



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:43 AM GMT

PDB ID : 3D7T
Title : Structural basis for the recognition of c-Src by its inactivator Csk
Authors : Levinson, N.M.; Seeliger, M.A.; Cole, P.A.; Kuriyan, J.
Deposited on : 2008-05-21
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

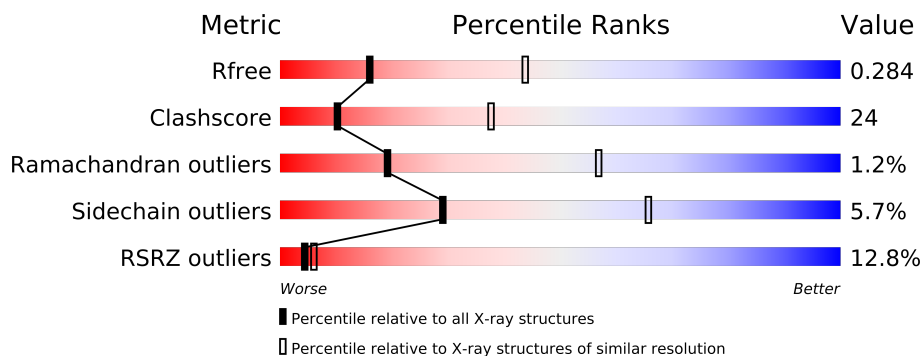
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	269	
2	B	286	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4174 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1969	1261	337	358	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	GLY	-	EXPRESSION TAG	UNP P41240
A	183	PRO	-	EXPRESSION TAG	UNP P41240
A	184	LEU	-	EXPRESSION TAG	UNP P41240
A	185	GLY	-	EXPRESSION TAG	UNP P41240
A	186	SER	-	EXPRESSION TAG	UNP P41240
A	187	GLY	-	EXPRESSION TAG	UNP P41240
A	361	ALA	LYS	ENGINEERED	UNP P41240
A	362	ALA	LYS	ENGINEERED	UNP P41240

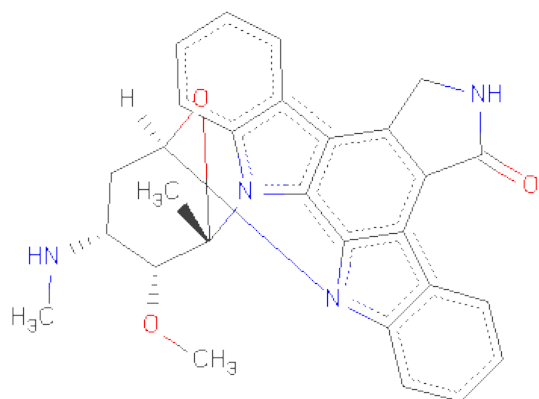
- Molecule 2 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	265	2135	1372	357	389	17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	248	GLY	-	EXPRESSION TAG	UNP P00523
B	249	HIS	-	EXPRESSION TAG	UNP P00523
B	250	MET	-	EXPRESSION TAG	UNP P00523

- Molecule 3 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).

