



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 AM GMT

PDB ID : 2OND  
Title : Crystal Structure of the HAT-C domain of murine CstF-77  
Authors : Bai, Y.; Auperin, T.C.; Chou, C.-Y.; Chang, G.-G.; Manley, J.L.; Tong, L.  
Deposited on : 2007-01-23  
Resolution : 2.80 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](mailto: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

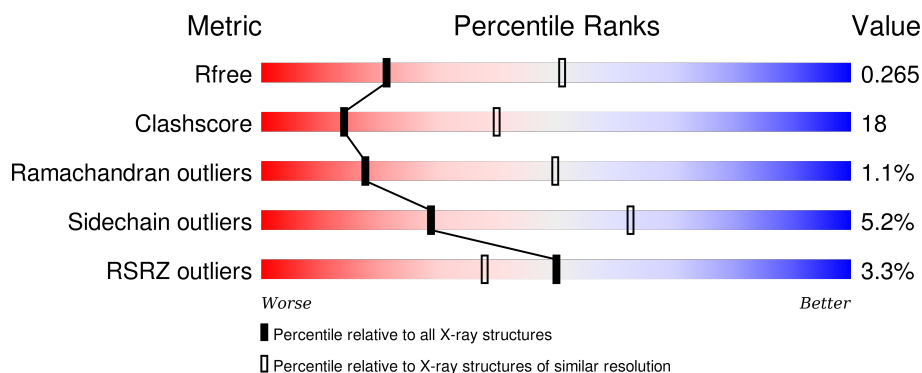
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	308	<div> <div>3%</div> <div>58%</div> <div>38%</div> <div>.</div> </div>
1	B	308	<div> <div>4%</div> <div>61%</div> <div>35%</div> <div>.</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5099 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 Cleavage stimulation factor 77 kDa subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	Se	0	0	0
			2549	1641	424	472	3	9			
1	B	308	Total	C	N	O	S	Se	0	0	0
			2550	1641	424	473	3	9			

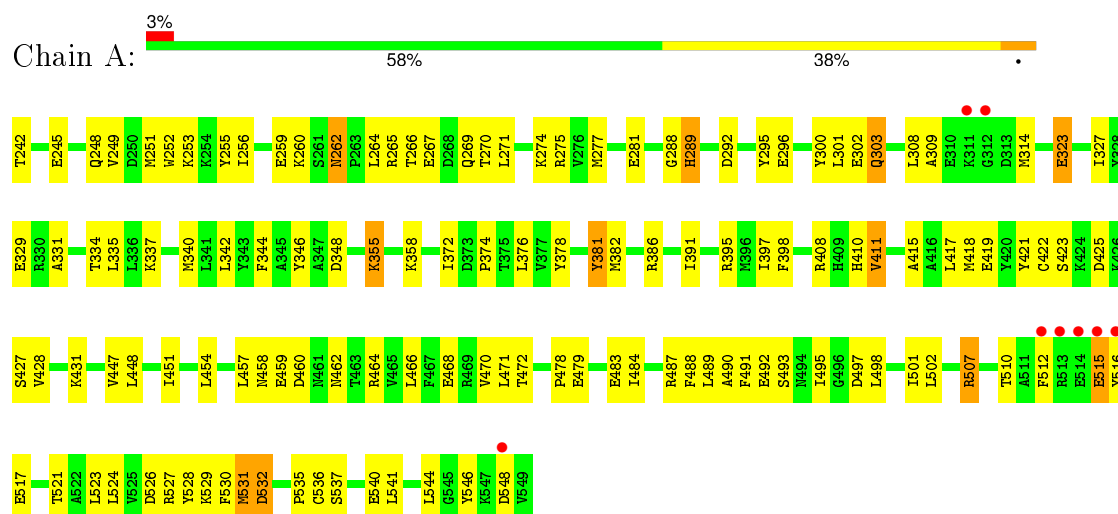
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	277	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	314	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	340	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	354	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	382	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	396	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	418	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
A	531	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	251	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	277	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	314	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	340	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	354	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	382	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	396	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	418	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7
B	531	MSE	MET	MODIFIED RESIDUE	UNP Q99LI7

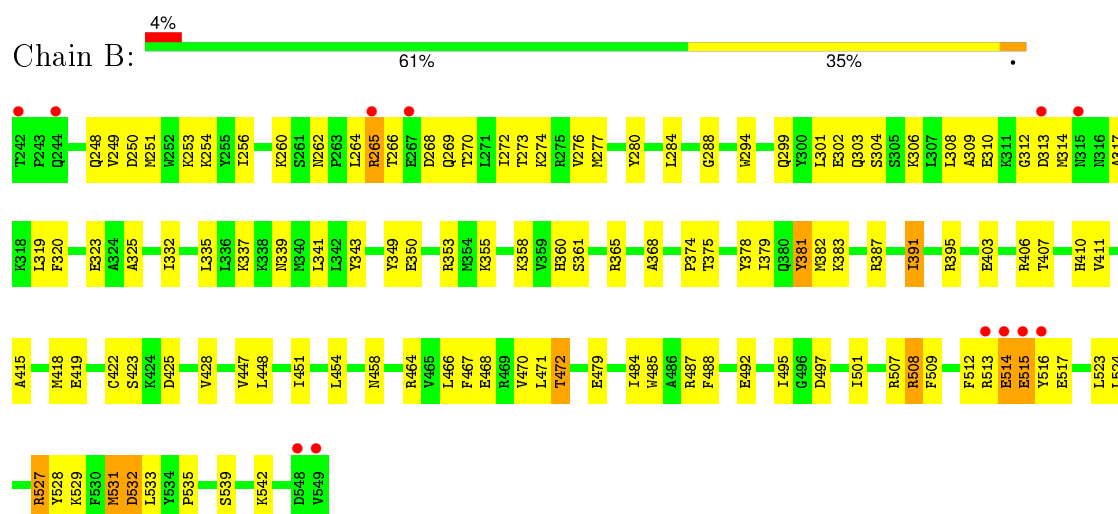
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: Cleavage stimulation factor 77 kDa subunit



