



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:45 PM GMT

PDB ID : 4PUZ
Title : Crystal structure of spleen tyrosine kinase (Syk) in complex with GS-9973
Authors : Lansdon, E.B.; Mitchell, S.A.
Deposited on : 2014-03-14
Resolution : 2.08 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

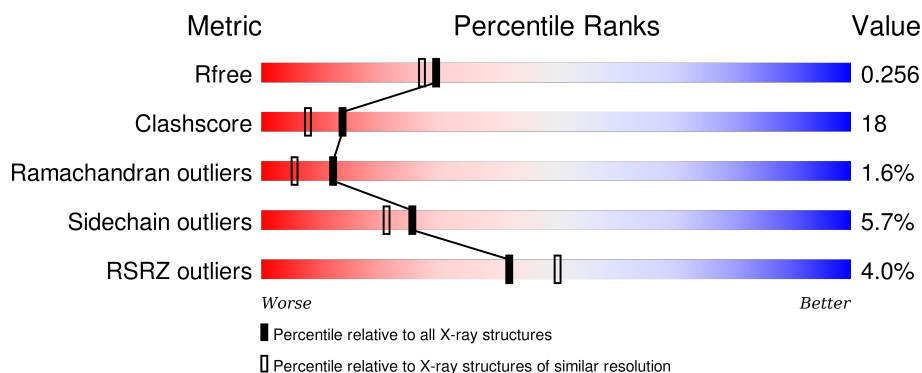
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	4546 (2.10-2.06)
Clashscore	102246	5101 (2.10-2.06)
Ramachandran outliers	100387	5048 (2.10-2.06)
Sidechain outliers	100360	5049 (2.10-2.06)
RSRZ outliers	91569	4556 (2.10-2.06)

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 $\leq 5\%$. 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	A	291	<div> <div>3%</div> <div>57%</div> <div>30%</div> <div>•</div> <div>10%</div> </div>
1	B	291	<div> <div>4%</div> <div>60%</div> <div>29%</div> <div>•</div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4479 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.

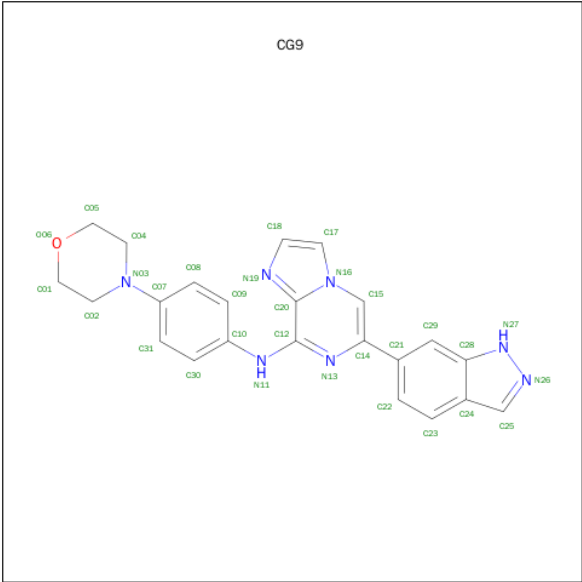
- Molecule 1 is a protein called Tyrosine-protein kinase SYK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2145	1381	359	386	19			
1	B	265	Total	C	N	O	S	0	0	0
			2160	1390	362	389	19			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	MET	ALA	CONFLICT	UNP P43405
A	354	ALA	ASP	CONFLICT	UNP P43405
A	355	LEU	PRO	CONFLICT	UNP P43405
A	636	GLU	-	EXPRESSION TAG	UNP P43405
A	637	GLY	-	EXPRESSION TAG	UNP P43405
A	638	HIS	-	EXPRESSION TAG	UNP P43405
A	639	HIS	-	EXPRESSION TAG	UNP P43405
A	640	HIS	-	EXPRESSION TAG	UNP P43405
A	641	HIS	-	EXPRESSION TAG	UNP P43405
A	642	HIS	-	EXPRESSION TAG	UNP P43405
A	643	HIS	-	EXPRESSION TAG	UNP P43405
B	353	MET	ALA	CONFLICT	UNP P43405
B	354	ALA	ASP	CONFLICT	UNP P43405
B	355	LEU	PRO	CONFLICT	UNP P43405
B	636	GLU	-	EXPRESSION TAG	UNP P43405
B	637	GLY	-	EXPRESSION TAG	UNP P43405
B	638	HIS	-	EXPRESSION TAG	UNP P43405
B	639	HIS	-	EXPRESSION TAG	UNP P43405
B	640	HIS	-	EXPRESSION TAG	UNP P43405
B	641	HIS	-	EXPRESSION TAG	UNP P43405
B	642	HIS	-	EXPRESSION TAG	UNP P43405
B	643	HIS	-	EXPRESSION TAG	UNP P43405

