



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:45 AM GMT

PDB ID : 3PQZ  
Title : Grb7 SH2 with peptide  
Authors : Wilce, J.A.  
Deposited on : 2010-11-29  
Resolution : 2.41 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

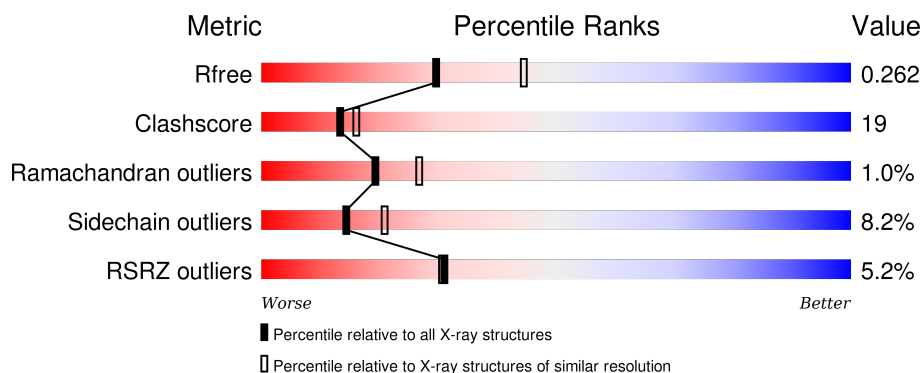
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	117	<div> <div>2%</div> <div>68% 20% • 11%</div> </div>
1	B	117	<div> <div>5%</div> <div>62% 19% 7% • 10%</div> </div>
1	C	117	<div> <div>4%</div> <div>51% 26% • • 17%</div> </div>
1	D	117	<div> <div>8%</div> <div>56% 21% 6% • 17%</div> </div>
2	L	11	<div> <div>64% 36%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	M	11	 64% 36%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3537 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 Growth factor receptor-bound protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			841	534	157	145	5			
1	B	105	Total	C	N	O	S	0	0	0
			848	538	161	144	5			
1	C	97	Total	C	N	O	S	0	0	0
			791	505	145	136	5			
1	D	97	Total	C	N	O	S	0	0	0
			754	484	134	131	5			

- Molecule 2 is a protein called cyclic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	11	Total	C	N	O	S	0	0	0
			100	67	13	19	1			
2	M	11	Total	C	N	O	S	0	0	0
			100	67	13	19	1			

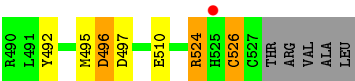
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	32	Total	O	0	0
			32	32		
3	C	21	Total	O	0	0
			21	21		
3	D	21	Total	O	0	0
			21	21		
3	L	1	Total	O	0	0
			1	1		

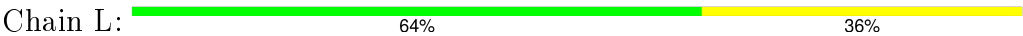


- Molecule 1: Growth factor receptor-bound protein 7





● Molecule 2: cyclic peptide



● Molecule 2: cyclic peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.66 Å 79.11 Å 54.69 Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	32.88 – 2.41 37.36 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.8 (32.88-2.41) 92.8 (37.36-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.42 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7 _650)	Depositor
R, $R_{free}$	0.238 , 0.277 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	779 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 67.3	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 15604 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.78 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.4551e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.66	0/858	0.79	1/1154 (0.1%)
1	B	0.74	2/863 (0.2%)	0.71	3/1159 (0.3%)
1	C	0.53	0/807	0.67	1/1086 (0.1%)
1	D	0.68	0/770	0.68	2/1040 (0.2%)
2	L	0.27	0/96	0.33	0/131
2	M	0.26	0/96	0.32	0/131
All	All	0.64	2/3490 (0.1%)	0.70	7/4701 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	GLN	CD-NE2	-5.89	1.18	1.32
1	B	442	GLN	CD-OE1	-5.07	1.12	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	438	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	D	496	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	497	ASP	CB-CG-OD1	5.75	123.47	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	506	LEU	CB-CG-CD2	5.45	120.26	111.00
1	B	425	ILE	CB-CA-C	-5.44	100.73	111.60
1	B	425	ILE	CG1-CB-CG2	-5.38	99.55	111.40
1	D	463	ASN	N-CA-C	-5.18	97.00	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	425	ILE	Peptide
1	D	462	ARG	Peptide

