



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:04 AM GMT

PDB ID : 2FHD
Title : Crystal structure of Crb2 tandem tudor domains
Authors : Lee, J.; Botuyan, M.V.; Thompson, J.R.; Mer, G.
Deposited on : 2005-12-23
Resolution : 2.40 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

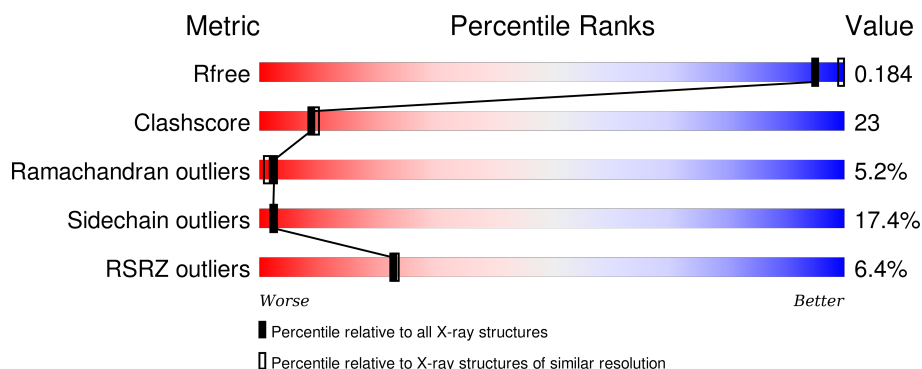
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 ≥ 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	153	<div> <div>3%</div> <div>61%</div> <div>27%</div> <div>8%</div> <div>• •</div> </div>
1	B	153	<div> <div>11%</div> <div>50%</div> <div>24%</div> <div>9%</div> <div>8%</div> <div>8%</div> </div>
1	C	153	<div> <div>3%</div> <div>60%</div> <div>20%</div> <div>10%</div> <div>•</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	301[A]	-	-	-	X
2	PO4	A	301[B]	-	-	-	X
2	PO4	A	312	-	-	-	X
2	PO4	C	302	-	-	-	X
2	PO4	C	305	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3722 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 DNA repair protein rhp9/CRB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	Se	0	4	0
			1230	788	213	223	6			
1	B	140	Total	C	N	O	Se	0	1	0
			1124	721	196	204	3			
1	C	142	Total	C	N	O	Se	0	1	0
			1137	733	193	207	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	INSERTION	GB 1449177
A	356	HIS	-	INSERTION	GB 1449177
A	357	MSE	-	INSERTION	GB 1449177
B	355	GLY	-	INSERTION	GB 1449177
B	356	HIS	-	INSERTION	GB 1449177
B	357	MSE	-	INSERTION	GB 1449177
C	355	GLY	-	INSERTION	GB 1449177
C	356	HIS	-	INSERTION	GB 1449177
C	357	MSE	-	INSERTION	GB 1449177

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	1
			10	8	2		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	1
			10	8	2		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	11
			78	78		
3	B	47	Total	O	0	6
			49	49		

Continued on next page...

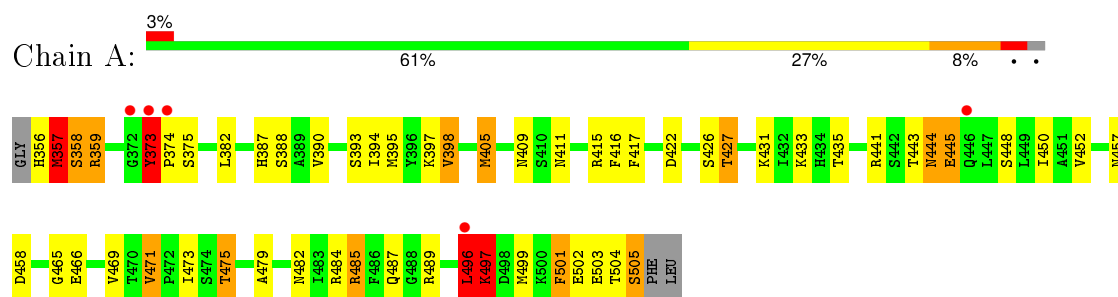
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	40	Total	O	0	4
			44	44		

