HE21	1:B:310:ASP:N	2.15	0.45
1:B:464:GLU:O	1:B:468:GLY:N	2.48	0.45
1:A:228:VAL:HG12	1:A:233:ILE:HD12	1.99	0.45
1:A:523:ARG:HG3	1:A:523:ARG:HH11	1.81	0.45
1:A:73:ALA:O	1:A:76:SER:HB2	2.16	0.45
1:B:373:ALA:HB3	1:B:474:LEU:HD22	1.99	0.45
1:A:31:LEU:HD11	1:A:492:LEU:HD22	1.98	0.45
1:B:158:ARG:NH1	1:B:158:ARG:HG3	2.32	0.44
1:B:268:ASN:HB3	1:B:274:CYS:SG	2.57	0.44
1:B:464:GLU:OE2	1:B:538:PRO:HA	2.17	0.44
1:B:433:LEU:HD22	1:B:438:GLN:O	2.18	0.44
1:A:258:GLU:HA	1:A:262:ILE:HD13	2.00	0.44
1:B:470:SER:O	1:B:474:LEU:HG	2.17	0.44
1:A:215:MET:HG3	1:A:332:ASP:OD2	2.17	0.44
1:B:36:MET:O	1:B:146:CYS:HA	2.17	0.44
1:A:375:ASP:OD1	1:A:377:SER:N	2.51	0.44
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.83	0.44
1:B:538:PRO:O	1:B:539:ILE:O	2.35	0.44
1:B:313:MET:HE3	3:B:699:HOH:O	2.18	0.44
1:B:322:VAL:HG12	1:B:323:ILE:N	2.32	0.44
1:A:50:LYS:HG2	1:A:50:LYS:O	2.17	0.44
1:B:254:ARG:HH12	1:B:258:GLU:HG3	1.82	0.44
1:B:309:GLN:HE21	1:B:310:ASP:H	1.66	0.43
1:A:204:LEU:HD21	1:A:314:LEU:CD2	2.48	0.43
1:A:212:LYS:N	1:A:325:GLU:OE1	2.47	0.43
1:B:454:ILE:CG2	1:B:455:GLU:N	2.80	0.43
1:A:99:SER:HB2	1:A:165:LEU:HB3	2.00	0.43
1:B:191:TYR:CZ	1:B:193:PHE:HB2	2.54	0.43
1:B:22:PRO:O	1:B:25:PRO:HG3	2.19	0.43
1:A:459:LEU:HB2	1:A:460:PRO:HD3	2.00	0.43
1:B:187:MET:HG2	1:B:296:TYR:CD1	2.53	0.43
1:A:294:THR:HG23	3:A:770:HOH:O	2.18	0.43
1:B:416:ALA:HB1	1:B:463:ILE:HG23	2.00	0.43
1:A:81:LYS:HG2	1:A:177:ASP:CG	2.38	0.43
1:B:539:ILE:HG23	1:B:540:PRO:HD2	2.00	0.43
1:B:21:LEU:HD12	1:B:34:HIS:HB2	2.01	0.43
1:A:416:ALA:N	1:A:417:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:OG	1:A:199:GLN:HG3	2.19	0.43
1:A:458:ASP:HA	1:A:461:GLN:NE2	2.34	0.43
1:B:508:ARG:HH11	1:B:508:ARG:HG2	1.84	0.43
1:B:409:LEU:O	1:B:410:GLY:C	2.55	0.42
1:B:200:ARG:NH2	1:B:365:SER:OG	2.37	0.42
1:B:385:THR:OG1	1:B:386:ARG:N	2.52	0.42
1:B:531:ARG:HD3	1:B:532:THR:HG23	2.01	0.42
1:A:508:ARG:NH1	1:A:508:ARG:HG2	2.34	0.42
1:A:375:ASP:C	1:A:375:ASP:OD1	2.57	0.42
1:A:313:MET:SD	1:A:322:VAL:HG22	2.59	0.42
1:B:458:ASP:OD1	1:B:461:GLN:OE1	2.38	0.42
1:B:217:PHE:CE1	1:B:322:VAL:HB	2.55	0.42
1:B:187:MET:HE2	1:B:187:MET:HB2	1.93	0.42
1:B:459:LEU:O	1:B:463:ILE:HG13	2.19	0.42
1:B:165:LEU:O	1:B:169:VAL:HG23	2.19	0.42
1:A:3:SER:HB3	1:A:56:ARG:HD2	2.01	0.42
1:A:508:ARG:HH11	1:A:508:ARG:HG2	1.84	0.42
1:B:129:ASP:HB3	1:B:259:ARG:NH1	2.35	0.42