## 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	841	0	830	20	0
1	B	848	0	842	35	0
1	C	791	0	783	41	0
1	D	754	0	715	29	0
2	L	100	0	75	5	0
2	M	100	0	75	4	0
3	A	28	0	0	3	0
3	B	32	0	0	6	0
3	C	21	0	0	2	0
3	D	21	0	0	2	0
3	L	1	0	0	0	0
All	All	3537	0	3320	127	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 19.

All (127) 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:C:496:ASP:HB2	1:C:499:GLN:NE2	1.40	1.36

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:HIS:HB3	1:D:436:ILE:HD11	1.21	1.18
1:C:496:ASP:CB	1:C:499:GLN:NE2	2.07	1.15
1:C:433:HIS:HB3	1:C:436:ILE:HD11	1.24	1.12
1:B:425:ILE:HG22	1:B:426:HIS:N	1.64	1.09
1:B:463:ASN:HD22	1:B:465:GLN:CB	1.68	1.06
1:C:496:ASP:HB2	1:C:499:GLN:HE22	1.20	0.98
1:B:463:ASN:ND2	1:B:465:GLN:CB	2.30	0.94
1:D:433:HIS:CB	1:D:436:ILE:HD11	1.97	0.94
1:C:490:ARG:N	3:C:93:HOH:O	2.02	0.92
1:C:496:ASP:HB2	1:C:499:GLN:HE21	1.36	0.90
1:B:425:ILE:HG22	1:B:426:HIS:H	1.37	0.90
1:B:425:ILE:CG2	1:B:426:HIS:H	1.82	0.88
1:C:433:HIS:CB	1:C:436:ILE:HD11	2.05	0.87
1:B:465:GLN:N	3:B:85:HOH:O	2.07	0.86
1:C:499:GLN:N	1:C:499:GLN:OE1	2.09	0.85
1:B:424:ALA:O	1:B:425:ILE:HB	1.75	0.84
1:C:496:ASP:CB	1:C:499:GLN:HE22	1.80	0.83
1:B:492:TYR:HB2	1:B:502:PHE:O	1.82	0.80
1:D:510:GLU:OE1	3:D:29:HOH:O	2.01	0.77
1:C:430:LEU:HD13	1:C:432:PHE:H	1.50	0.76
1:B:486:GLU:HA	1:B:491:LEU:HG	1.67	0.76
1:B:425:ILE:CG2	1:B:426:HIS:N	2.29	0.75
1:D:431:TRP:HB3	1:D:526:CYS:SG	2.27	0.75
1:B:487:GLU:OE1	1:C:474:LEU:HD11	1.85	0.75
1:C:431:TRP:HB3	1:C:526:CYS:SG	2.27	0.75
1:C:496:ASP:CG	1:C:499:GLN:NE2	2.40	0.74
1:A:459:GLU:O	3:A:28:HOH:O	2.07	0.72
1:B:424:ALA:O	1:B:425:ILE:CB	2.37	0.72
1:A:460:SER:OG	1:A:464:PRO:HD2	1.91	0.71
1:A:438:ARG:O	1:A:442:GLN:HG3	1.92	0.70
1:C:439:GLU:HG3	1:C:443:ARG:HE	1.58	0.68
1:C:451:VAL:HG23	1:C:454:LEU:HB2	1.76	0.67
1:A:485:SER:OG	1:A:492:TYR:CZ	2.48	0.67
1:D:451:VAL:HG23	1:D:454:LEU:HB2	1.76	0.66
1:B:425:ILE:O	1:B:427:ARG:N	2.27	0.65
1:B:425:ILE:HG22	1:B:426:HIS:CA	2.26	0.65
1:C:496:ASP:O	1:C:499:GLN:NE2	2.29	0.64
1:D:476:LYS:NZ	1:D:478:LYS:NZ	2.46	0.64
1:C:476:LYS:NZ	1:C:478:LYS:NZ	2.45	0.64