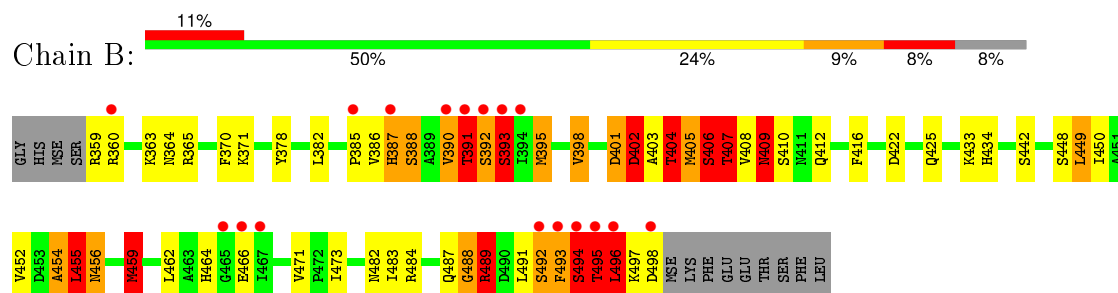
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

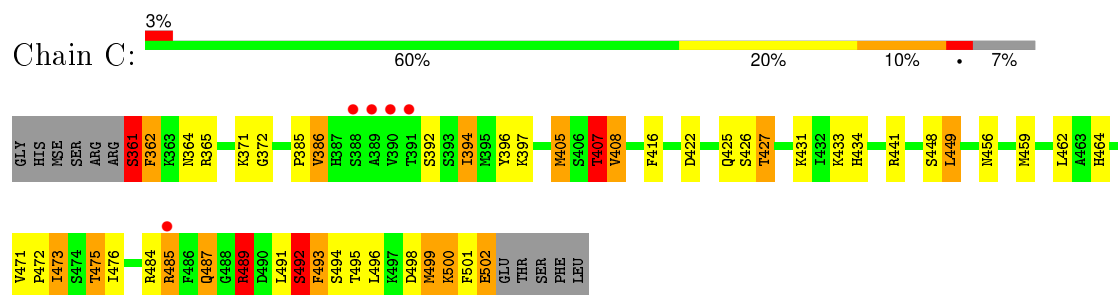
• Molecule 1: DNA repair protein rhp9/CRB2



• Molecule 1: DNA repair protein rhp9/CRB2



• Molecule 1: DNA repair protein rhp9/CRB2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 116.92Å 87.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.00 – 2.40 33.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.00-2.40) 100.0 (33.00-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	45.76 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.256 0.196 , 0.184	Depositor DCC
R_{free} test set	1366 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 75.1	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27191 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3722	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: PO4

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	1.37	7/1249 (0.6%)	1.30	11/1676 (0.7%)
1	B	1.22	2/1143 (0.2%)	1.28	10/1541 (0.6%)
1	C	1.21	1/1156 (0.1%)	1.25	10/1556 (0.6%)
All	All	1.27	10/3548 (0.3%)	1.28	31/4773 (0.6%)

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	A	0	2
1	B	0	12
1	C	0	4
All	All	0	18