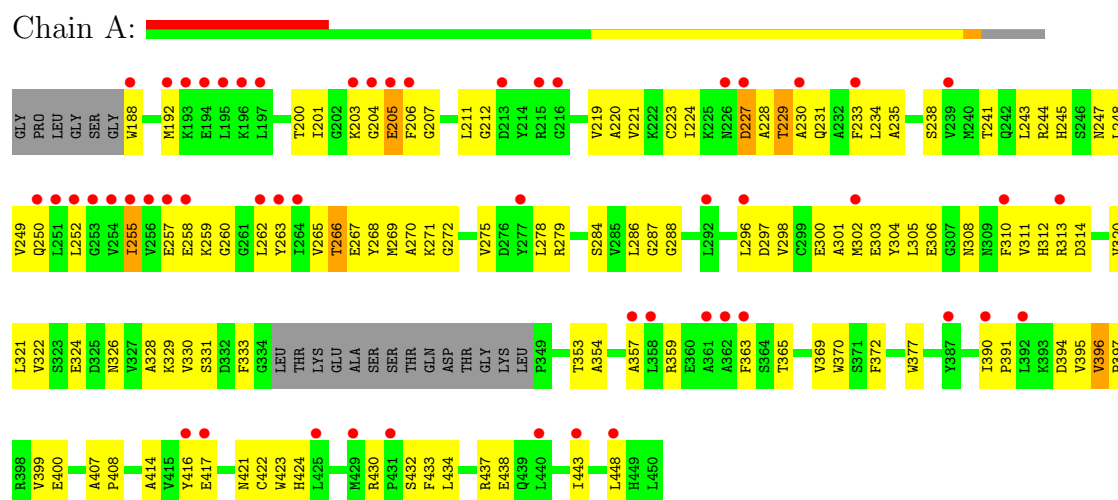


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			35	28	4	3		
3	A	1	Total	C	N	O	0	0
			35	28	4	3		

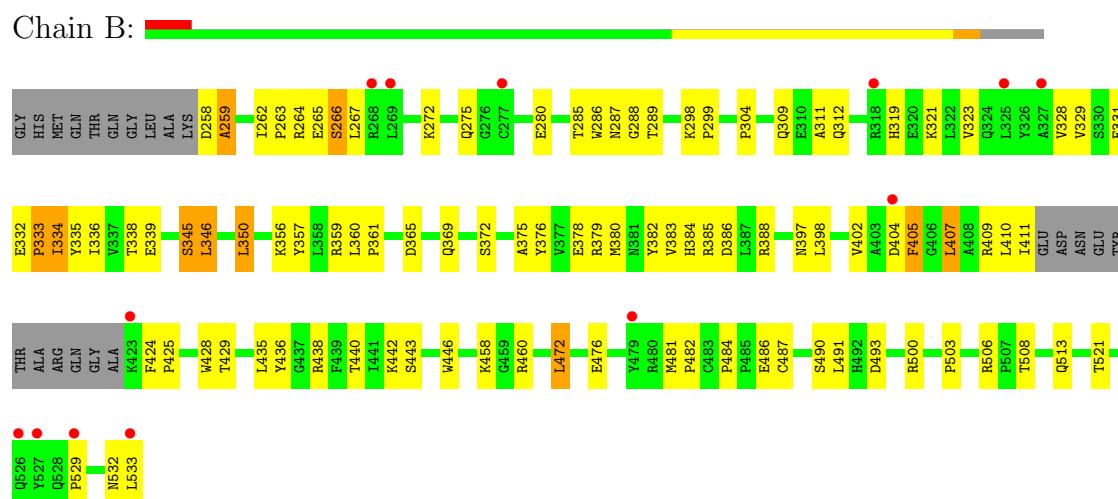
3 Residue-property plots

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



• Molecule 2: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.65Å 99.65Å 137.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.69 – 2.90 45.69 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (45.69-2.90) 99.3 (45.69-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.237 , 0.278 0.242 , 0.284	Depositor DCC
R_{free} test set	912 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.6	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 17900 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4174	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: STU

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	0.33	0/2011	0.51	0/2716
2	B	0.41	0/2187	0.62	0/2960
All	All	0.38	0/4198	0.57	0/5676

