Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:32 AM GMT

PDB ID	:	3F3U
Title	:	Kinase domain of cSrc in complex with inhibitor RL37 (Type III)
Authors	:	Gruetter, C.; Klueter, S.; Getlik, M.; Rauh, D.
Deposited on	:	2008-10-31
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

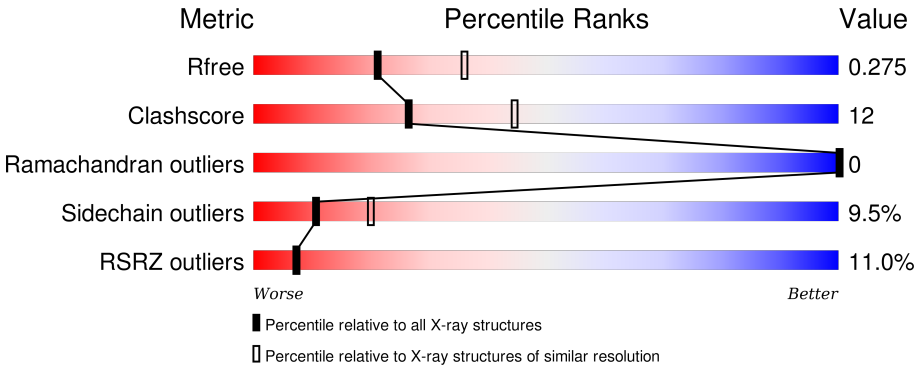
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	286	8% 63% 26% • 9%
1	B	286	12% 61% 26% • • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4355 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.

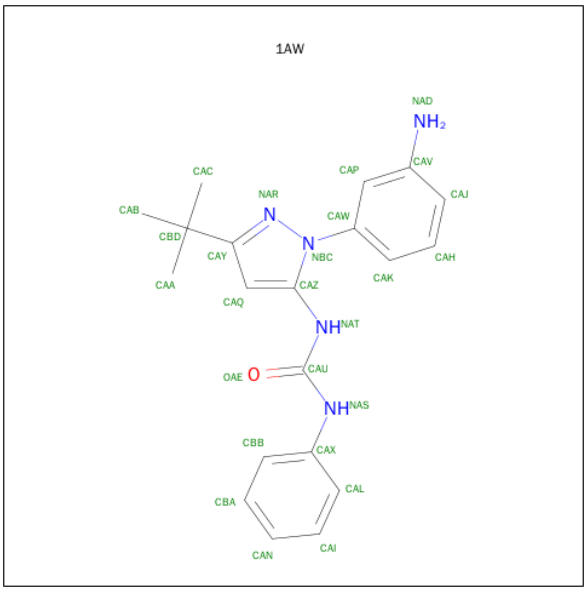
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2103	1351	350	384	18			
1	B	259	Total	C	N	O	S	0	0	0
			2088	1342	348	381	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	EXPRESSION TAG	UNP P00523
A	249	HIS	-	EXPRESSION TAG	UNP P00523
A	250	MET	-	EXPRESSION TAG	UNP P00523
A	345	CYS	SER	ENGINEERED	UNP P00523
B	248	GLY	-	EXPRESSION TAG	UNP P00523
B	249	HIS	-	EXPRESSION TAG	UNP P00523
B	250	MET	-	EXPRESSION TAG	UNP P00523
B	345	CYS	SER	ENGINEERED	UNP P00523

- Molecule 2 is 1-[1-(3-AMINOPHENYL)-3-TERT-BUTYL-1H-PYRAZOL-5-YL]-3-PHENYLUREA (three-letter code: 1AW) (formula: $C_{20}H_{23}N_5O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 26 20 5 1	0	0
2	A	1	Total C N O 26 20 5 1	0	0
2	B	1	Total C N O 26 20 5 1	0	0

- Molecule 3 is water.