1:C:496:ASP:C	1:C:499:GLN:HE22	2.02	0.63
1:A:485:SER:OG	1:A:492:TYR:CE1	2.51	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ASP:CA	1:C:499:GLN:HE22	2.13	0.61
1:B:487:GLU:HG2	1:B:492:TYR:OH	2.01	0.61
1:C:430:LEU:CD1	1:C:432:PHE:H	2.15	0.59
1:B:487:GLU:OE1	1:C:474:LEU:CD1	2.50	0.59
1:D:462:ARG:O	1:D:463:ASN:CB	2.47	0.59
1:A:433:HIS:CE1	1:A:444:LEU:HD13	2.39	0.58
1:C:440:GLU:HG3	1:C:443:ARG:NH2	2.19	0.58
1:B:516:ARG:NH2	3:B:30:HOH:O	2.36	0.57
1:A:459:GLU:CD	3:A:94:HOH:O	2.42	0.57
1:A:462:ARG:C	1:A:464:PRO:HD3	2.24	0.57
1:C:462:ARG:CD	1:C:463:ASN:HB2	2.34	0.57
1:B:433:HIS:CE1	1:B:444:LEU:HD13	2.39	0.57
3:B:24:HOH:O	2:M:8:THR:HG22	2.05	0.56
1:B:486:GLU:CA	1:B:491:LEU:HG	2.36	0.55
1:B:425:ILE:C	1:B:427:ARG:H	2.08	0.55
1:C:439:GLU:HG3	1:C:443:ARG:NE	2.22	0.55
1:B:509:VAL:O	1:B:513:GLN:HG3	2.07	0.55
1:D:433:HIS:HB3	1:D:436:ILE:CD1	2.15	0.53
1:B:443:ARG:NH2	3:B:65:HOH:O	2.41	0.52
1:B:516:ARG:HD3	1:B:521:CYS:HA	1.91	0.52
1:D:436:ILE:HG22	1:D:440:GLU:OE1	2.11	0.51
1:C:462:ARG:HD2	1:C:463:ASN:HB2	1.92	0.51
1:D:438:ARG:HG2	1:D:442:GLN:HE21	1.75	0.51
1:C:438:ARG:HG2	1:C:442:GLN:HE21	1.76	0.51
1:B:433:HIS:CE1	1:B:529:ARG:HA	2.46	0.51
2:L:9:PHE:HB2	2:L:10:PRO:HD2	1.93	0.50
1:B:435:ARG:HB2	1:B:459:GLU:OE1	2.11	0.50
1:B:438:ARG:HG3	1:B:479:HIS:CE1	2.47	0.50
1:A:438:ARG:HG3	1:A:479:HIS:CE1	2.47	0.50
1:A:487:GLU:OE1	1:D:474:LEU:CD1	2.59	0.50
1:A:435:ARG:HB2	1:A:459:GLU:OE1	2.11	0.50
1:D:435:ARG:HG3	1:D:435:ARG:HH11	1.77	0.49
1:B:425:ILE:C	1:B:427:ARG:N	2.61	0.49
1:D:434:GLY:O	1:D:459:GLU:HG3	2.13	0.49
2:M:9:PHE:HB2	2:M:10:PRO:HD2	1.93	0.48
1:A:482:ILE:HG12	1:A:495:MET:HG2	1.95	0.48
1:D:462:ARG:C	1:D:463:ASN:O	2.50	0.48
1:D:484:PRO:HA	1:D:492:TYR:O	2.13	0.48
1:C:432:PHE:CE2	1:C:434:GLY:HA2	2.48	0.48
1:C:462:ARG:HD3	1:C:463:ASN:HB2	1.95	0.48
1:C:484:PRO:HA	1:C:492:TYR:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ASP:O	1:C:499:GLN:OE1	2.31	0.47
1:D:496:ASP:HB3	2:L:10:PRO:HB3	1.97	0.47
1:D:435:ARG:HG2	1:D:459:GLU:CD	2.34	0.47
1:A:506:LEU:HD11	1:A:510:GLU:OE2	2.14	0.47
2:L:5:TYR:OH	2:M:3:GLU:HG2	2.15	0.47