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1969	0	1978	112	1
2	B	2135	0	2129	69	0
3	A	35	0	26	10	0
3	B	35	0	26	10	0
All	All	4174	0	4159	196	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (196) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:244:ARG:HD2	1:A:250:GLN:HE22	1.17	1.03
1:A:252:LEU:HB2	1:A:265:VAL:HG12	1.47	0.94
1:A:247:ASN:HB3	1:A:301:ALA:HB2	1.50	0.90
3:B:6334:STU:H16	3:B:6334:STU:H261	1.56	0.87
2:B:331:GLU:O	2:B:334:ILE:HG12	1.75	0.86
3:A:6335:STU:H261	3:A:6335:STU:H16	1.56	0.85
1:A:206:PHE:CE2	1:A:233:PHE:HE2	1.94	0.85
1:A:200:THR:HG21	1:A:203:LYS:HE2	1.61	0.82
2:B:264:ARG:NH2	2:B:333:PRO:HD2	1.95	0.80
2:B:407:LEU:HD23	2:B:407:LEU:H	1.48	0.78
3:A:6335:STU:N4	3:A:6335:STU:H273	2.01	0.74
1:A:270:ALA:CB	1:A:324:GLU:HG3	2.17	0.74
1:A:311:VAL:HG11	1:A:363:PHE:O	1.88	0.74
3:B:6334:STU:H241	3:B:6334:STU:H272	1.70	0.73
1:A:221:VAL:HG22	1:A:265:VAL:HG22	1.70	0.73
1:A:188:TRP:CZ2	1:A:241:THR:HB	2.25	0.72
3:A:6335:STU:HN4	3:A:6335:STU:H273	1.57	0.70
1:A:257:GLU:HG2	1:A:258:GLU:H	1.56	0.70
1:A:257:GLU:HG2	1:A:258:GLU:N	2.07	0.69
1:A:258:GLU:O	1:A:260:GLY:N	2.26	0.69
1:A:247:ASN:CB	1:A:301:ALA:HB2	2.24	0.68
2:B:409:ARG:HE	2:B:411:ILE:HG13	1.58	0.68
1:A:219:VAL:CG1	1:A:265:VAL:HG13	2.24	0.68
1:A:245:HIS:HD2	1:A:247:ASN:HB2	1.60	0.67
1:A:396:VAL:HG13	1:A:397:PRO:CD	2.25	0.67
2:B:405:PHE:CD1	2:B:405:PHE:N	2.61	0.66
2:B:272:LYS:HE3	2:B:280:GLU:OE1	1.96	0.66
1:A:269:MET:SD	1:A:329:LYS:HB2	2.35	0.66
2:B:484:PRO:HG2	2:B:487:CYS:HB3	1.78	0.65
2:B:338:THR:HG22	2:B:339:GLU:N	2.10	0.65
2:B:287:ASN:O	2:B:289:THR:HG23	1.97	0.65
2:B:484:PRO:HG2	2:B:487:CYS:CB	2.27	0.64
1:A:228:ALA:C	1:A:230:ALA:H	2.01	0.64
1:A:223:CYS:HB3	1:A:263:TYR:HE1	1.63	0.63
1:A:245:HIS:HB3	1:A:248:LEU:HG	1.80	0.63
2:B:376:TYR:HD1	2:B:379:ARG:NH2	1.95	0.63
1:A:220:ALA:HB3	1:A:266:THR:HG22	1.82	0.62
2:B:263:PRO:HB2	2:B:265:GLU:OE1	2.00	0.62
3:A:6335:STU:C16	3:A:6335:STU:H261	2.26	0.60
2:B:264:ARG:CZ	2:B:333:PRO:HD2	2.31	0.60
1:A:245:HIS:CD2	1:A:247:ASN:HB2	2.37	0.59
2:B:359:ARG:HD2	2:B:533:LEU:OXT	2.01	0.59
2:B:365:ASP:O	2:B:369:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:396:VAL:O	1:A:400:GLU:HG3	2.02	0.59
1:A:247:ASN:ND2	1:A:300:GLU:HB2	2.18	0.59