- Molecule 2 is 6-(1H-INDAZOL-6-YL)-N-[4-(MORPHOLIN-4-YL)PHENYL]IMIDAZO[1,2-A]PYRAZIN-8-AMINE (three-letter code: CG9) (formula: C₂₃H₂₁N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	23	7	1		
2	B	1	Total	C	N	O	0	0
			31	23	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	64	Total	O	0	0
			64	64		

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.

Chain A:

57% 30% 3% 10%

Sequence logo for Chain A (48 amino acids):

Position	Amino Acid	Category
1	V433	Yellow
2	A441	Yellow
3	E442	Yellow
4	S443	Yellow
5	W444	Yellow
6	M450	Yellow
7	A451	Yellow
8	E452	Yellow
9	Y459	Yellow
10	Q462	Green
11	M463	Green
12	L464	Green
13	H465	Orange
14	V466	Orange
15	K467	Orange
16	D468	Orange
17	I471	Orange
18	I472	Orange
19	E473	Orange
20	Q477	Yellow
21	M482	Yellow
22	K483	Yellow
23	E486	Yellow
24	E487	Yellow
25	F490	Yellow
26	V491	Yellow
27	H492	Yellow
28	K493	Yellow
29	Q505	Orange
30	H506	Orange
31	Y507	Yellow
32	A508	Green
33	K509	Green
34	L510	Yellow
35	S516	Yellow
36	V517	Yellow
37	A518	Yellow
38	L519	Yellow
39	R520	Yellow
40	A521	Yellow
41	D522	Yellow
42	Q529	Green
43	THR	Grey
44	HIS	Grey
45	GLY	Grey
46	K533	Green
47	H534	Grey
48	D535	Grey

Chain B:

60% 29% 9%

Residue	Category
Q529	Green
THR	Green
HIS	Green
HIS	Green
K593	Green
A540	Green
K552	Green
V555	Green
W556	Green
L561	Green
S567	Green
K577	Green
G578	Green
S579	Green
E580	Green
A583	Green
K587	Green
M591	Green
G592	Green
C593	Green
P594	Green
C597	Green
P598	Green
M601	Green
Y602	Green
M605	Green
M606	Green
L607	Green
P617	Green
G618	Green
V622	Green
G623	Green
L624	Green
G625	Green
L626	Green
Y631	Green
D632	Green
V633	Green
G634	Green
M635	Green
GLU	Green
GLY	Green
HIS	Green
HIS	Green
HIS	Green
Q425	Green
Q426	Green
N429	Green
P430	Green
M435	Green
I436	Green
G437	Green
I438	Green
A441	Green
E442	Green
S443	Green
W444	Green
N445	Green
L446	Green
E449	Green
M450	Green
A451	Green
E452	Green
N463	Green
R464	Green
H465	Green
V466	Green
K467	Green
D468	Green
K469	Green
I472	Green
H476	Green
K483	Green
Y484	Green
L485	Green
E486	Green
E487	Green
H492	Green
R493	Green
V500	Green
L501	Green
V502	Green
V503	Green
Y504	Green
Y507	Green
L515	Green
S516	Green
K517	Green
N524	Green
Y525	Green
Y526	Green
M363	Yellow
D366	Yellow
R367	Yellow
K368	Yellow
L369	Yellow
I370	Yellow
T371	Yellow
D374	Yellow
L377	Yellow
G378	Yellow
N381	Yellow
F382	Yellow
G383	Yellow
K386	Yellow
K387	Yellow
G388	Yellow
Q391	Yellow
M392	Yellow
K393	Yellow
K394	Yellow
V395	Yellow
V396	Yellow
L404	Yellow
K405	Yellow
ASN	Yellow
GLU	Yellow
ALA	Yellow
ASN	Yellow
ASP	Yellow
P411	Yellow
A412	Yellow
L413	Yellow
K414	Yellow
D415	Yellow
E416	Yellow
I417	Yellow
L418	Yellow
A419	Yellow
E420	Yellow
A421	Yellow
N422	Yellow
Y423	Yellow
M424	Yellow
ALA	Grey
GLU	Grey
ALA	Grey
ASN	Grey
ASP	Grey
P411	Grey
A412	Grey
L413	Grey
K414	Grey
D415	Grey
E416	Grey
I417	Grey
L418	Grey
A419	Grey
E420	Grey
A421	Grey
N422	Grey
Y423	Grey
M424	Grey