- Molecule 1: Cleavage stimulation factor 77 kDa subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.40 Å   155.40 Å   161.60 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	29.84 – 2.80 29.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.84-2.80) 98.6 (29.84-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.71 (at 2.80 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224   ,   0.262 0.231   ,   0.265	Depositor DCC
$R_{free}$ test set	2104 reflections (7.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53498 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5099	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.42	0/2597	0.61	0/3484
1	B	0.38	0/2598	0.59	0/3484
All	All	0.40	0/5195	0.60	0/6968

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	2549	0	2534	104	0
1	B	2550	0	2534	95	0
All	All	5099	0	5068	186	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 (186) 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:340:MSE:HE1	1:A:376:LEU:HD23	1.48	0.96
1:A:262:ASN:HD21	1:A:266:THR:HG22	1.31	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLU:O	1:B:472:THR:HB	1.73	0.89
1:A:468:GLU:O	1:A:472:THR:HG22	1.74	0.88
1:A:512:PHE:HB3	1:A:515:GLU:HB3	1.56	0.87
1:B:269:GLN:HA	1:B:272:ILE:HD12	1.58	0.85
1:B:266:THR:HG22	1:B:268:ASP:H	1.42	0.85
1:A:340:MSE:CE	1:A:376:LEU:HD23	2.10	0.80
1:B:515:GLU:HG3	1:B:516:TYR:CD1	2.20	0.77
1:A:301:LEU:HD13	1:A:323:GLU:HB3	1.67	0.76
1:B:249:VAL:O	1:B:253:LYS:HG2	1.86	0.74
1:A:248:GLN:HA	1:A:251:MSE:HE2	1.73	0.70
1:A:466:LEU:O	1:A:470:VAL:HG13	1.91	0.70
1:A:245:GLU:HA	1:A:248:GLN:NE2	2.07	0.70
1:B:332:ILE:O	1:B:337:LYS:HA	1.93	0.69
1:A:489:LEU:HD11	1:A:501:ILE:HG23	1.76	0.67
1:A:537:SER:O	1:A:541:LEU:HB2	1.94	0.67
1:A:259:GLU:OE2	1:A:275:ARG:NH1	2.28	0.67
1:B:485:TRP:HB3	1:B:508:ARG:HG2	1.77	0.67
1:A:493:SER:HA	1:A:501:ILE:HD11	1.76	0.66
1:A:329:GLU:HG2	1:A:346:TYR:OH	1.95	0.66
1:A:288:GLY:HA3	1:A:335:LEU:HD13	1.78	0.65
1:A:262:ASN:ND2	1:A:266:THR:HG22	2.07	0.65
1:A:242:THR:HG23	1:A:245:GLU:HB2	1.79	0.65
1:B:248:GLN:HA	1:B:251:MSE:HE2	1.78	0.64
1:A:471:LEU:HD21	1:A:484:ILE:HB	1.79	0.64