2:B:323:VAL:HG23	2:B:402:VAL:O	2.03	0.59
2:B:272:LYS:HZ1	2:B:275:GLN:HG3	1.68	0.58
2:B:409:ARG:HE	2:B:411:ILE:CG1	2.16	0.58
1:A:303:GLU:HB2	1:A:433:PHE:O	2.05	0.57
2:B:360:LEU:HB3	2:B:361:PRO:HD3	1.85	0.57
1:A:204:GLY:C	1:A:206:PHE:H	2.06	0.57
1:A:243:LEU:HD21	1:A:308:ASN:HB3	1.87	0.57
2:B:376:TYR:O	2:B:380:MET:HG2	2.06	0.56
1:A:369:VAL:O	1:A:422:CYS:HB3	2.04	0.56
1:A:278:LEU:HD23	1:A:286:LEU:HD12	1.88	0.56
1:A:248:LEU:HD23	1:A:301:ALA:HB1	1.88	0.56
1:A:313:ARG:HG2	1:A:363:PHE:HB2	1.88	0.56
2:B:258:ASP:O	2:B:259:ALA:HB3	2.06	0.56
1:A:219:VAL:HG11	1:A:265:VAL:HG13	1.87	0.55
1:A:443:ILE:HA	1:A:448:LEU:HD12	1.88	0.55
2:B:266:SER:HB3	2:B:286:TRP:CD1	2.40	0.55
1:A:417:GLU:O	1:A:421:ASN:HB2	2.07	0.55
1:A:224:ILE:HG22	1:A:230:ALA:HB2	1.88	0.55
2:B:388:ARG:HB3	2:B:428:TRP:CD1	2.42	0.55
2:B:304:PRO:HB3	2:B:334:ILE:CD1	2.37	0.55
1:A:219:VAL:HG13	1:A:265:VAL:HG13	1.88	0.54
2:B:409:ARG:NE	2:B:411:ILE:HG13	2.20	0.54
2:B:264:ARG:HH21	2:B:331:GLU:HB2	1.71	0.54
1:A:223:CYS:HA	1:A:263:TYR:CD1	2.43	0.54
2:B:329:VAL:HB	2:B:335:TYR:HB2	1.90	0.54
1:A:244:ARG:CD	1:A:250:GLN:HE22	2.06	0.54
1:A:313:ARG:HG2	1:A:363:PHE:CB	2.38	0.53
1:A:321:LEU:HD21	3:A:6335:STU:H272	1.91	0.53
1:A:230:ALA:HB3	1:A:262:LEU:HD23	1.90	0.53
1:A:249:VAL:HG23	1:A:330:VAL:O	2.08	0.53
3:B:6334:STU:C16	3:B:6334:STU:H261	2.29	0.53
2:B:490:SER:O	2:B:493:ASP:HB3	2.08	0.53
1:A:268:TYR:CE2	1:A:270:ALA:HA	2.42	0.53
1:A:396:VAL:HG13	1:A:397:PRO:HD3	1.89	0.53
2:B:332:GLU:HB2	2:B:333:PRO:HD3	1.91	0.53
1:A:234:LEU:HD11	1:A:262:LEU:HD21	1.89	0.53
1:A:424:HIS:HB2	1:A:430:ARG:HG2	1.89	0.53
2:B:338:THR:CG2	2:B:339:GLU:N	2.72	0.53
3:B:6334:STU:H241	3:B:6334:STU:C27	2.37	0.52
2:B:356:LYS:HE3	2:B:357:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:GLY:O	1:A:321:LEU:HA	2.09	0.52
2:B:375:ALA:O	2:B:378:GLU:HB3	2.09	0.52
3:B:6334:STU:N4	3:B:6334:STU:H273	2.24	0.52
1:A:306:GLU:OE2	1:A:432:SER:HB2	2.10	0.51
1:A:407:ALA:HB2	1:A:416:TYR:CD2	2.46	0.51
2:B:372:SER:HA	2:B:513:GLN:OE1	2.10	0.50
1:A:244:ARG:HD2	1:A:250:GLN:NE2	2.03	0.50
1:A:245:HIS:HD2	1:A:247:ASN:H	1.58	0.50
2:B:262:ILE:HD11	2:B:267:LEU:HD11	1.94	0.50
2:B:304:PRO:HB3	2:B:334:ILE:HD12	1.94	0.49
1:A:271:LYS:NZ	1:A:326:ASN:OD1	2.45	0.49