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.88Å 41.88Å 87.41Å 98.67° 90.43° 101.38°	Depositor
Resolution (Å)	43.17 – 2.08 43.17 – 2.09	Depositor EDS
% Data completeness (in resolution range)	81.3 (43.17-2.08) 78.7 (43.17-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.209 , 0.261 0.208 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (8.10%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28645 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4479	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CG9

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	0.44	0/2193	0.59	0/2952
1	B	0.46	0/2208	0.59	0/2973
All	All	0.45	0/4401	0.59	0/5925

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 [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	2145	0	2143	79	0
1	B	2160	0	2158	81	0
2	A	31	0	21	3	0
2	B	31	0	21	4	0
3	A	48	0	0	3	0
3	B	64	0	0	3	0
All	All	4479	0	4343	161	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 18.

All (161) 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:414:LYS:HE3	1:A:444:TRP:NE1	1.75	0.99
1:A:382:PHE:HA	1:A:413:LEU:HD23	1.51	0.92
1:A:414:LYS:HE3	1:A:444:TRP:HE1	1.33	0.88
1:B:594:PRO:HG2	1:B:597:CYS:HB2	1.61	0.83
1:A:450:MET:HG3	1:A:452:GLU:HG2	1.62	0.80
1:A:590:ARG:HB2	1:B:396:VAL:HG12	1.65	0.79
1:A:390:TYR:HD2	1:A:392:MET:HE2	1.48	0.77
1:B:634:VAL:O	1:B:634:VAL:HG12	1.85	0.77
1:A:390:TYR:HD2	1:A:392:MET:CE	1.97	0.76
1:B:529:GLN:HA	1:B:529:GLN:OE1	1.85	0.75
1:A:601:MET:O	1:A:605:MET:HG3	1.87	0.75
2:A:701:CG9:H20	2:A:701:CG9:N13	2.02	0.74
1:A:471:ILE:HD12	1:A:471:ILE:N	2.03	0.73
1:B:404:LEU:HD11	1:B:414:LYS:HA	1.72	0.72
1:B:503:VAL:HG21	1:B:507:TYR:CD1	2.24	0.72
1:A:414:LYS:CE	1:A:444:TRP:HE1	2.04	0.71
1:A:471:ILE:CD1	1:A:471:ILE:N	2.55	0.69
1:A:594:PRO:HG2	1:A:597:CYS:HB2	1.73	0.69
2:B:701:CG9:H20	2:B:701:CG9:N13	2.10	0.67
1:A:459:TYR:OH	1:A:505:GLN:HG3	1.95	0.67
1:B:503:VAL:HG23	1:B:504:THR:N	2.11	0.66
1:A:404:LEU:HD11	1:A:414:LYS:HA	1.78	0.65
1:B:503:VAL:CG2	1:B:507:TYR:HB3	2.26	0.65