1:B:425:ILE:HG22	1:B:426:HIS:HA	1.96	0.46
1:B:425:ILE:O	1:B:427:ARG:HG3	2.15	0.46
1:B:461:GLN:NE2	3:B:20:HOH:O	2.48	0.46
1:C:430:LEU:HD13	1:C:431:TRP:N	2.31	0.46
1:D:432:PHE:CE2	1:D:434:GLY:HA2	2.50	0.46
1:D:461:GLN:HA	1:D:462:ARG:HA	1.34	0.46
1:C:481:LEU:HG	1:C:483:LEU:HG	1.99	0.45
1:A:460:SER:OG	1:A:464:PRO:CD	2.63	0.45
1:B:433:HIS:ND1	1:B:444:LEU:HD13	2.32	0.45
1:D:462:ARG:O	1:D:463:ASN:O	2.33	0.45
1:A:433:HIS:ND1	1:A:444:LEU:HD13	2.31	0.45
1:C:476:LYS:NZ	1:C:478:LYS:HZ2	2.15	0.44
1:D:476:LYS:NZ	1:D:478:LYS:HZ2	2.15	0.44
1:A:461:GLN:HG3	1:A:462:ARG:N	2.30	0.44
1:C:476:LYS:HZ1	1:C:478:LYS:NZ	2.15	0.44
1:C:435:ARG:HH11	1:C:435:ARG:HG3	1.83	0.44
1:D:460:SER:OG	1:D:462:ARG:O	2.29	0.43
2:L:9:PHE:HB2	2:L:10:PRO:CD	2.48	0.43
1:A:487:GLU:OE1	1:D:474:LEU:HD13	2.18	0.43
1:B:426:HIS:C	1:B:428:THR:N	2.71	0.43
2:M:9:PHE:HB2	2:M:10:PRO:CD	2.48	0.43
1:A:431:TRP:HB3	1:A:526:CYS:SG	2.59	0.43
1:D:476:LYS:HZ1	1:D:478:LYS:NZ	2.16	0.43
1:C:468:VAL:HG11	1:C:479:HIS:HB3	2.01	0.42
1:B:492:TYR:OH	1:B:501:ARG:NH1	2.52	0.42
1:D:468:VAL:HG11	1:D:479:HIS:HB3	2.02	0.42
1:D:453:GLY:HA3	1:D:524:ARG:HD2	2.02	0.42
1:D:495:MET:HB2	3:D:106:HOH:O	2.19	0.42
3:A:11:HOH:O	2:L:8:THR:HG22	2.19	0.42
1:B:497:ASP:HA	3:B:38:HOH:O	2.19	0.41
1:A:429:GLN:HG3	1:A:431:TRP:CZ2	2.55	0.41
1:C:453:GLY:HA3	1:C:524:ARG:HD2	2.02	0.41
1:D:448:GLN:HB3	1:D:454:LEU:HD21	2.03	0.41
1:C:512:HIS:NE2	3:C:9:HOH:O	2.36	0.41
1:C:496:ASP:C	1:C:499:GLN:NE2	2.73	0.41
1:B:506:LEU:HD22	1:B:510:GLU:HG3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ASN:HA	1:C:464:PRO:HD3	1.91	0.40
1:A:487:GLU:OE1	1:D:474:LEU:HD11	2.21	0.40
1:C:476:LYS:HZ2	1:C:478:LYS:HZ2	1.68	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	100/117 (86%)	97 (97%)	3 (3%)	0	100	100
1	B	99/117 (85%)	96 (97%)	1 (1%)	2 (2%)	9	10
1	C	93/117 (80%)	88 (95%)	4 (4%)	1 (1%)	17	24
1	D	93/117 (80%)	89 (96%)	3 (3%)	1 (1%)	17	24
2	L	9/11 (82%)	9 (100%)	0	0	100	100
2	M	9/11 (82%)	9 (100%)	0	0	100	100
All	All	403/490 (82%)	388 (96%)	11 (3%)	4 (1%)	19	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	425	ILE
1	B	426	HIS
1	C	462	ARG
1	D	463	ASN