1:A:289:HIS:CD2	1:A:289:HIS:H	2.15	0.63
1:A:447:VAL:O	1:A:451:ILE:HG12	1.99	0.62
1:A:454:LEU:HD22	1:A:466:LEU:HD22	1.83	0.61
1:A:340:MSE:HE2	1:B:535:PRO:HA	1.83	0.60
1:A:340:MSE:HE1	1:A:376:LEU:CD2	2.29	0.60
1:B:513:ARG:O	1:B:517:GLU:HB2	2.01	0.60
1:B:309:ALA:HB2	1:B:317:ALA:HB1	1.81	0.60
1:A:270:THR:O	1:A:274:LYS:HG3	2.01	0.59
1:A:382:MSE:HE1	1:A:415:ALA:HA	1.85	0.59
1:A:252:TRP:O	1:A:256:ILE:HG13	2.02	0.58
1:B:250:ASP:OD1	1:B:254:LYS:HE3	2.03	0.58
1:B:309:ALA:O	1:B:314:MSE:HE1	2.03	0.57
1:B:515:GLU:HG3	1:B:516:TYR:HD1	1.68	0.57
1:A:524:LEU:CD2	1:B:341:LEU:HD11	2.35	0.57
1:B:447:VAL:HG11	1:B:470:VAL:CG1	2.34	0.57
1:B:379:ILE:O	1:B:383:LYS:HG2	2.05	0.56
1:B:272:ILE:O	1:B:276:VAL:HG23	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLN:HB3	1:B:308:LEU:HD21	1.86	0.56
1:B:319:LEU:O	1:B:323:GLU:HG2	2.06	0.56
1:B:265:ARG:HG3	1:B:265:ARG:O	2.05	0.56
1:A:340:MSE:HE1	1:A:376:LEU:HB3	1.88	0.55
1:A:245:GLU:O	1:A:249:VAL:HG23	2.07	0.55
1:B:270:THR:O	1:B:274:LYS:HG3	2.07	0.55
1:B:516:TYR:CG	1:B:523:LEU:HD21	2.41	0.55
1:A:531:MSE:O	1:A:532:ASP:OD1	2.25	0.55
1:A:528:TYR:HB2	1:A:535:PRO:CG	2.37	0.55
1:A:531:MSE:HE2	1:B:410:HIS:CD2	2.41	0.54
1:A:529:LYS:HG3	1:A:529:LYS:O	2.06	0.54
1:B:309:ALA:HB2	1:B:317:ALA:CB	2.37	0.54
1:A:292:ASP:O	1:A:296:GLU:HG3	2.08	0.54
1:B:350:GLU:OE1	1:B:350:GLU:HA	2.08	0.54
1:B:485:TRP:HB3	1:B:508:ARG:CG	2.38	0.54
1:B:485:TRP:CB	1:B:508:ARG:HG2	2.37	0.53
1:A:427:SER:O	1:A:431:LYS:HG3	2.07	0.53
1:B:288:GLY:HA3	1:B:335:LEU:CD1	2.38	0.53
1:B:471:LEU:HD21	1:B:484:ILE:HB	1.90	0.53
1:A:515:GLU:HG3	1:A:516:TYR:HD1	1.73	0.53
1:A:275:ARG:HH11	1:A:275:ARG:HB3	1.72	0.53
1:B:306:LYS:O	1:B:310:GLU:HB2	2.09	0.52
1:B:468:GLU:OE1	1:B:507:ARG:NH2	2.43	0.52
1:B:497:ASP:O	1:B:501:ILE:HG13	2.09	0.52
1:B:516:TYR:HB2	1:B:523:LEU:HD11	1.91	0.52
1:A:374:PRO:HB2	1:A:378:TYR:CE1	2.43	0.52
1:B:299:GLN:O	1:B:303:GLN:HG3	2.10	0.52
1:A:521:THR:HG22	1:A:544:LEU:HD13	1.90	0.52
1:B:454:LEU:HD22	1:B:466:LEU:HD22	1.92	0.52
1:B:264:LEU:O	1:B:265:ARG:C	2.48	0.52
1:B:350:GLU:OE2	1:B:358:LYS:NZ	2.39	0.52
1:A:355:LYS:HB2	1:A:358:LYS:HB3	1.92	0.52
1:A:495:ILE:HG22	1:B:422:CYS:SG	2.50	0.52
1:B:468:GLU:CD	1:B:507:ARG:HH22	2.13	0.51