1:A:312:HIS:CE1	1:A:314:ASP:HB3	2.47	0.49
1:A:223:CYS:HB3	1:A:263:TYR:CE1	2.46	0.49
1:A:357:ALA:HB1	1:A:363:PHE:CE1	2.47	0.48
2:B:382:TYR:HA	2:B:409:ARG:HA	1.94	0.48
2:B:409:ARG:HG3	2:B:411:ILE:HG12	1.94	0.48
1:A:396:VAL:HG13	1:A:397:PRO:HD2	1.94	0.48
1:A:228:ALA:O	1:A:230:ALA:N	2.47	0.48
2:B:388:ARG:HE	2:B:425:PRO:HG2	1.79	0.48
2:B:384:HIS:O	2:B:385:ARG:HB2	2.13	0.48
2:B:346:LEU:HD22	2:B:350:LEU:HD22	1.96	0.47
1:A:247:ASN:HD22	1:A:300:GLU:HB2	1.78	0.47
1:A:321:LEU:HD21	3:A:6335:STU:C27	2.45	0.47
1:A:312:HIS:NE2	1:A:333:PHE:HA	2.29	0.47
1:A:211:LEU:HD12	1:A:212:GLY:H	1.80	0.47
1:A:245:HIS:CD2	1:A:247:ASN:H	2.33	0.46
1:A:296:LEU:C	1:A:298:VAL:H	2.17	0.46
1:A:353:THR:HG22	1:A:354:ALA:O	2.16	0.46
2:B:331:GLU:HB3	2:B:332:GLU:H	1.60	0.46
3:A:6335:STU:C18	3:A:6335:STU:H272	2.46	0.46
2:B:442:LYS:HD2	2:B:503:PRO:O	2.16	0.46
1:A:201:ILE:HD12	3:A:6335:STU:C4	2.45	0.46
1:A:434:LEU:O	1:A:438:GLU:HG2	2.15	0.46
2:B:258:ASP:O	2:B:259:ALA:CB	2.64	0.46
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.80	0.46
1:A:229:THR:HG22	1:A:229:THR:O	2.16	0.46
1:A:205:GLU:H	1:A:205:GLU:CD	2.19	0.46
1:A:320:VAL:HG12	1:A:321:LEU:N	2.30	0.46
1:A:228:ALA:C	1:A:230:ALA:N	2.68	0.46
1:A:192:MET:HB2	1:A:255:ILE:HG21	1.97	0.45
2:B:345:SER:HB3	3:B:6334:STU:H273	1.98	0.45
2:B:266:SER:HB3	2:B:286:TRP:HD1	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:ALA:O	1:A:238:SER:HB3	2.16	0.45
1:A:395:VAL:O	1:A:399:VAL:HG23	2.16	0.45
3:A:6335:STU:N4	3:A:6335:STU:C27	2.74	0.45
1:A:248:LEU:CD2	1:A:301:ALA:HB1	2.45	0.45
2:B:309:GLN:HA	2:B:312:GLN:HG2	1.98	0.45
2:B:500:ARG:O	2:B:506:ARG:HD2	2.17	0.45
3:B:6334:STU:HN4	3:B:6334:STU:H273	1.82	0.45
1:A:370:TRP:CE3	1:A:423:TRP:HA	2.52	0.45
2:B:472:LEU:HD22	2:B:476:GLU:OE2	2.17	0.45
1:A:304:TYR:CD2	1:A:305:LEU:HD23	2.52	0.44
2:B:424:PHE:HB2	2:B:429:THR:OG1	2.18	0.44
3:B:6334:STU:C24	3:B:6334:STU:H272	2.43	0.44
1:A:414:ALA:HB1	1:A:443:ILE:HG12	1.98	0.44
1:A:333:PHE:CD1	1:A:333:PHE:N	2.85	0.44
3:B:6334:STU:C24	3:B:6334:STU:C27	2.96	0.44
1:A:206:PHE:CE2	1:A:233:PHE:CE2	2.87	0.44
1:A:297:ASP:HB2	1:A:328:ALA:HB3	2.00	0.44
1:A:357:ALA:HB1	1:A:363:PHE:CD1	2.53	0.44
1:A:227:ASP:HB3	1:A:228:ALA:H	1.45	0.44