### 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	91/104 (88%)	88 (97%)	3 (3%)	45	65
1	B	91/104 (88%)	80 (88%)	11 (12%)	6	7
1	C	87/104 (84%)	78 (90%)	9 (10%)	9	12
1	D	78/104 (75%)	71 (91%)	7 (9%)	12	17
2	L	9/9 (100%)	9 (100%)	0	100	100
2	M	9/9 (100%)	9 (100%)	0	100	100
All	All	365/434 (84%)	335 (92%)	30 (8%)	14	21

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	435	ARG
1	A	490	ARG
1	A	514	LEU
1	B	425	ILE
1	B	428	THR
1	B	430	LEU
1	B	435	ARG
1	B	461	GLN
1	B	463	ASN
1	B	487	GLU
1	B	490	ARG
1	B	492	TYR
1	B	506	LEU
1	B	529	ARG
1	C	435	ARG
1	C	436	ILE
1	C	461	GLN
1	C	462	ARG
1	C	465	GLN
1	C	475	GLN
1	C	497	ASP
1	C	524	ARG
1	C	526	CYS
1	D	435	ARG
1	D	436	ILE
1	D	439	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	460	SER
1	D	497	ASP
1	D	524	ARG
1	D	526	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	461	GLN
1	B	463	ASN
1	C	442	GLN
1	D	442	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	CCS	L	11	2	7,8,10	1.09	0	3,8,12	0.99	0
2	CCS	M	11	2	7,8,10	1.41	1 (14%)	3,8,12	1.25	0

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	CCS	L	11	2	-	0/4/7/10	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CCS	M	11	2	-	0/4/7/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	11	CCS	CD-SG	3.00	1.84	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

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	104/117 (88%)	0.18	2 (1%) 70 69	13, 26, 62, 75	0
1	B	105/117 (89%)	0.17	6 (5%) 27 27	14, 26, 57, 95	0
1	C	97/117 (82%)	0.34	5 (5%) 31 30	14, 33, 67, 89	0
1	D	97/117 (82%)	0.44	9 (9%) 11 10	18, 33, 59, 80	0
2	L	10/11 (90%)	-0.15	0 100 100	19, 23, 33, 45	0
2	M	10/11 (90%)	-0.02	0 100 100	20, 23, 33, 46	0
All	All	423/490 (86%)	0.26	22 (5%) 31 30	13, 29, 61, 95	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	462	ARG	4.4
1	B	492	TYR	4.0
1	D	447	GLN	3.9
1	D	448	GLN	3.8
1	D	450	LEU	3.7
1	D	446	GLY	3.4
1	B	451	VAL	3.3
1	C	488	GLU	3.1
1	D	451	VAL	2.9
1	D	525	HIS	2.9
1	C	449	GLY	2.8
1	D	487	GLU	2.8
1	D	430	LEU	2.7
1	C	447	GLN	2.5
1	B	489	GLY	2.5
1	D	444	LEU	2.5
1	A	465	GLN	2.3
1	C	461	GLN	2.3
1	B	491	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	423	ALA	2.1
1	B	474	LEU	2.0
1	A	492	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CCS	L	11	9/11	0.96	0.13	-	18,21,29,34	0
2	CCS	M	11	9/11	0.93	0.16	-	17,22,33,34	0

## 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.