1:B:417:LEU:HB3	1:B:444:TRP:CZ3	2.32	0.65
1:B:415:ASP:O	1:B:418:LEU:HG	1.98	0.64
1:B:363:VAL:HG12	1:B:363:VAL:O	1.97	0.64
1:B:463:ASN:O	1:B:466:VAL:HG23	1.99	0.63
1:B:634:VAL:O	1:B:634:VAL:CG1	2.46	0.63
1:B:418:LEU:HD12	1:B:419:ALA:N	2.14	0.63
1:A:483:LYS:O	1:A:487:GLU:HG3	1.99	0.63
1:A:467:LYS:O	1:A:471:ILE:HD11	1.99	0.63
1:B:476:HIS:HA	1:B:626:LEU:HD13	1.80	0.63
1:B:393:LYS:O	1:B:393:LYS:HG3	1.99	0.63
1:B:567:SER:OG	1:B:594:PRO:HB3	1.99	0.62
1:A:486:GLU:HG3	1:A:551:SER:CB	2.29	0.62
1:A:490:PHE:CE2	1:A:518:ALA:HB2	2.34	0.62
1:A:520:ARG:NH1	1:A:522:ASP:OD2	2.29	0.62
1:A:413:LEU:HD12	1:A:413:LEU:H	1.65	0.61
1:A:373:GLU:HA	1:A:373:GLU:OE1	1.99	0.61
1:B:483:LYS:O	1:B:487:GLU:HG3	2.01	0.61
1:A:467:LYS:O	1:A:471:ILE:CD1	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TYR:CD2	1:A:392:MET:HE2	2.36	0.59
1:B:366:ASP:HB3	1:B:369:LEU:HG	1.85	0.58
1:B:383:GLY:HA2	1:B:405:LYS:HG3	1.85	0.58
1:B:469:LYS:HG2	1:B:469:LYS:O	2.03	0.58
1:B:420:GLU:O	1:B:424:MET:HG3	2.04	0.57
1:B:450:MET:HG3	1:B:452:GLU:HG2	1.86	0.57
1:B:503:VAL:HG23	1:B:504:THR:H	1.68	0.57
1:A:468:ASP:HA	1:A:471:ILE:HD13	1.87	0.57
1:A:628:ASN:O	1:A:630:TYR:N	2.37	0.57
1:B:415:ASP:HA	1:B:418:LEU:HG	1.87	0.56
1:B:607:LEU:HG	1:B:617:PRO:HG3	1.87	0.56
1:B:383:GLY:CA	1:B:405:LYS:HG3	2.35	0.56
1:A:618:GLY:O	1:A:622:VAL:HG23	2.07	0.55
1:A:391:GLN:CD	3:A:809:HOH:O	2.45	0.55
1:B:503:VAL:HG22	1:B:507:TYR:O	2.07	0.54
1:B:501:LEU:HD13	2:B:701:CG9:C20	2.38	0.54
1:B:601:MET:O	1:B:605:MET:HG3	2.08	0.54
1:B:493:ARG:HD3	1:B:515:LEU:O	2.07	0.54
1:B:625:ARG:NH2	3:B:850:HOH:O	2.37	0.54
1:A:486:GLU:HG3	1:A:551:SER:OG	2.08	0.54
1:B:561:LEU:HD23	1:B:561:LEU:C	2.28	0.54
1:A:450:MET:CG	1:A:452:GLU:HG2	2.37	0.54
1:A:628:ASN:O	1:A:629:TYR:C	2.45	0.53
1:A:390:TYR:CD2	1:A:392:MET:CE	2.87	0.53
1:A:593:CYS:H	1:B:391:GLN:HE22	1.57	0.52
1:A:466:VAL:HG12	1:A:467:LYS:O	2.08	0.52
1:B:435:MET:HG3	1:B:446:LEU:HD11	1.91	0.52
1:B:449:GLU:HG2	1:B:449:GLU:O	2.09	0.52
1:A:466:VAL:O	1:A:467:LYS:O	2.28	0.52
1:B:503:VAL:HG21	1:B:507:TYR:CG	2.44	0.52
1:B:369:LEU:N	1:B:369:LEU:HD23	2.24	0.52