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	ASP	CB-CG	-9.28	1.32	1.51
1	B	459	MSE	N-CA	9.25	1.64	1.46
1	A	496	LEU	N-CA	8.14	1.62	1.46
1	A	469	VAL	CB-CG2	-6.08	1.40	1.52
1	A	417	PHE	CD2-CE2	5.79	1.50	1.39
1	B	395	MSE	SE-CE	5.30	2.26	1.95
1	A	485	ARG	CB-CG	5.16	1.66	1.52
1	A	416	PHE	CD2-CE2	5.10	1.49	1.39
1	C	493	PHE	N-CA	5.03	1.56	1.46
1	A	496	LEU	CA-C	5.00	1.66	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	489	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	A	458	ASP	CB-CG-OD1	-11.44	108.01	118.30
1	A	484	ARG	NE-CZ-NH1	-9.19	115.71	120.30
1	B	455	LEU	N-CA-C	9.18	135.80	111.00
1	A	359	ARG	N-CA-C	-8.96	86.80	111.00
1	C	407	THR	C-N-CA	8.71	143.49	121.70
1	A	458	ASP	N-CA-CB	-7.66	96.81	110.60
1	C	489	ARG	CG-CD-NE	-7.66	95.71	111.80
1	B	406	SER	N-CA-C	7.18	130.39	111.00
1	A	398	VAL	CG1-CB-CG2	6.94	122.00	110.90
1	C	459	MSE	CG-SE-CE	6.47	113.14	98.90
1	C	407	THR	CA-C-N	6.37	131.22	117.20
1	C	361	SER	CB-CA-C	-6.35	98.03	110.10
1	C	427	THR	CA-CB-CG2	6.21	121.09	112.40
1	B	406	SER	CB-CA-C	-6.17	98.38	110.10
1	B	402	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	373	TYR	N-CA-C	5.74	126.50	111.00
1	B	459	MSE	N-CA-C	5.67	126.30	111.00
1	C	441	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	497	LYS	CD-CE-NZ	-5.52	99.00	111.70
1	B	409	ASN	CB-CA-C	-5.49	99.42	110.40
1	B	407	THR	N-CA-C	5.38	125.52	111.00
1	A	458	ASP	OD1-CG-OD2	5.28	133.32	123.30
1	C	408	VAL	CB-CA-C	5.20	121.28	111.40
1	C	361	SER	C-N-CA	5.19	134.66	121.70
1	B	494	SER	N-CA-C	5.16	124.94	111.00
1	A	485	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	454	ALA	N-CA-C	5.09	124.76	111.00
1	B	489	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	450	ILE	CG1-CB-CG2	-5.05	100.29	111.40
1	A	441	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	SER	Peptide
1	A	373	TYR	Peptide
1	B	387	HIS	Peptide
1	B	390	VAL	Peptide
1	B	391	THR	Peptide
1	B	392	SER	Peptide
1	B	401	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	402	ASP	Peptide
1	B	405	MSE	Peptide
1	B	406	SER	Peptide
1	B	454	ALA	Peptide
1	B	488	GLY	Peptide
1	B	494	SER	Peptide
1	B	495	THR	Peptide
1	C	361	SER	Peptide
1	C	491	LEU	Peptide
1	C	492	SER	Peptide
1	C	499	MSE	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	1230	0	1258	51	0
1	B	1124	0	1150	77	0
1	C	1137	0	1162	46	0
2	A	25	0	0	0	0
2	B	10	0	0	1	0
2	C	25	0	0	0	0
3	A	78	0	0	6	1
3	B	49	0	0	3	0
3	C	44	0	0	2	1
All	All	3722	0	3570	166	1

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 23.