2:B:486:GLU:OE1	2:B:532:ASN:HB2	2.18	0.44
1:A:330:VAL:HG12	1:A:331:SER:H	1.83	0.43
2:B:311:ALA:HB2	2:B:336:ILE:HD13	1.99	0.43
2:B:440:THR:O	2:B:443:SER:HB3	2.18	0.43
1:A:223:CYS:HA	1:A:263:TYR:HD1	1.83	0.43
1:A:310:PHE:CD2	1:A:311:VAL:N	2.86	0.43
1:A:204:GLY:C	1:A:206:PHE:N	2.72	0.43
1:A:258:GLU:C	1:A:260:GLY:H	2.21	0.43
1:A:422:CYS:O	1:A:430:ARG:HD3	2.18	0.43
2:B:264:ARG:HH21	2:B:331:GLU:CB	2.31	0.43
3:A:6335:STU:C16	3:A:6335:STU:C26	2.95	0.43
1:A:228:ALA:O	1:A:231:GLN:HG3	2.18	0.43
3:B:6334:STU:C16	3:B:6334:STU:C26	2.95	0.43
2:B:384:HIS:HE1	2:B:386:ASP:O	2.02	0.43
1:A:219:VAL:HG22	1:A:252:LEU:CD1	2.49	0.43
2:B:436:TYR:CD2	2:B:438:ARG:NH1	2.87	0.43
1:A:287:GLY:O	1:A:288:GLY:C	2.57	0.43
1:A:207:GLY:HA2	1:A:224:ILE:CD1	2.49	0.42
2:B:388:ARG:NE	2:B:425:PRO:HG2	2.34	0.42
1:A:298:VAL:CG1	1:A:372:PHE:HE1	2.32	0.42
1:A:300:GLU:HG2	1:A:437:ARG:HD2	2.00	0.42
1:A:304:TYR:CZ	1:A:308:ASN:ND2	2.87	0.42
2:B:272:LYS:HE3	2:B:280:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:LEU:HD23	1:A:286:LEU:CD1	2.49	0.42
2:B:359:ARG:HA	2:B:359:ARG:HD3	1.75	0.42
1:A:377:TRP:CD1	1:A:408:PRO:HG3	2.54	0.42
1:A:302:MET:HE2	1:A:433:PHE:CZ	2.54	0.42
1:A:305:LEU:HB3	1:A:310:PHE:HB3	2.02	0.42
1:A:432:SER:C	1:A:434:LEU:H	2.23	0.42
1:A:245:HIS:HB2	1:A:304:TYR:CD2	2.55	0.42
2:B:398:LEU:HA	2:B:398:LEU:HD23	1.82	0.42
1:A:271:LYS:HB2	1:A:322:VAL:HB	2.02	0.41
2:B:446:TRP:CD1	2:B:446:TRP:C	2.94	0.41
2:B:298:LYS:HA	2:B:299:PRO:HD3	1.94	0.41
1:A:313:ARG:HD3	1:A:363:PHE:CD2	2.56	0.41
2:B:435:LEU:O	2:B:436:TYR:CD1	2.73	0.41
1:A:192:MET:HE3	1:A:257:GLU:HB2	2.03	0.41
1:A:230:ALA:CB	1:A:262:LEU:HD23	2.50	0.41
1:A:443:ILE:HG23	1:A:448:LEU:HB2	2.02	0.41
2:B:383:VAL:O	2:B:407:LEU:HA	2.20	0.41
1:A:250:GLN:N	1:A:267:GLU:HG2	2.35	0.41
2:B:458:LYS:HB3	2:B:458:LYS:HE2	1.72	0.41
2:B:521:THR:HG22	2:B:521:THR:O	2.20	0.41
1:A:279:ARG:O	2:B:508:THR:HG23	2.21	0.41
1:A:304:TYR:CE1	1:A:308:ASN:ND2	2.88	0.40
1:A:270:ALA:HB3	1:A:324:GLU:N	2.35	0.40
1:A:296:LEU:C	1:A:298:VAL:N	2.75	0.40
2:B:435:LEU:HA	2:B:435:LEU:HD23	1.88	0.40
2:B:319:HIS:CD2	2:B:321:LYS:H	2.40	0.40
2:B:481:MET:HA	2:B:482:PRO:HD2	1.93	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:258:GLU:O	1:A:258:GLU:O[4.465]	1.89	0.31