1:B:469:LYS:HA	1:B:472:ILE:HD12	1.91	0.52
1:A:441:ALA:HB1	1:A:442:GLU:OE2	2.10	0.51
1:A:551:SER:O	1:A:555:VAL:HG23	2.11	0.51
1:A:473:GLU:O	1:A:477:GLN:HG3	2.10	0.51
1:A:413:LEU:HD12	1:A:413:LEU:N	2.25	0.51
1:A:414:LYS:HE3	1:A:444:TRP:CE2	2.43	0.50
1:B:503:VAL:CG2	1:B:504:THR:N	2.74	0.50
1:A:629:TYR:O	1:A:633:VAL:HG23	2.12	0.50
1:A:567:SER:O	1:A:570:GLN:HG3	2.12	0.50
1:B:503:VAL:CG2	1:B:504:THR:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LEU:HD23	1:A:561:LEU:C	2.32	0.49
1:B:594:PRO:HG2	1:B:597:CYS:CB	2.38	0.49
1:A:471:ILE:CD1	1:A:471:ILE:H	2.25	0.49
1:B:417:LEU:CD2	1:B:444:TRP:HZ3	2.26	0.49
1:A:630:TYR:O	1:A:633:VAL:N	2.40	0.49
1:B:517:LYS:HE3	1:B:526:TYR:CZ	2.48	0.49
1:B:552:LYS:O	1:B:555:VAL:HB	2.12	0.48
1:B:429:ASN:CG	1:B:430:PRO:HD2	2.33	0.48
1:A:590:ARG:HB2	1:B:396:VAL:CG1	2.42	0.48
1:B:597:CYS:SG	1:B:598:PRO:HD2	2.54	0.48
1:B:393:LYS:O	1:B:394:LYS:HB2	2.13	0.47
1:A:472:ILE:CG2	1:A:630:TYR:HB2	2.45	0.47
1:A:600:GLU:O	1:A:604:LEU:N	2.46	0.47
1:A:621:ALA:O	1:A:624:LEU:HB3	2.15	0.47
1:B:441:ALA:C	1:B:443:SER:N	2.68	0.47
1:A:367:ARG:NH1	1:A:370:LEU:O	2.48	0.47
1:B:463:ASN:C	1:B:465:HIS:H	2.16	0.47
1:B:503:VAL:HG23	1:B:507:TYR:HB3	1.95	0.47
1:B:441:ALA:C	1:B:443:SER:H	2.18	0.47
1:A:483:LYS:NZ	1:A:487:GLU:OE1	2.29	0.46
1:A:413:LEU:CD1	1:A:413:LEU:H	2.27	0.46
1:B:393:LYS:O	1:B:394:LYS:CB	2.64	0.46
1:A:373:GLU:CD	1:A:374:ASP:H	2.19	0.46
1:B:374:ASP:O	1:B:386:LYS:HE3	2.15	0.46
1:B:500:VAL:HG21	1:B:561:LEU:HD11	1.97	0.46
1:B:422:ASN:O	1:B:426:GLN:HG3	2.15	0.46
1:A:535:PRO:HG2	1:A:539:TYR:CE2	2.50	0.46
1:B:503:VAL:CG2	1:B:507:TYR:CG	2.99	0.45
1:B:449:GLU:HG2	3:B:811:HOH:O	2.16	0.45
1:B:533:LYS:N	3:B:833:HOH:O	2.48	0.45
1:A:546:TYR:O	1:A:547:TYR:HB2	2.17	0.45
1:B:371:THR:O	1:B:388:GLY:HA2	2.17	0.45
2:A:701:CG9:C30	2:A:701:CG9:N13	2.70	0.44
1:A:397:LYS:HD3	3:A:807:HOH:O	2.16	0.44
1:A:433:VAL:HA	1:A:509:LYS:HE2	1.99	0.44
1:B:363:VAL:CG1	1:B:437:GLY:HA2	2.48	0.44
2:B:701:CG9:C30	2:B:701:CG9:N13	2.76	0.43
1:A:411:PRO:O	1:A:412:ALA:HB2	2.18	0.43
1:B:485:LEU:HA	1:B:485:LEU:HD12	1.80	0.43