1:B:284:LEU:HD22	1:B:294:TRP:CE2	2.45	0.51
1:A:498:LEU:O	1:A:502:LEU:HG	2.10	0.51
1:B:516:TYR:CD1	1:B:523:LEU:HD21	2.45	0.51
1:A:266:THR:OG1	1:A:267:GLU:N	2.43	0.51
1:A:253:LYS:NZ	1:A:296:GLU:OE2	2.43	0.51
1:A:448:LEU:HG	1:A:484:ILE:CD1	2.41	0.50
1:B:451:ILE:HD13	1:B:467:PHE:CE2	2.46	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:HD23	1:B:341:LEU:HD11	1.93	0.50
1:B:288:GLY:HA3	1:B:335:LEU:HD13	1.94	0.50
1:A:515:GLU:HG3	1:A:516:TYR:CD1	2.47	0.50
1:B:360:HIS:HD2	1:B:381:TYR:OH	1.94	0.50
1:B:361:SER:O	1:B:365:ARG:HG3	2.12	0.49
1:A:459:GLU:HG3	1:A:462:ASN:HB2	1.95	0.49
1:A:275:ARG:NH1	1:A:275:ARG:HB3	2.28	0.49
1:A:260:LYS:HE2	1:A:300:TYR:CD1	2.48	0.49
1:A:528:TYR:HB2	1:A:535:PRO:HG2	1.94	0.48
1:B:447:VAL:HG11	1:B:470:VAL:HG11	1.95	0.48
1:B:355:LYS:O	1:B:358:LYS:HB3	2.12	0.48
1:A:334:THR:O	1:A:337:LYS:HE3	2.13	0.48
1:A:478:PRO:HD2	1:A:479:GLU:OE1	2.13	0.48
1:B:374:PRO:HG3	1:B:406:ARG:CZ	2.43	0.48
1:B:391:ILE:O	1:B:395:ARG:HG3	2.14	0.48
1:B:448:LEU:HD22	1:B:487:ARG:CZ	2.44	0.48
1:B:419:GLU:OE1	1:B:419:GLU:HA	2.14	0.47
1:B:419:GLU:O	1:B:423:SER:HB2	2.14	0.47
1:A:408:ARG:HH21	1:A:410:HIS:CE1	2.32	0.47
1:B:382:MSE:HE2	1:B:418:MSE:CE	2.45	0.47
1:A:454:LEU:HD12	1:A:457:LEU:HD12	1.96	0.47
1:B:447:VAL:HG11	1:B:470:VAL:HG13	1.96	0.47
1:A:309:ALA:HA	1:A:314:MSE:HE2	1.97	0.47
1:A:269:GLN:HB3	1:A:308:LEU:HD21	1.97	0.47
1:A:497:ASP:HA	1:B:387:ARG:HD2	1.98	0.46
1:B:266:THR:HG22	1:B:268:ASP:N	2.20	0.46
1:B:304:SER:O	1:B:308:LEU:HG	2.16	0.46
1:A:536:CYS:HB2	1:A:541:LEU:HD13	1.96	0.46
1:B:325:ALA:HB2	1:B:353:ARG:HH12	1.80	0.46
1:A:398:PHE:HE2	1:A:411:VAL:HG13	1.81	0.46
1:A:292:ASP:N	1:A:292:ASP:OD1	2.49	0.46
1:A:242:THR:HG23	1:A:245:GLU:CB	2.44	0.45
1:B:382:MSE:HE1	1:B:415:ALA:HA	1.97	0.45
1:B:517:GLU:OE1	1:B:517:GLU:HA	2.16	0.45
1:A:528:TYR:HB2	1:A:535:PRO:HG3	1.98	0.45
1:A:425:ASP:OD2	1:A:427:SER:HB3	2.16	0.45
1:B:256:ILE:HG22	1:B:260:LYS:HE3	1.99	0.45
1:A:524:LEU:HG	1:B:341:LEU:HD11	1.99	0.45
1:A:546:TYR:OH	1:A:548:ASP:HB2	2.17	0.45
1:A:391:ILE:HG21	1:A:395:ARG:NH2	2.32	0.45
1:A:408:ARG:NH2	1:B:533:LEU:HD21	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:HIS:CD2	1:B:531:MSE:HE2	2.51	0.45