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/269 (91%)	204 (83%)	39 (16%)	2 (1%)	27	68
2	B	261/286 (91%)	234 (90%)	23 (9%)	4 (2%)	15	50
All	All	506/555 (91%)	438 (87%)	62 (12%)	6 (1%)	19	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	LYS
1	A	229	THR
2	B	259	ALA
2	B	529	PRO
2	B	333	PRO
2	B	288	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/226 (93%)	201 (95%)	10 (5%)	36	75
2	B	230/245 (94%)	215 (94%)	15 (6%)	24	58
All	All	441/471 (94%)	416 (94%)	25 (6%)	29	66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	GLU
1	A	227	ASP
1	A	255	ILE
1	A	266	THR
1	A	275	VAL
1	A	284	SER
1	A	359	ARG
1	A	365	THR
1	A	394	ASP
1	A	396	VAL
2	B	266	SER

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Mol	Chain	Res	Type
2	B	285	THR
2	B	328	VAL
2	B	334	ILE
2	B	345	SER
2	B	346	LEU
2	B	350	LEU
2	B	397	ASN
2	B	404	ASP
2	B	405	PHE
2	B	407	LEU
2	B	410	LEU
2	B	460	ARG
2	B	472	LEU
2	B	491	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	245	HIS
1	A	247	ASN
1	A	250	GLN
2	B	275	GLN
2	B	287	ASN
2	B	319	HIS
2	B	324	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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$
3	STU	A	6335	-	40,42,42	1.05	2 (5%)	62,68,68	2.29	15 (24%)
3	STU	B	6334	-	40,42,42	1.08	3 (7%)	62,68,68	2.57	14 (22%)