All (166) 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:405:MSE:SE	1:A:405:MSE:CE	2.15	1.44
1:A:357:MSE:SE	1:A:357:MSE:CE	2.15	1.43
1:A:499[A]:MSE:CE	1:A:499[A]:MSE:SE	2.16	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:MSE:SE	1:B:395:MSE:CE	2.26	1.33
1:A:388:SER:HB2	1:A:395:MSE:CE	1.67	1.23
1:C:492:SER:OG	1:C:493:PHE:HA	1.47	1.12
1:A:496:LEU:HA	1:A:497:LYS:HB2	1.27	1.12
1:B:406:SER:OG	1:B:407:THR:HA	1.51	1.09
1:C:492:SER:HB3	1:C:496:LEU:HG	1.25	1.08
1:C:487:GLN:HA	1:C:487:GLN:HE21	1.23	1.01
1:C:492:SER:CB	1:C:496:LEU:HG	1.89	1.01
1:B:360:ARG:HH21	1:B:497:LYS:CD	1.74	1.01
1:A:356:HIS:O	3:A:87:HOH:O	1.77	1.00
1:B:360:ARG:HH21	1:B:497:LYS:HD2	1.23	1.00
1:C:492:SER:OG	1:C:493:PHE:CA	2.09	1.00
1:C:361:SER:OG	1:C:362:PHE:N	1.88	1.00
1:A:388:SER:HB2	1:A:395:MSE:HE2	1.45	0.99
1:C:492:SER:HB2	1:C:496:LEU:H	1.25	0.98
1:A:388:SER:HB2	1:A:395:MSE:HE1	1.45	0.98
1:B:398:VAL:O	1:B:406:SER:HB3	1.64	0.98
1:C:487:GLN:HA	1:C:487:GLN:NE2	1.79	0.95
1:B:488:GLY:H	1:B:489:ARG:NH1	1.65	0.95
1:B:493:PHE:HB2	1:B:495:THR:N	1.82	0.94
1:B:406:SER:OG	1:B:407:THR:CA	2.16	0.94
1:B:403:ALA:C	1:B:404:THR:HG22	1.89	0.93
1:A:496:LEU:O	1:A:496:LEU:HD23	1.68	0.92
1:B:403:ALA:O	1:B:404:THR:HG22	1.68	0.92
1:B:398:VAL:HG12	1:B:406:SER:HB2	1.50	0.91
1:B:493:PHE:HD1	1:B:494:SER:HA	1.35	0.87
1:B:403:ALA:O	1:B:404:THR:CB	2.23	0.84
1:B:493:PHE:CD1	1:B:494:SER:HA	2.13	0.83
1:B:403:ALA:O	1:B:404:THR:CG2	2.26	0.82
1:B:406:SER:HG	1:B:407:THR:HA	1.40	0.82
1:B:406:SER:OG	1:B:407:THR:N	2.08	0.79
1:C:422:ASP:OD2	1:C:489:ARG:NH2	2.15	0.79
1:A:496:LEU:C	1:A:496:LEU:HD23	2.02	0.79
1:B:409:ASN:HB2	1:B:412:GLN:OE1	1.83	0.78
1:C:492:SER:HB2	1:C:496:LEU:N	1.99	0.78
1:C:361:SER:HB2	1:C:364:ASN:HD22	1.49	0.78
1:C:492:SER:HA	1:C:495:THR:HB	1.65	0.77
1:C:433:LYS:O	1:C:464:HIS:HD2	1.69	0.76
1:B:365:ARG:HD3	1:B:449:LEU:HD22	1.68	0.75
1:A:496:LEU:HA	1:A:497:LYS:CB	2.13	0.74
1:B:403:ALA:O	1:B:404:THR:HB	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:SER:CB	1:A:395:MSE:HE2	2.17	0.74
1:B:360:ARG:NH2	1:B:497:LYS:HD2	2.01	0.73
1:B:398:VAL:H	1:B:406:SER:HB3	1.53	0.73
1:A:465:GLY:HA3	3:A:9:HOH:O	1.89	0.73
1:B:488:GLY:N	1:B:489:ARG:NH1	2.36	0.72
1:B:488:GLY:N	1:B:489:ARG:HH11	1.86	0.72
1:B:488:GLY:H	1:B:489:ARG:HH11	1.35	0.72
1:A:388:SER:CB	1:A:395:MSE:CE	2.60	0.72
1:B:360:ARG:HH21	1:B:497:LYS:CE	2.03	0.71
1:B:493:PHE:HB2	1:B:495:THR:H	1.53	0.71
1:C:499:MSE:HA	1:C:500:LYS:HB2	1.71	0.71