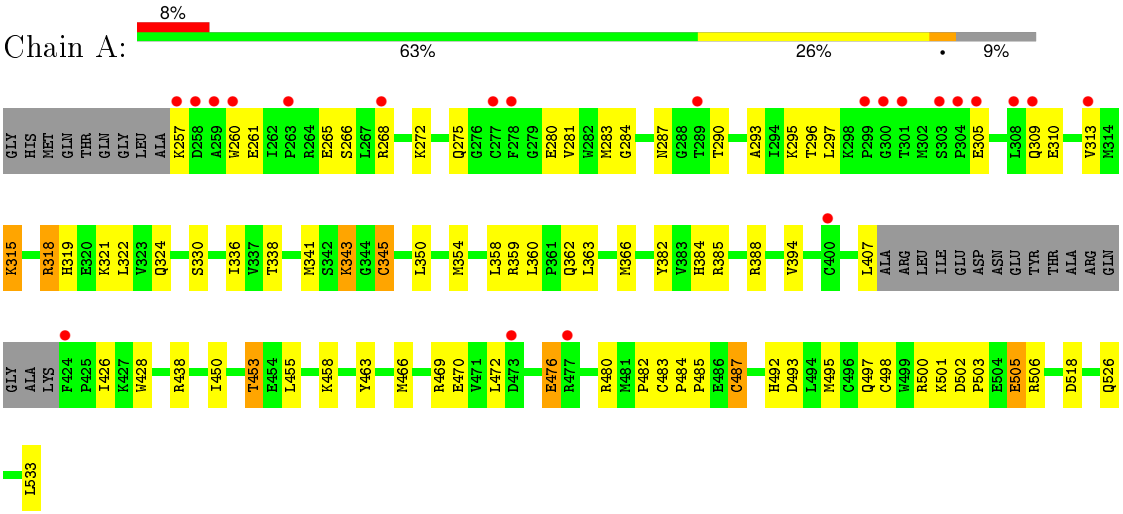
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	45	Total O 45 45	0	0

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.

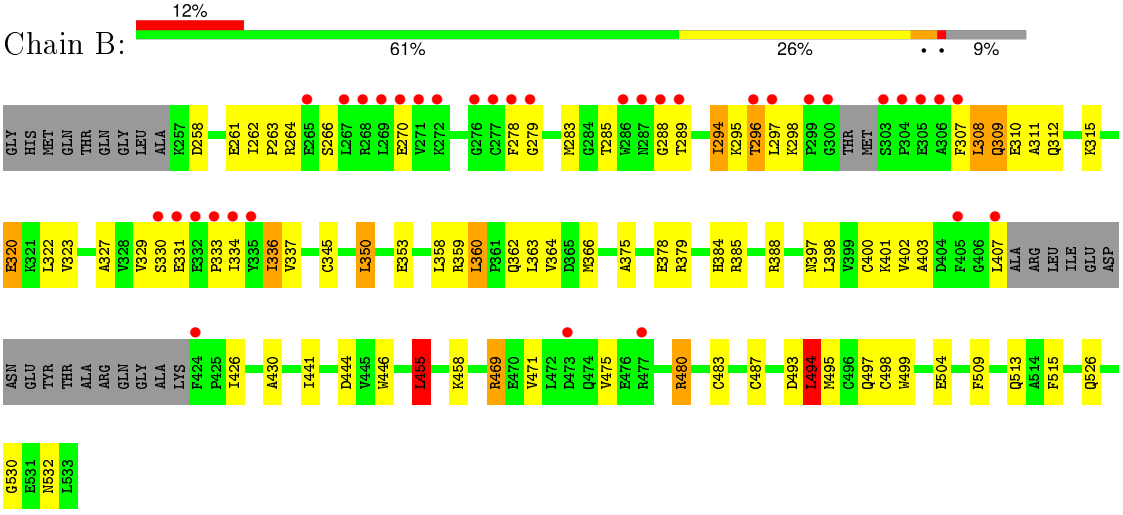
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain A:



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.09Å 63.53Å 73.99Å 78.94° 89.37° 90.06°	Depositor
Resolution (Å)	36.59 – 2.50 36.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.59-2.50) 91.6 (36.59-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.281 0.219 , 0.275	Depositor DCC
R_{free} test set	1014 reflections (4.17%)	DCC
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.1	EDS
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 25330 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4355	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.49% 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: 1AW