1:A:417:LEU:HD22	1:A:421:TYR:HE1	1.81	0.44
1:A:540:GLU:OE2	1:B:339:ASN:ND2	2.50	0.44
1:A:382:MSE:HB3	1:A:418:MSE:HE1	1.97	0.44
1:A:491:PHE:CZ	1:A:495:ILE:HD11	2.53	0.44
1:B:374:PRO:HB2	1:B:378:TYR:CE1	2.53	0.44
1:A:516:TYR:CD2	1:A:523:LEU:HB2	2.53	0.44
1:A:517:GLU:OE1	1:A:517:GLU:HA	2.16	0.44
1:B:512:PHE:O	1:B:513:ARG:C	2.56	0.44
1:A:526:ASP:HA	1:A:529:LYS:HG2	1.99	0.44
1:B:302:GLU:HG3	1:B:349:TYR:CE1	2.52	0.44
1:A:271:LEU:O	1:A:275:ARG:HG3	2.19	0.43
1:A:546:TYR:CZ	1:A:548:ASP:HB2	2.52	0.43
1:B:512:PHE:HB3	1:B:515:GLU:HB3	2.01	0.43
1:B:365:ARG:O	1:B:368:ALA:HB3	2.18	0.43
1:B:531:MSE:HG3	1:B:531:MSE:O	2.19	0.43
1:B:425:ASP:CG	1:B:428:VAL:HG23	2.38	0.43
1:A:537:SER:OG	1:A:540:GLU:HB2	2.18	0.43
1:B:531:MSE:O	1:B:532:ASP:OD1	2.37	0.43
1:B:407:THR:CG2	1:B:411:VAL:HG21	2.48	0.43
1:B:528:TYR:HB2	1:B:535:PRO:CG	2.48	0.43
1:B:256:ILE:HD13	1:B:280:TYR:CD2	2.54	0.43
1:A:340:MSE:HE3	1:A:344:PHE:CZ	2.53	0.43
1:A:507:ARG:O	1:A:510:THR:HB	2.19	0.43
1:A:460:ASP:OD2	1:A:460:ASP:N	2.51	0.43
1:A:425:ASP:C	1:A:425:ASP:OD2	2.58	0.43
1:A:331:ALA:HB1	1:A:342:LEU:HD13	2.01	0.43
1:A:530:PHE:O	1:A:531:MSE:C	2.56	0.42
1:A:259:GLU:CD	1:A:275:ARG:NH1	2.72	0.42
1:B:524:LEU:O	1:B:527:ARG:HB3	2.18	0.42
1:B:539:SER:O	1:B:542:LYS:HB3	2.19	0.42
1:B:485:TRP:CG	1:B:508:ARG:HG2	2.55	0.42
1:B:425:ASP:OD1	1:B:428:VAL:HG23	2.19	0.42
1:B:273:THR:HG21	1:B:320:PHE:CE2	2.54	0.42
1:A:303:GLN:H	1:A:303:GLN:HG2	1.68	0.42
1:A:483:GLU:O	1:A:487:ARG:HG2	2.20	0.41
1:A:372:ILE:C	1:A:372:ILE:HD12	2.40	0.41
1:B:447:VAL:CG1	1:B:470:VAL:HG11	2.49	0.41
1:B:528:TYR:HB2	1:B:535:PRO:HG3	2.03	0.41
1:B:248:GLN:CA	1:B:251:MSE:HE2	2.49	0.41
1:B:375:THR:O	1:B:379:ILE:HG13	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:MSE:O	1:A:281:GLU:HG2	2.20	0.41
1:A:457:LEU:HA	1:A:457:LEU:HD23	1.92	0.41
1:B:312:GLY:O	1:B:314:MSE:N	2.54	0.41
1:A:264:LEU:O	1:A:265:ARG:HB2	2.20	0.41
1:B:337:LYS:O	1:B:343:TYR:OH	2.28	0.41
1:A:295:TYR:CZ	1:B:524:LEU:HD22	2.56	0.41
1:B:514:GLU:O	1:B:515:GLU:C	2.59	0.41
1:A:490:ALA:O	1:A:493:SER:HB3	2.21	0.41
1:A:419:GLU:HG3	1:A:428:VAL:HG12	2.03	0.41
1:B:464:ARG:NE	1:B:492:GLU:OE2	2.51	0.41
1:B:277:MSE:SE	1:B:301:LEU:HG	2.70	0.41