1:A:387:HIS:H	1:A:499[A]:MSE:HE1	1.56	0.70
1:B:398:VAL:CG1	1:B:406:SER:HB2	2.21	0.69
1:C:361:SER:OG	1:C:362:PHE:CA	2.42	0.69
1:C:426:SER:OG	1:C:475:THR:HG23	1.93	0.68
1:C:487:GLN:CA	1:C:487:GLN:NE2	2.56	0.68
1:A:409:ASN:OD1	1:A:411:ASN:HB2	1.94	0.68
1:B:403:ALA:C	1:B:404:THR:CG2	2.59	0.67
1:B:360:ARG:HG2	1:B:364:ASN:ND2	2.09	0.67
1:B:455:LEU:H	1:B:455:LEU:HD13	1.61	0.64
1:B:398:VAL:H	1:B:406:SER:CB	2.11	0.64
1:B:493:PHE:HB2	1:B:494:SER:C	2.18	0.63
1:B:401:ASP:O	1:B:402:ASP:HB2	1.98	0.63
1:A:505:SER:HB3	1:B:371:LYS:HB2	1.80	0.63
1:A:496:LEU:HD22	3:A:221:HOH:O	1.98	0.62
1:A:382:LEU:HG	1:A:497:LYS:HE3	1.80	0.62
1:A:471:VAL:HG13	1:A:475:THR:HG21	1.82	0.62
1:C:365:ARG:HD3	1:C:449:LEU:HD22	1.82	0.62
1:C:433:LYS:O	1:C:464:HIS:CD2	2.52	0.61
1:B:494:SER:O	1:B:495:THR:O	2.19	0.61
1:A:504:THR:HG22	1:B:406:SER:O	2.01	0.61
1:C:492:SER:HG	1:C:493:PHE:HA	1.62	0.61
1:B:360:ARG:NH2	1:B:497:LYS:HE3	2.17	0.60
1:A:504:THR:OG1	3:A:75[B]:HOH:O	2.16	0.60
1:A:356:HIS:HB2	1:A:357:MSE:O	2.02	0.59
1:B:360:ARG:HH21	1:B:497:LYS:HE3	1.68	0.58
1:A:427:THR:HG21	3:A:227:HOH:O	2.03	0.57
1:B:455:LEU:N	1:B:455:LEU:CD1	2.68	0.57
1:C:397:LYS:HD2	1:C:405:MSE:HG2	1.85	0.57
1:C:396:TYR:O	1:C:407:THR:HA	2.04	0.57
1:A:479:ALA:HB3	1:A:482:ASN:HD22	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:CA	1:A:497:LYS:HB2	2.18	0.57
1:A:426:SER:OG	1:A:475:THR:HG23	2.04	0.56
1:C:487:GLN:O	1:C:489:ARG:HD3	2.06	0.56
1:A:501:PHE:CD1	1:A:501:PHE:C	2.78	0.56
1:B:398:VAL:O	1:B:406:SER:CB	2.49	0.56
1:C:416:PHE:CZ	1:C:473:ILE:HD12	2.40	0.56
1:C:422:ASP:CG	1:C:489:ARG:HH22	2.08	0.56
1:A:496:LEU:C	1:A:496:LEU:CD2	2.72	0.56
1:B:495:THR:HA	1:B:498:ASP:HB2	1.88	0.55
1:C:501:PHE:O	1:C:502:GLU:HB2	2.06	0.55
1:B:398:VAL:HG12	1:B:406:SER:CB	2.31	0.55
1:B:359:ARG:HG2	3:B:88:HOH:O	2.07	0.54
1:A:496:LEU:O	1:A:496:LEU:CD2	2.49	0.54
1:A:485:ARG:NH1	1:A:487:GLN:HE21	2.05	0.54
1:A:471:VAL:HG13	1:A:475:THR:CG2	2.36	0.54
1:B:391:THR:OG1	1:B:393:SER:HB2	2.07	0.54
1:C:397:LYS:HD3	1:C:407:THR:HG22	1.89	0.54
1:B:422:ASP:OD1	1:B:489:ARG:NH2	2.41	0.53
1:B:455:LEU:N	1:B:455:LEU:HD13	2.23	0.53
1:B:494:SER:OG	1:B:495:THR:HG23	2.10	0.52
1:C:492:SER:CB	1:C:496:LEU:CG	2.78	0.51
1:A:485:ARG:HH11	1:A:487:GLN:HE21	1.59	0.51
1:C:386:VAL:N	3:C:21[B]:HOH:O	1.76	0.51
1:C:496:LEU:O	1:C:499:MSE:HG2	2.10	0.51
1:C:426:SER:OG	1:C:475:THR:CG2	2.59	0.51
1:B:492:SER:HA	1:B:493:PHE:CG	2.46	0.50