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	0.82	1/2155 (0.0%)	0.83	2/2917 (0.1%)
1	B	0.83	2/2139 (0.1%)	0.87	6/2894 (0.2%)
All	All	0.82	3/4294 (0.1%)	0.85	8/5811 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	CYS	CB-SG	-7.71	1.69	1.82
1	A	505	GLU	CG-CD	6.03	1.60	1.51
1	B	400	CYS	CB-SG	-5.99	1.72	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	480	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	480	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	480	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	350	LEU	CA-CB-CG	6.06	129.25	115.30
1	B	494	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	480	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	444	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	455	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2103	0	2089	47	0
1	B	2088	0	2072	54	0
2	A	52	0	46	7	0
2	B	26	0	23	3	0
3	A	41	0	0	3	0
3	B	45	0	0	3	0
All	All	4355	0	4230	104	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 12.

All (104) 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:A:345:CYS:SG	2:A:534:1AW:NAD	2.32	1.01
1:B:294:ILE:HG23	1:B:337:VAL:HG22	1.52	0.90
1:B:285:THR:HG22	1:B:288:GLY:HA2	1.57	0.86
1:A:363:LEU:HD13	1:A:455:LEU:O	1.77	0.85
1:B:263:PRO:HD2	1:B:266:SER:OG	1.83	0.79
1:B:359:ARG:H	1:B:362:GLN:HE21	1.33	0.76
1:B:469:ARG:CG	1:B:469:ARG:HH11	1.98	0.74
1:B:310:GLU:HG3	2:B:1:1AW:CAV	2.18	0.74
1:A:453:THR:HG23	3:A:18:HOH:O	1.87	0.74
1:B:493:ASP:O	1:B:497:GLN:HG3	1.88	0.74
1:B:469:ARG:HH11	1:B:469:ARG:HG2	1.53	0.73
1:B:285:THR:CG2	1:B:288:GLY:HA2	2.19	0.73
1:A:322:LEU:HD13	2:A:1:1AW:HAB	1.72	0.72
1:A:266:SER:HB2	1:A:287:ASN:HD22	1.58	0.69
1:B:298:LYS:HB3	1:B:333:PRO:HB3	1.73	0.68
1:B:526:GLN:HG2	3:B:8:HOH:O	1.94	0.68
1:A:500:ARG:HD3	1:A:505:GLU:HB3	1.76	0.67
1:B:494:LEU:HG	1:B:515:PHE:CE1	2.30	0.67
1:A:313:VAL:HG11	1:A:382:TYR:OH	1.94	0.67
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.31	0.65
1:B:359:ARG:H	1:B:362:GLN:NE2	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLU:OE1	1:A:476:GLU:HA	1.97	0.64
1:B:323:VAL:HG21	1:B:403:ALA:HB2	1.81	0.62
1:A:281:VAL:HG23	2:A:534:1AW:HABB	1.84	0.60
1:B:310:GLU:HG3	2:B:1:1AW:CAP	2.35	0.57
1:B:323:VAL:HG23	1:B:402:VAL:O	2.05	0.57
1:A:450:ILE:O	1:A:453:THR:HG22	2.06	0.56
1:A:426:ILE:HD11	1:A:472:LEU:HD21	1.87	0.56
1:A:518:ASP:OD2	3:A:85:HOH:O	2.18	0.54
1:A:280:GLU:H	1:A:296:THR:HB	1.72	0.54
1:A:260:TRP:CZ2	1:A:315:LYS:HG2	2.43	0.54
1:B:378:GLU:HB2	1:B:441:ILE:HG12	1.89	0.54
1:B:322:LEU:HD22	1:B:402:VAL:HB	1.90	0.53
1:B:363:LEU:HD13	1:B:455:LEU:O	2.09	0.53
1:B:430:ALA:HB2	1:B:446:TRP:CB	2.38	0.53
1:A:463:TYR:HA	3:A:48:HOH:O	2.08	0.52
1:B:320:GLU:O	1:B:401:LYS:HE2	2.10	0.52
1:A:319:HIS:CD2	1:A:321:LYS:H	2.28	0.52
1:A:266:SER:HB2	1:A:287:ASN:ND2	2.25	0.51
1:B:469:ARG:CG	1:B:469:ARG:NH1	2.64	0.51
1:B:261:GLU:OE1	1:B:330:SER:HB2	2.11	0.51
1:B:311:ALA:O	1:B:315:LYS:HG3	2.11	0.50
1:B:264:ARG:HE	1:B:329:VAL:HG11	1.76	0.50