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
3	STU	A	6335	-	-	0/4/42/42	0/0/8/8
3	STU	B	6334	-	-	0/4/42/42	0/0/8/8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	6335	STU	C19-N3	-2.95	1.35	1.39
3	B	6334	STU	C19-N3	-2.84	1.35	1.39
3	B	6334	STU	O4-C21	-2.11	1.39	1.44
3	A	6335	STU	O4-C25	-2.10	1.39	1.43
3	B	6334	STU	O4-C25	-2.01	1.39	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6334	STU	C28-N4-C23	-13.90	106.07	113.82
3	A	6335	STU	C28-N4-C23	-8.65	109.00	113.82
3	A	6335	STU	C26-C21-N2	-6.32	107.66	111.09
3	A	6335	STU	C10-C9-N1	5.62	106.12	101.45
3	B	6334	STU	C10-C9-N1	5.48	106.01	101.45
3	A	6335	STU	C6-C7-C8	5.26	133.03	128.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6334	STU	O6-C22-C23	4.85	118.97	108.14
3	B	6334	STU	C26-C21-N2	-4.53	108.63	111.09
3	B	6334	STU	C6-C7-C8	4.22	132.21	128.93
3	B	6334	STU	C26-C21-C22	-3.75	103.94	112.87
3	A	6335	STU	C7-C8-N1	3.60	110.30	106.39
3	A	6335	STU	C26-C21-C22	-3.57	104.36	112.87
3	A	6335	STU	O6-C22-C23	3.56	116.09	108.14
3	B	6334	STU	C9-N1-C8	-3.52	108.85	113.15
3	A	6335	STU	C9-N1-C8	-3.48	108.90	113.15
3	B	6334	STU	C24-C25-N3	3.35	116.33	112.48
3	A	6335	STU	O4-C25-N3	3.34	114.06	108.95
3	B	6334	STU	C7-C8-N1	3.25	109.92	106.39
3	B	6334	STU	C9-C10-C7	-2.84	106.48	109.21
3	A	6335	STU	C24-C25-N3	-2.65	109.43	112.48
3	A	6335	STU	C9-C10-C7	-2.57	106.75	109.21
3	B	6334	STU	C3-C4-C5	-2.45	116.40	120.74
3	A	6335	STU	O4-C21-C22	2.43	115.64	109.80
3	B	6334	STU	C4-C5-C20	2.43	122.46	119.39
3	A	6335	STU	O4-C21-N2	2.37	114.33	109.37
3	B	6334	STU	C25-C24-C23	-2.20	109.19	112.35
3	A	6335	STU	C3-C4-C5	-2.10	117.02	120.74
3	A	6335	STU	C14-C13-C12	-2.05	117.10	120.74
3	B	6334	STU	O4-C25-N3	2.02	112.05	108.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/269 (92%)	1.26	53 (21%) 1 2	75, 128, 181, 196	0
2	B	265/286 (92%)	0.34	13 (4%) 28 34	63, 84, 114, 136	0
All	All	514/555 (92%)	0.79	66 (12%) 4 6	63, 100, 173, 196	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	VAL	16.0
1	A	255	ILE	8.9
1	A	194	GLU	8.7
1	A	197	LEU	8.1
1	A	206	PHE	6.5
1	A	195	LEU	6.4
1	A	188	TRP	6.0
1	A	196	LYS	5.9
1	A	264	ILE	5.8
1	A	193	LYS	5.7
1	A	254	VAL	5.3
1	A	417	GLU	5.2
1	A	227	ASP	5.0
1	A	448	LEU	4.7
2	B	526	GLN	4.5
1	A	387	TYR	4.5
1	A	251	LEU	4.5
2	B	533	LEU	4.3
1	A	203	LYS	4.3
1	A	425	LEU	4.2
1	A	363	PHE	4.0
1	A	392	LEU	3.7
1	A	230	ALA	3.6
1	A	216	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	192	MET	3.5
1	A	233	PHE	3.5
1	A	205	GLU	3.4
1	A	204	GLY	3.3
1	A	215	ARG	3.3
2	B	327	ALA	3.2
1	A	357	ALA	3.2
1	A	429	MET	3.1
2	B	529	PRO	3.1
2	B	527	TYR	3.0
1	A	252	LEU	3.0
2	B	277	CYS	3.0
1	A	239	VAL	2.9
1	A	443	ILE	2.9
2	B	268	ARG	2.9
1	A	277	TYR	2.8
1	A	390	ILE	2.8
1	A	431	PRO	2.8
1	A	262	LEU	2.7
2	B	325	LEU	2.7
1	A	361	ALA	2.6
2	B	269	LEU	2.6
1	A	226	ASN	2.6
1	A	310	PHE	2.6
1	A	263	TYR	2.5
2	B	404	ASP	2.5
2	B	318	ARG	2.5
1	A	250	GLN	2.5
1	A	416	TYR	2.4
2	B	479	TYR	2.4
1	A	313	ARG	2.4
1	A	358	LEU	2.4
1	A	258	GLU	2.4
1	A	440	LEU	2.3
1	A	362	ALA	2.3
1	A	257	GLU	2.2
1	A	296	LEU	2.2
1	A	253	GLY	2.1
1	A	302	MET	2.1
1	A	213	ASP	2.1
1	A	292	LEU	2.0
2	B	423	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	STU	A	6335	35/35	0.29	0.29	104,125,129,129	0
3	STU	B	6334	35/35	0.21	-0.38	58,65,71,84	0

6.5 Other polymers

There are no such residues in this entry.