1:A:464:ARG:NE	1:A:492:GLU:OE2	2.49	0.41
1:A:382:MSE:HE1	1:A:415:ALA:CA	2.50	0.41
1:A:309:ALA:HA	1:A:314:MSE:CE	2.51	0.40
1:A:419:GLU:O	1:A:423:SER:HB2	2.20	0.40
1:A:340:MSE:HE3	1:A:344:PHE:CE1	2.56	0.40
1:A:348:ASP:OD2	1:B:527:ARG:NH1	2.54	0.40
1:A:381:TYR:CE1	1:A:397:ILE:HD12	2.57	0.40
1:A:323:GLU:O	1:A:327:ILE:HG12	2.22	0.40
1:A:422:CYS:SG	1:B:495:ILE:HG22	2.62	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	306/308 (99%)	291 (95%)	13 (4%)	2 (1%)	26	62
1	B	306/308 (99%)	285 (93%)	16 (5%)	5 (2%)	12	38
All	All	612/616 (99%)	576 (94%)	29 (5%)	7 (1%)	17	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	515	GLU
1	A	531	MSE
1	B	265	ARG
1	B	313	ASP
1	B	514	GLU
1	A	515	GLU
1	B	531	MSE

### 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	270/261 (103%)	255 (94%)	15 (6%)	26	59
1	B	270/261 (103%)	257 (95%)	13 (5%)	31	66
All	All	540/522 (103%)	512 (95%)	28 (5%)	29	62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	TYR
1	A	262	ASN
1	A	289	HIS
1	A	302	GLU
1	A	303	GLN
1	A	323	GLU
1	A	355	LYS
1	A	381	TYR
1	A	386	ARG
1	A	411	VAL
1	A	458	ASN
1	A	488	PHE
1	A	507	ARG
1	A	527	ARG
1	A	532	ASP
1	B	262	ASN
1	B	381	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	391	ILE
1	B	403	GLU
1	B	458	ASN
1	B	472	THR
1	B	479	GLU
1	B	488	PHE
1	B	508	ARG
1	B	509	PHE
1	B	527	ARG
1	B	529	LYS
1	B	532	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	A	262	ASN
1	A	289	HIS
1	A	458	ASN
1	A	462	ASN
1	B	247	GLN
1	B	303	GLN
1	B	316	ASN
1	B	360	HIS
1	B	458	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	299/308 (97%)	-0.16	8 (2%) 58 45	28, 48, 94, 106	0
1	B	299/308 (97%)	-0.06	12 (4%) 42 30	29, 54, 99, 109	0
All	All	598/616 (97%)	-0.11	20 (3%) 50 38	28, 51, 97, 109	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	TYR	5.0
1	B	549	VAL	4.4
1	A	548	ASP	4.0
1	B	265	ARG	3.3
1	B	315	ASN	3.1
1	A	513	ARG	3.0
1	A	514	GLU	2.8
1	B	267	GLU	2.8
1	B	516	TYR	2.8
1	B	515	GLU	2.7
1	A	515	GLU	2.6
1	B	313	ASP	2.5
1	B	514	GLU	2.5
1	B	548	ASP	2.3
1	B	242	THR	2.3
1	A	312	GLY	2.3
1	B	244	GLN	2.1
1	A	512	PHE	2.1
1	B	513	ARG	2.1
1	A	311	LYS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.