1:B:279:GLY:HA3	1:B:296:THR:O	2.12	0.50
1:A:438:ARG:HH21	1:A:503:PRO:HG2	1.75	0.50
1:A:261:GLU:OE1	1:A:330:SER:HB2	2.11	0.49
1:B:307:PHE:HE2	1:B:334:ILE:CD1	2.25	0.49
1:B:309:GLN:HA	1:B:312:GLN:HG2	1.93	0.49
1:B:397:ASN:O	1:B:398:LEU:HB2	2.11	0.49
1:A:384:HIS:O	1:A:385:ARG:HB2	2.12	0.49
1:A:309:GLN:NE2	1:A:309:GLN:HA	2.27	0.49
1:B:359:ARG:HB2	1:B:362:GLN:HE22	1.78	0.49
1:B:310:GLU:OE1	1:B:336:ILE:HD12	2.13	0.49
2:B:1:1AW:HAP	2:B:1:1AW:NAT	2.28	0.49
1:A:341:MET:H	2:A:534:1AW:HAN	1.76	0.48
1:A:493:ASP:O	1:A:497:GLN:HG3	2.13	0.48
1:B:307:PHE:CE2	1:B:334:ILE:HD11	2.49	0.48
1:A:318:ARG:NH1	1:A:318:ARG:HB3	2.28	0.48
2:A:1:1AW:HAL	2:A:1:1AW:OAE	2.14	0.48
1:B:285:THR:HG22	1:B:288:GLY:CA	2.35	0.48
1:B:358:LEU:O	1:B:458:LYS:NZ	2.46	0.47
1:B:307:PHE:HE2	1:B:334:ILE:HD11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:GLN:CG	3:B:8:HOH:O	2.57	0.47
1:A:483:CYS:SG	1:A:487:CYS:O	2.72	0.47
1:A:426:ILE:CD1	1:A:472:LEU:HD21	2.45	0.47
1:A:260:TRP:HE1	1:A:315:LYS:HD2	1.80	0.46
1:B:530:GLY:HA3	3:B:77:HOH:O	2.15	0.46
1:A:492:HIS:O	1:A:495:MET:HB2	2.16	0.46
1:A:426:ILE:O	1:A:426:ILE:HG13	2.15	0.46
1:A:319:HIS:HD2	1:A:321:LYS:H	1.63	0.46
1:A:283:MET:HG2	1:A:284:GLY:N	2.30	0.45
1:A:358:LEU:O	1:A:458:LYS:NZ	2.49	0.45
1:A:272:LYS:CE	1:A:275:GLN:HB3	2.47	0.45
1:A:295:LYS:HB3	1:A:336:ILE:HB	1.99	0.45
1:A:293:ALA:HB3	1:A:338:THR:OG1	2.16	0.45
1:B:471:VAL:O	1:B:475:VAL:HG13	2.17	0.44
1:B:362:GLN:O	1:B:366:MET:HG3	2.18	0.44
1:B:308:LEU:HD22	1:B:308:LEU:HA	1.80	0.44
1:B:295:LYS:HE2	1:B:307:PHE:HZ	1.82	0.43
1:B:480:ARG:NH2	1:B:499:TRP:O	2.50	0.43
1:A:482:PRO:O	1:A:484:PRO:HD3	2.18	0.43
1:B:262:ILE:HG12	1:B:327:ALA:HB1	2.00	0.43
1:A:343:LYS:HB2	1:A:394:VAL:O	2.18	0.43
1:A:358:LEU:O	1:A:359:ARG:NH1	2.40	0.43
1:B:384:HIS:O	1:B:385:ARG:HB2	2.19	0.43
2:A:534:1AW:OAE	2:A:534:1AW:HAL	2.18	0.43
1:B:334:ILE:HD12	1:B:334:ILE:C	2.39	0.43
1:B:458:LYS:NZ	1:B:532:ASN:O	2.52	0.42
1:A:466:MET:HA	1:A:470:GLU:OE1	2.19	0.42
1:A:485:PRO:O	1:A:533:LEU:HD12	2.19	0.42
1:B:495:MET:O	1:B:498:CYS:HB2	2.19	0.42
1:A:318:ARG:NH2	1:A:324:GLN:NE2	2.67	0.42
1:B:294:ILE:CG2	1:B:337:VAL:HG22	2.35	0.42
1:B:483:CYS:SG	1:B:487:CYS:O	2.78	0.42
1:B:509:PHE:O	1:B:513:GLN:N	2.45	0.41
1:A:310:GLU:HA	2:A:1:1AW:CAH	2.50	0.41
1:A:502:ASP:HB3	1:A:505:GLU:OE1	2.19	0.41
1:A:426:ILE:HD11	1:A:472:LEU:CD2	2.51	0.41
1:B:375:ALA:O	1:B:379:ARG:HG3	2.21	0.41
1:A:498:CYS:O	1:A:506:ARG:HD3	2.19	0.41
1:A:362:GLN:O	1:A:366:MET:HG3	2.21	0.40
1:B:262:ILE:HD12	1:B:266:SER:HB2	2.04	0.40
1:B:360:LEU:HD22	1:B:364:VAL:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:GLU:HB2	1:B:441:ILE:CD1	2.52	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	257/286 (90%)	242 (94%)	15 (6%)	0	100	100
1	B	253/286 (88%)	235 (93%)	18 (7%)	0	100	100
All	All	510/572 (89%)	477 (94%)	33 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	227/245 (93%)	207 (91%)	20 (9%)	12	23
1	B	225/245 (92%)	202 (90%)	23 (10%)	9	17
All	All	452/490 (92%)	409 (90%)	43 (10%)	11	20