1:A:492:HIS:O	1:A:493:ARG:HB2	2.19	0.43
1:A:404:LEU:CD1	1:A:414:LYS:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:GLY:O	1:B:622:VAL:HG23	2.19	0.43
1:A:571:LYS:NZ	3:A:829:HOH:O	2.52	0.43
1:B:591:MET:O	1:B:602:TYR:OH	2.26	0.43
1:B:363:VAL:O	1:B:363:VAL:CG1	2.66	0.42
1:A:628:ASN:O	1:A:631:TYR:N	2.51	0.42
1:A:391:GLN:HA	1:A:396:VAL:HG23	2.01	0.42
1:A:612:ASP:O	1:A:613:VAL:C	2.58	0.42
1:A:491:VAL:O	1:A:516:SER:HA	2.19	0.42
1:A:463:ASN:HB3	1:A:466:VAL:HG23	2.00	0.42
1:A:466:VAL:C	1:A:467:LYS:O	2.58	0.42
1:B:404:LEU:HD23	1:B:404:LEU:HA	1.78	0.42
1:A:552:LYS:O	1:A:555:VAL:HB	2.20	0.42
1:B:463:ASN:O	1:B:465:HIS:N	2.53	0.42
1:B:387:LYS:HG3	1:B:450:MET:CE	2.50	0.42
1:A:420:GLU:O	1:A:424:MET:HG3	2.20	0.42
1:A:482:MET:SD	1:A:510:ILE:HD13	2.60	0.42
1:B:378:GLY:HA3	2:B:701:CG9:H16	2.02	0.41
1:B:463:ASN:C	1:B:465:HIS:N	2.74	0.41
1:A:378:GLY:HA3	2:A:701:CG9:H16	2.03	0.41
1:A:463:ASN:O	1:A:464:ARG:C	2.58	0.41
1:B:626:LEU:HD23	1:B:626:LEU:HA	1.80	0.41
1:B:561:LEU:HD23	1:B:561:LEU:O	2.21	0.41
1:B:583:ALA:O	1:B:587:LYS:HG3	2.21	0.41
1:A:387:LYS:HG3	1:A:450:MET:CE	2.50	0.41
1:B:593:CYS:HA	1:B:602:TYR:CE1	2.56	0.41
1:B:540:ALA:HB2	1:B:556:TRP:CB	2.50	0.41
1:B:577:LYS:HG3	1:B:580:GLU:CD	2.41	0.41
1:A:573:TYR:CE2	1:A:591:MET:HG3	2.56	0.41
1:A:366:ASP:HB3	1:A:369:LEU:HD13	2.02	0.41
1:B:492:HIS:O	1:B:493:ARG:HB2	2.21	0.40
1:A:599:ARG:HG2	1:A:600:GLU:N	2.37	0.40
1:A:363:VAL:HG13	1:A:363:VAL:O	2.20	0.40
1:B:503:VAL:CG2	1:B:507:TYR:CB	2.98	0.40
1:B:417:LEU:HD23	1:B:444:TRP:HZ3	1.86	0.40
1:A:385:VAL:HG22	1:A:402:LYS:HG2	2.04	0.40
1:A:404:LEU:O	1:A:405:LYS:C	2.59	0.40
1:A:600:GLU:CD	1:A:600:GLU:H	2.24	0.40
1:B:624:LEU:HD12	1:B:624:LEU:HA	1.96	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	257/291 (88%)	233 (91%)	18 (7%)	6 (2%)	8	3
1	B	259/291 (89%)	243 (94%)	14 (5%)	2 (1%)	24	17
All	All	516/582 (89%)	476 (92%)	32 (6%)	8 (2%)	12	5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	ALA
1	A	467	LYS
1	B	394	LYS
1	A	595	ALA
1	A	628	ASN
1	A	629	TYR
1	A	536	VAL
1	B	634	VAL