1:B:309:GLN:CA	1:B:309:GLN:HE21	2.32	0.42
1:B:233:ILE:CD1	1:B:261:TYR:O	2.68	0.42
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.67	0.42
1:B:93:PRO:HG3	1:B:561:TYR:HB2	2.02	0.42
1:B:405:ILE:HG23	1:B:445:CYS:HA	2.02	0.41
1:A:452:TYR:OH	1:A:562:HIS:HD2	2.04	0.41
1:A:211:LYS:HE2	1:A:324:CYS:CA	2.50	0.41
1:B:459:LEU:N	1:B:460:PRO:CD	2.83	0.41
1:A:21:LEU:HA	1:A:22:PRO:HD3	1.91	0.41
1:A:336:LEU:HD23	1:A:336:LEU:HA	1.85	0.41
1:B:175:LEU:HD21	1:B:253:ILE:HG12	2.03	0.41
1:B:390:THR:O	1:B:391:PRO:C	2.58	0.41
1:A:51:LYS:HE2	1:A:223:CYS:SG	2.61	0.41
1:A:24:ASN:CG	1:A:25:PRO:HD2	2.40	0.41
1:A:146:CYS:O	1:A:147:VAL:C	2.58	0.41
1:A:254:ARG:NH1	3:A:733:HOH:O	2.50	0.41
1:B:30:LEU:HD23	1:B:396:ALA:HA	2.03	0.41
1:B:407:SER:O	1:B:411:ASN:ND2	2.54	0.41
1:B:49:GLN:HG3	1:B:159:LEU:HD11	2.01	0.41
1:B:466:LEU:HD21	1:B:551:PHE:HE2	1.86	0.41
1:B:547:LEU:O	1:B:550:TRP:HB2	2.20	0.41
1:A:82:LEU:HD12	1:A:173:MET:O	2.20	0.41
1:B:197:PRO:O	1:B:201:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:O	1:B:114:ARG:C	2.55	0.41
1:A:385:THR:OG1	1:A:386:ARG:N	2.54	0.41
1:A:7:THR:HG23	1:A:275:GLY:HA2	2.02	0.41
1:A:524:TYR:CD2	1:A:536:LEU:HD22	2.55	0.41
1:B:67:VAL:HG12	1:B:297:LEU:HD12	2.03	0.41
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.99	0.41
1:B:508:ARG:HG2	1:B:508:ARG:NH1	2.36	0.41
1:A:30:LEU:HB2	1:A:428:HIS:CE1	2.57	0.40
1:B:361:GLU:HG2	1:B:370:VAL:O	2.21	0.40
1:A:72:LYS:HB3	1:B:76:SER:HB2	2.03	0.40
1:A:86:GLU:HG2	1:A:111:LEU:HD11	2.04	0.40
1:A:197:PRO:O	1:A:201:VAL:HG23	2.20	0.40
1:B:336:LEU:HD21	1:B:354:PRO:O	2.22	0.40
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.77	0.40
1:B:433:LEU:HA	1:B:433:LEU:HD23	1.95	0.40
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.74	0.40
1:A:561:TYR:CE2	1:A:563:SER:HA	2.56	0.40
1:A:292:THR:HG23	1:A:315:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/576 (96%)	525 (95%)	28 (5%)	2 (0%)	39	56
1	B	554/576 (96%)	516 (93%)	31 (6%)	7 (1%)	15	21
All	All	1109/1152 (96%)	1041 (94%)	59 (5%)	9 (1%)	24	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	525	LEU
1	B	538	PRO
1	B	310	ASP
1	B	533	LYS
1	A	15	ALA
1	A	82	LEU
1	B	526	PHE
1	B	539	ILE
1	B	23	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	477/491 (97%)	463 (97%)	14 (3%)	50 71
1	B	475/491 (97%)	463 (98%)	12 (2%)	55 76
All	All	952/982 (97%)	926 (97%)	26 (3%)	52 73