1:C:492:SER:OG	1:C:493:PHE:N	2.43	0.50
1:B:455:LEU:H	1:B:455:LEU:CD1	2.23	0.50
1:A:504:THR:CG2	1:B:407:THR:N	2.76	0.49
1:B:493:PHE:HD1	1:B:494:SER:CA	2.18	0.49
1:A:503:GLU:HA	1:A:503:GLU:OE1	2.13	0.49
1:A:444:ASN:HD22	1:A:444:ASN:H	1.61	0.49
1:A:397:LYS:HE3	1:A:405:MSE:SE	2.62	0.48
1:A:485:ARG:HH11	1:A:487:GLN:NE2	2.11	0.48
1:B:370:PHE:HB2	1:B:378:TYR:HD2	1.78	0.48
1:C:425:GLN:NE2	1:C:434:HIS:HD2	2.11	0.48
1:A:501:PHE:HD1	1:A:501:PHE:C	2.16	0.48
1:B:360:ARG:NH2	1:B:497:LYS:CD	2.59	0.48
1:A:485:ARG:NH1	1:A:487:GLN:NE2	2.62	0.48
1:B:360:ARG:NH2	1:B:497:LYS:CE	2.72	0.47
1:C:499:MSE:O	3:C:8:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:THR:HG23	1:B:407:THR:N	2.30	0.47
1:B:388:SER:HA	1:B:391:THR:CG2	2.45	0.46
1:A:499[B]:MSE:HG3	1:C:392[B]:SER:O	2.16	0.46
1:B:392:SER:O	1:B:393:SER:O	2.32	0.46
1:B:484:ARG:HD2	3:B:140:HOH:O	2.15	0.46
1:B:391:THR:OG1	1:B:393:SER:CB	2.65	0.45
1:C:472:PRO:O	1:C:475:THR:HB	2.16	0.45
1:B:398:VAL:CB	1:B:406:SER:HB2	2.46	0.45
1:B:385:PRO:HG3	1:B:498:ASP:C	2.38	0.45
1:B:434:HIS:HB3	1:B:462:LEU:HB3	2.00	0.44
1:A:433:LYS:NZ	1:A:482:ASN:HD21	2.16	0.44
1:C:484:ARG:HB3	1:C:485:ARG:NH2	2.33	0.44
1:C:487:GLN:CA	1:C:487:GLN:HE21	2.04	0.44
1:A:443:THR:OG1	1:A:445:GLU:HG2	2.18	0.44
1:A:503:GLU:CA	1:A:503:GLU:OE1	2.65	0.44
1:C:498:ASP:O	1:C:500:LYS:HD3	2.19	0.43
1:A:452:VAL:HA	1:A:457:ASN:O	2.18	0.43
1:C:471:VAL:HB	1:C:475:THR:HG21	2.01	0.43
1:C:425:GLN:O	1:C:476:ILE:HA	2.18	0.43
1:B:442:SER:HB3	1:B:459:MSE:HG3	2.01	0.43
1:B:425:GLN:NE2	3:B:197:HOH:O	2.52	0.42
1:A:394:ILE:HD13	1:C:499:MSE:HE3	2.01	0.42
1:C:385:PRO:HD2	1:C:500:LYS:O	2.20	0.42
1:B:409:ASN:HB2	1:B:412:GLN:CD	2.39	0.42
1:A:504:THR:CG2	1:B:406:SER:C	2.87	0.42
1:B:388:SER:HA	1:B:391:THR:HG22	2.02	0.42
1:B:459:MSE:HA	1:B:471:VAL:O	2.19	0.42
1:A:496:LEU:HD12	1:C:394:ILE:HG23	2.02	0.42
1:B:363:LYS:HB3	1:B:496:LEU:HD21	2.01	0.42
1:B:455:LEU:O	1:B:456:ASN:CB	2.66	0.41
1:C:492:SER:OG	1:C:493:PHE:C	2.58	0.41
1:C:397:LYS:HD2	1:C:405:MSE:CG	2.50	0.41
1:B:433:LYS:NZ	1:B:482:ASN:HD21	2.18	0.41
1:B:456:ASN:ND2	2:B:311[B]:PO4:O4	2.26	0.41
1:B:456:ASN:HD22	1:B:456:ASN:HA	1.64	0.41
1:B:401:ASP:O	1:B:402:ASP:CB	2.67	0.41
1:A:422:ASP:O	1:A:435:THR:HA	2.21	0.41
1:B:360:ARG:N	1:B:360:ARG:HD2	2.36	0.40
1:A:466:GLU:HG2	3:A:9:HOH:O	2.22	0.40
1:B:404:THR:OG1	1:B:405:MSE:O	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:121:HOH:O	3:C:122:HOH:O[3_665]	1.63	0.57