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	229/253 (90%)	215 (94%)	14 (6%)	23	18
1	B	231/253 (91%)	219 (95%)	12 (5%)	29	25
All	All	460/506 (91%)	434 (94%)	26 (6%)	25	21

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

Mol	Chain	Res	Type
1	A	363	VAL
1	A	379	SER
1	A	396	VAL
1	A	415	ASP
1	A	418	LEU
1	A	426	GLN
1	A	443	SER
1	A	464	ARG
1	A	471	ILE
1	A	473	GLU
1	A	505	GLN
1	A	507	TYR
1	A	577	LYS
1	A	599	ARG
1	B	368	LYS
1	B	381	ASN
1	B	396	VAL
1	B	417	LEU
1	B	418	LEU
1	B	425	GLN
1	B	438	ILE
1	B	442	GLU
1	B	449	GLU
1	B	507	TYR
1	B	524	ASN
1	B	579	SER

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	425	GLN
1	A	470	ASN
1	A	505	GLN
1	A	506	HIS
1	B	463	ASN
1	B	465	HIS

5.3.3 RNA ⓘ

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](#)

2 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	CG9	A	701	-	29,36,36	1.20	3 (10%)	35,51,51	1.25	3 (8%)
2	CG9	B	701	-	29,36,36	1.24	2 (6%)	35,51,51	1.21	3 (8%)

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	CG9	A	701	-	-	0/12/20/20	0/6/6/6
2	CG9	B	701	-	-	0/12/20/20	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CG9	C15-C14	-2.74	1.35	1.39
2	B	701	CG9	C15-C14	-2.61	1.35	1.39
2	A	701	CG9	C23-C22	2.25	1.41	1.36
2	A	701	CG9	C14-N13	3.86	1.40	1.34
2	B	701	CG9	C14-N13	4.45	1.41	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CG9	C21-C29-C28	-3.87	116.79	120.80
2	A	701	CG9	C18-C17-N16	-3.52	103.97	107.02
2	B	701	CG9	C21-C29-C28	-2.92	117.77	120.80
2	B	701	CG9	C18-C17-N16	-2.41	104.93	107.02
2	A	701	CG9	C22-C21-C29	2.03	121.20	118.11
2	B	701	CG9	C02-N03-C04	3.78	119.54	111.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CG9	3	0
2	B	701	CG9	4	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, 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	A	263/291 (90%)	0.28	10 (3%) 44 52	34, 50, 75, 88	0
1	B	265/291 (91%)	0.12	11 (4%) 40 48	33, 47, 71, 87	0
All	All	528/582 (90%)	0.20	21 (3%) 42 50	33, 49, 74, 88	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	630	TYR	6.7
1	B	631	TYR	5.2
1	B	415	ASP	4.1
1	A	624	LEU	3.9
1	A	631	TYR	3.9
1	B	635	ASN	3.1
1	A	418	LEU	3.1
1	A	633	VAL	3.0
1	A	533	LYS	3.0
1	B	468	ASP	2.8
1	A	374	ASP	2.8
1	B	418	LEU	2.8
1	A	465	HIS	2.6
1	B	411	PRO	2.5
1	A	629	TYR	2.5
1	A	462	GLN	2.5
1	B	634	VAL	2.3
1	B	413	LEU	2.1
1	B	377	LEU	2.1
1	B	393	LYS	2.1
1	B	633	VAL	2.1

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CG9	A	701	31/31	0.95	0.12	-0.17	40,47,64,70	0
2	CG9	B	701	31/31	0.94	0.12	-0.24	36,45,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.