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	31	LEU
1	A	32	ARG
1	A	81	LYS
1	A	184	GLN
1	A	248	GLU
1	A	273	ASN
1	A	274	CYS
1	A	336	LEU
1	A	337	ARG
1	A	381	VAL
1	A	461	GLN
1	A	488	CYS
1	A	547	LEU
1	B	32	ARG

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Mol	Chain	Res	Type
1	B	182	LEU
1	B	197	PRO
1	B	309	GLN
1	B	310	ASP
1	B	319	ASP
1	B	398	GLU
1	B	431	SER
1	B	465	ARG
1	B	514	GLN
1	B	531	ARG
1	B	545	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	273	ASN
1	A	374	HIS
1	A	406	ASN
1	A	438	GLN
1	A	483	ASN
1	A	514	GLN
1	A	544	GLN
1	A	562	HIS
1	B	95	HIS
1	B	110	ASN
1	B	251	GLN
1	B	273	ASN
1	B	309	GLN
1	B	527	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	1JL	A	601	-	26,29,29	2.89	13 (50%)	37,41,41	0.93	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1JL	A	601	-	-	0/15/19/19	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1JL	C23-C22	2.01	1.43	1.38
2	A	601	1JL	C25-C26	2.09	1.43	1.38
2	A	601	1JL	C5-C6	2.10	1.42	1.38
2	A	601	1JL	C22-C21	2.38	1.43	1.38
2	A	601	1JL	C1-C6	2.39	1.42	1.38
2	A	601	1JL	C26-C21	2.87	1.44	1.38
2	A	601	1JL	C16-C11	3.06	1.44	1.39
2	A	601	1JL	C16-C15	3.29	1.44	1.38
2	A	601	1JL	O8-S7	3.47	1.47	1.43
2	A	601	1JL	O9-S7	3.97	1.47	1.43
2	A	601	1JL	C11-N10	4.10	1.50	1.42
2	A	601	1JL	C12-C11	4.28	1.46	1.40
2	A	601	1JL	S7-N10	8.68	1.78	1.63

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	1JL	C13-C12-C11	2.98	120.67	117.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	1JL	1	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	559/576 (97%)	0.39	13 (2%) 64 63	19, 32, 47, 61	0
1	B	558/576 (96%)	0.83	72 (12%) 5 5	20, 40, 57, 62	0
All	All	1117/1152 (96%)	0.61	85 (7%) 17 16	19, 35, 54, 62	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	ALA	7.2
1	B	23	ILE	6.3
1	B	547	LEU	5.5
1	A	23	ILE	5.4
1	B	153	GLY	5.1
1	B	27	SER	4.7
1	B	469	LEU	4.3
1	B	468	GLY	3.9
1	B	528	TRP	3.9
1	B	532	THR	3.8
1	B	474	LEU	3.8
1	B	526	PHE	3.8
1	B	530	VAL	3.7
1	B	525	LEU	3.7
1	B	541	ALA	3.7
1	B	457	LEU	3.4
1	B	529	ALA	3.3
1	B	15	ALA	3.3
1	B	531	ARG	3.3
1	B	24	ASN	3.3
1	B	536	LEU	3.2
1	B	14	CYS	3.1
1	A	545	LEU	3.0
1	B	440	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	550	TRP	3.0
1	B	39	ALA	2.9
1	B	30	LEU	2.9
1	B	524	TYR	2.8
1	B	303	CYS	2.7
1	A	31	LEU	2.7
1	B	511	LEU	2.7
1	B	438	GLN	2.7
1	B	31	LEU	2.7
1	B	527	ASN	2.6
1	A	402	HIS	2.6
1	B	10	LEU	2.6
1	B	545	LEU	2.6
1	B	306	ALA	2.6
1	B	402	HIS	2.6
1	B	367	SER	2.6
1	A	544	GLN	2.6
1	B	534	LEU	2.5
1	B	561	TYR	2.5
1	B	329	THR	2.5
1	B	535	LYS	2.5
1	B	507	VAL	2.5
1	B	307	LYS	2.5
1	B	543	SER	2.5
1	B	26	LEU	2.5
1	B	159	LEU	2.5
1	B	539	ILE	2.5
1	B	546	ASP	2.4
1	B	533	LYS	2.4
1	B	423	MET	2.4
1	B	95	HIS	2.4
1	B	25	PRO	2.3
1	B	308	LEU	2.3
1	B	312	THR	2.3
1	B	373	ALA	2.3
1	B	514	GLN	2.3
1	B	362	LEU	2.3
1	A	110	ASN	2.3
1	B	477	TYR	2.3
1	B	466	LEU	2.3
1	B	18	GLU	2.2
1	B	330	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	498	ARG	2.2
1	B	471	ALA	2.2
1	B	405	ILE	2.1
1	B	430	PHE	2.1
1	B	451	CYS	2.1
1	A	309	GLN	2.1
1	B	439	LEU	2.1
1	B	540	PRO	2.1
1	A	14	CYS	2.1
1	A	57	LEU	2.1
1	B	433	LEU	2.1
1	A	563	SER	2.1
1	B	435	ALA	2.0
1	A	322	VAL	2.0
1	B	412	ILE	2.0
1	B	43	ARG	2.0
1	A	405	ILE	2.0
1	A	550	TRP	2.0
1	B	473	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	1JL	A	601	27/27	0.84	0.27	3.57	45,47,51,53	0

6.5 Other polymers (i)

There are no such residues in this entry.