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LYS
1	A	265	GLU
1	A	268	ARG
1	A	290	THR
1	A	297	LEU
1	A	305	GLU
1	A	315	LYS
1	A	318	ARG
1	A	343	LYS
1	A	345	CYS
1	A	350	LEU
1	A	354	MET
1	A	360	LEU
1	A	407	LEU
1	A	453	THR
1	A	469	ARG
1	A	476	GLU
1	A	487	CYS
1	A	501	LYS
1	A	526	GLN
1	B	258	ASP
1	B	270	GLU
1	B	278	PHE
1	B	283	MET
1	B	289	THR
1	B	294	ILE
1	B	296	THR
1	B	297	LEU
1	B	308	LEU
1	B	309	GLN
1	B	320	GLU
1	B	331	GLU
1	B	336	ILE
1	B	350	LEU
1	B	353	GLU
1	B	360	LEU
1	B	388	ARG
1	B	407	LEU
1	B	426	ILE
1	B	455	LEU
1	B	469	ARG
1	B	494	LEU
1	B	504	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
1	A	309	GLN
1	A	319	HIS
1	A	397	ASN
1	B	362	GLN
1	B	528	GLN

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)

3 ligands are 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	1AW	A	1	-	27,28,28	2.46	5 (18%)	32,40,40	1.34	3 (9%)
2	1AW	A	534	-	27,28,28	2.32	5 (18%)	32,40,40	1.50	3 (9%)
2	1AW	B	1	-	27,28,28	2.36	5 (18%)	32,40,40	1.50	4 (12%)