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	152/153 (99%)	140 (92%)	8 (5%)	4 (3%)	7	6
1	B	139/153 (91%)	116 (84%)	11 (8%)	12 (9%)	1	0
1	C	141/153 (92%)	129 (92%)	6 (4%)	6 (4%)	3	2
All	All	432/459 (94%)	385 (89%)	25 (6%)	22 (5%)	2	1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	LEU
1	A	497	LYS
1	B	388	SER
1	B	391	THR
1	B	393	SER
1	B	455	LEU
1	B	492	SER
1	B	495	THR
1	B	496	LEU
1	C	362	PHE
1	C	408	VAL
1	C	492	SER
1	C	500	LYS
1	B	390	VAL
1	B	402	ASP
1	B	459	MSE
1	A	357	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	404	THR
1	B	464	HIS
1	C	386	VAL
1	A	374	PRO
1	C	372	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	140/133 (105%)	117 (84%)	23 (16%)	3	3
1	B	127/133 (96%)	100 (79%)	27 (21%)	1	1
1	C	129/133 (97%)	110 (85%)	19 (15%)	4	4
All	All	396/399 (99%)	327 (83%)	69 (17%)	2	2

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	MSE
1	A	358	SER
1	A	359	ARG
1	A	373	TYR
1	A	375[A]	SER
1	A	375[B]	SER
1	A	390	VAL
1	A	393	SER
1	A	398	VAL
1	A	405	MSE
1	A	415	ARG
1	A	427	THR
1	A	431	LYS
1	A	444	ASN
1	A	445	GLU
1	A	448	SER
1	A	471	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	473	ILE
1	A	475	THR
1	A	489	ARG
1	A	501	PHE
1	A	502	GLU
1	A	505	SER
1	B	382	LEU
1	B	386	VAL
1	B	387	HIS
1	B	393	SER
1	B	398	VAL
1	B	404	THR
1	B	407	THR
1	B	408	VAL
1	B	409	ASN
1	B	410	SER
1	B	416	PHE
1	B	448	SER
1	B	449	LEU
1	B	450	ILE
1	B	452	VAL
1	B	455	LEU
1	B	456	ASN
1	B	459	MSE
1	B	466	GLU
1	B	473	ILE
1	B	483	ILE
1	B	487	GLN
1	B	489	ARG
1	B	491	LEU
1	B	493	PHE
1	B	495	THR
1	B	496	LEU
1	C	361	SER
1	C	371	LYS
1	C	394	ILE
1	C	405	MSE
1	C	407	THR
1	C	427	THR
1	C	431	LYS
1	C	448	SER
1	C	449	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	456	ASN
1	C	462	LEU
1	C	473	ILE
1	C	475	THR
1	C	485	ARG
1	C	487	GLN
1	C	489	ARG
1	C	492	SER
1	C	494	SER
1	C	502	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	HIS
1	A	444	ASN
1	A	446	GLN
1	A	482	ASN
1	A	487	GLN
1	B	399	GLN
1	B	425	GLN
1	B	444	ASN
1	B	456	ASN
1	B	482	ASN
1	C	364	ASN
1	C	425	GLN
1	C	434	HIS
1	C	456	ASN
1	C	464	HIS
1	C	487	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	PO4	A	301[A]	-	4,4,4	0.37	0	6,6,6	0.31	0
2	PO4	A	301[B]	-	4,4,4	0.23	0	6,6,6	0.35	0
2	PO4	A	306	-	4,4,4	0.32	0	6,6,6	0.28	0
2	PO4	A	307	-	4,4,4	0.24	0	6,6,6	0.28	0
2	PO4	A	312	-	4,4,4	0.83	0	6,6,6	0.28	0
2	PO4	B	311[A]	-	4,4,4	0.24	0	6,6,6	0.26	0