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	1AW	A	1	-	-	0/16/18/18	0/3/3/3
2	1AW	A	534	-	-	0/16/18/18	0/3/3/3
2	1AW	B	1	-	-	0/16/18/18	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	1AW	NAR-NBC	-8.86	1.23	1.39
2	B	1	1AW	NAR-NBC	-8.76	1.23	1.39
2	A	534	1AW	NAR-NBC	-8.35	1.24	1.39
2	B	1	1AW	CAQ-CAY	-4.93	1.33	1.39
2	A	534	1AW	CAW-NBC	-4.79	1.34	1.44
2	B	1	1AW	CAW-NBC	-4.52	1.34	1.44
2	A	1	1AW	CAW-NBC	-4.51	1.34	1.44
2	A	1	1AW	CAQ-CAY	-4.47	1.33	1.39
2	A	1	1AW	CAX-NAS	-4.17	1.33	1.41
2	A	534	1AW	CAQ-CAY	-3.46	1.35	1.39
2	A	534	1AW	CAX-NAS	-3.11	1.35	1.41
2	B	1	1AW	CAZ-NAT	-2.86	1.34	1.39
2	B	1	1AW	CAX-NAS	-2.03	1.37	1.41
2	A	1	1AW	CAP-CAW	2.20	1.41	1.38
2	A	534	1AW	CBD-CAY	3.80	1.58	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	534	1AW	CAW-NBC-CAZ	-4.80	123.50	129.02
2	B	1	1AW	CAQ-CAY-CBD	-2.98	125.47	129.15
2	B	1	1AW	CAK-CAW-CAP	-2.81	118.96	121.50
2	A	534	1AW	CAQ-CAY-CBD	-2.55	126.01	129.15
2	A	1	1AW	CAQ-CAY-CBD	-2.43	126.16	129.15
2	B	1	1AW	NAT-CAU-NAS	3.11	117.42	112.53
2	A	1	1AW	CAP-CAW-NBC	3.33	123.20	119.13
2	A	1	1AW	CBD-CAY-NAR	3.80	124.61	120.58
2	B	1	1AW	CBD-CAY-NAR	4.18	125.02	120.58
2	A	534	1AW	CBD-CAY-NAR	4.52	125.38	120.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	1AW	3	0
2	A	534	1AW	4	0
2	B	1	1AW	3	0

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, 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	261/286 (91%)	0.45	22 (8%) 14 14	2, 15, 45, 49	0
1	B	259/286 (90%)	0.68	35 (13%) 4 4	4, 15, 50, 54	0
All	All	520/572 (90%)	0.57	57 (10%) 7 7	2, 15, 48, 54	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	LEU	6.4
1	B	268	ARG	6.0
1	B	304	PRO	4.7
1	B	278	PHE	4.6
1	A	300	GLY	4.5
1	B	424	PHE	4.5
1	B	335	TYR	4.5
1	B	289	THR	4.4
1	A	257	LYS	4.4
1	B	306	ALA	4.4
1	A	305	GLU	4.3
1	B	305	GLU	4.3
1	B	267	LEU	4.2
1	B	277	CYS	4.2
1	A	304	PRO	4.0
1	B	330	SER	4.0
1	B	276	GLY	3.9
1	A	313	VAL	3.8
1	B	288	GLY	3.7
1	B	331	GLU	3.5
1	A	301	THR	3.3
1	A	473	ASP	3.2
1	A	289	THR	3.2
1	B	265	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	303	SER	3.1
1	A	309	GLN	3.0
1	A	424	PHE	3.0
1	A	277	CYS	3.0
1	A	303	SER	2.9
1	B	407	LEU	2.8
1	B	334	ILE	2.8
1	B	271	VAL	2.8
1	B	332	GLU	2.8
1	B	300	GLY	2.8
1	B	473	ASP	2.7
1	B	477	ARG	2.7
1	B	269	LEU	2.7
1	A	258	ASP	2.7
1	B	299	PRO	2.6
1	B	272	LYS	2.6
1	A	477	ARG	2.6
1	B	270	GLU	2.6
1	B	286	TRP	2.5
1	A	260	TRP	2.5
1	A	278	PHE	2.4
1	A	308	LEU	2.4
1	B	279	GLY	2.4
1	B	333	PRO	2.3
1	B	405	PHE	2.3
1	A	259	ALA	2.3
1	A	299	PRO	2.2
1	B	287	ASN	2.2
1	A	268	ARG	2.1
1	B	307	PHE	2.1
1	A	400	CYS	2.1
1	B	296	THR	2.0
1	A	263	PRO	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

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	1AW	A	534	26/26	0.88	0.21	1.42	49,54,55,55	0
2	1AW	B	1	26/26	0.87	0.21	0.37	57,63,64,64	0
2	1AW	A	1	26/26	0.93	0.17	-0.19	34,35,41,43	0

6.5 Other polymers

There are no such residues in this entry.