2	PO4	B	311[B]	-	4,4,4	0.80	0	6,6,6	0.29	0
2	PO4	C	302	-	4,4,4	0.23	0	6,6,6	0.28	0
2	PO4	C	303	-	4,4,4	0.56	0	6,6,6	0.26	0
2	PO4	C	304	-	4,4,4	0.19	0	6,6,6	0.29	0
2	PO4	C	305	-	4,4,4	0.52	0	6,6,6	0.26	0
2	PO4	C	309	-	4,4,4	0.37	0	6,6,6	0.26	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	PO4	A	301[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	A	301[B]	-	-	0/0/0/0	0/0/0/0
2	PO4	A	306	-	-	0/0/0/0	0/0/0/0
2	PO4	A	307	-	-	0/0/0/0	0/0/0/0
2	PO4	A	312	-	-	0/0/0/0	0/0/0/0
2	PO4	B	311[A]	-	-	0/0/0/0	0/0/0/0
2	PO4	B	311[B]	-	-	0/0/0/0	0/0/0/0
2	PO4	C	302	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	C	303	-	-	0/0/0/0	0/0/0/0
2	PO4	C	304	-	-	0/0/0/0	0/0/0/0
2	PO4	C	305	-	-	0/0/0/0	0/0/0/0
2	PO4	C	309	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	311[B]	PO4	1	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	145/153 (94%)	-0.16	5 (3%) 49 49	21, 31, 54, 66	0
1	B	137/153 (89%)	0.36	17 (12%) 5 5	25, 40, 79, 88	0
1	C	138/153 (90%)	-0.09	5 (3%) 46 47	22, 36, 58, 65	0
All	All	420/459 (91%)	0.03	27 (6%) 23 23	21, 35, 63, 88	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	TYR	9.7
1	B	392	SER	5.6
1	B	390	VAL	5.5
1	B	391	THR	5.4
1	B	496	LEU	5.3
1	C	389	ALA	5.3
1	B	465	GLY	4.9
1	B	498	ASP	4.9
1	B	466	GLU	4.3
1	C	390	VAL	4.1
1	B	467	ILE	3.6
1	A	496	LEU	3.6
1	B	360	ARG	3.4
1	A	374	PRO	3.3
1	B	394	ILE	3.1
1	C	485	ARG	3.1
1	C	388	SER	3.0
1	B	495	THR	2.9
1	B	385	PRO	2.8
1	B	393	SER	2.8
1	B	492	SER	2.7
1	B	494	SER	2.5
1	B	493	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	391	THR	2.4
1	B	387	HIS	2.4
1	A	446	GLN	2.2
1	A	372	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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(Å ²)	Q<0.9
2	PO4	A	312	5/5	0.63	0.46	10.39	120,120,122,122	0
2	PO4	A	301[B]	5/5	0.69	0.45	8.07	50,51,52,54	5
2	PO4	A	301[A]	5/5	0.69	0.45	7.32	54,56,57,59	5
2	PO4	C	302	5/5	0.69	0.23	4.69	125,125,125,126	0
2	PO4	C	305	5/5	0.92	0.40	2.77	90,91,92,93	0
2	PO4	B	311[B]	5/5	0.90	0.23	1.39	27,30,35,37	5
2	PO4	C	304	5/5	0.81	0.24	1.02	91,92,94,95	0
2	PO4	B	311[A]	5/5	0.90	0.23	0.30	57,60,61,62	5
2	PO4	C	309	5/5	0.89	0.16	-0.50	90,91,92,92	0
2	PO4	C	303	5/5	0.94	0.14	-	66,67,67,69	0
2	PO4	A	307	5/5	0.95	0.20	-	76,76,78,80	0
2	PO4	A	306	5/5	0.84	0.18	-	121,122,122,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.