



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:52 AM GMT

PDB ID : 3CGY  
Title : Crystal Structure of Salmonella Sensor Kinase PhoQ catalytic domain in complex with radicicol  
Authors : Guarnieri, M.T.; Zhang, L.; Shen, J.; Zhao, R.  
Deposited on : 2008-03-06  
Resolution : 2.60 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.

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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

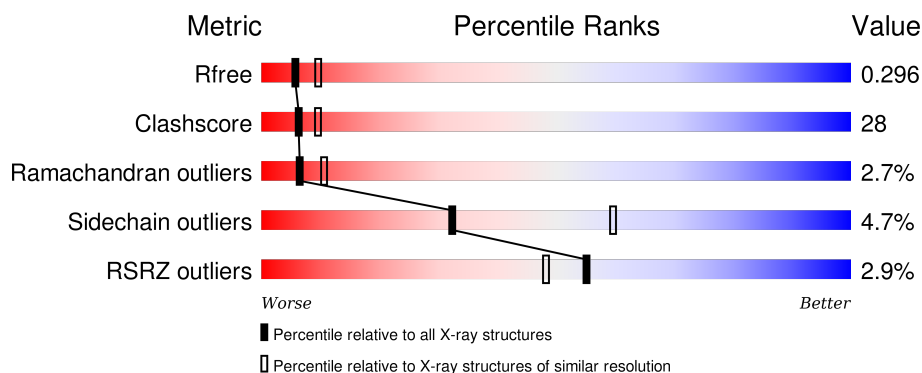
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	157	<div> <div>2%</div> <div>54%</div> <div>27%</div> <div>• •</div> <div>15%</div> </div>
1	B	157	<div> <div>%</div> <div>50%</div> <div>27%</div> <div>•</div> <div>22%</div> </div>
1	C	157	<div> <div>4%</div> <div>40%</div> <div>34%</div> <div>• •</div> <div>22%</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	RDC	B	700	-	-	-	X
2	RDC	C	700	-	-	X	-

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2993 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.

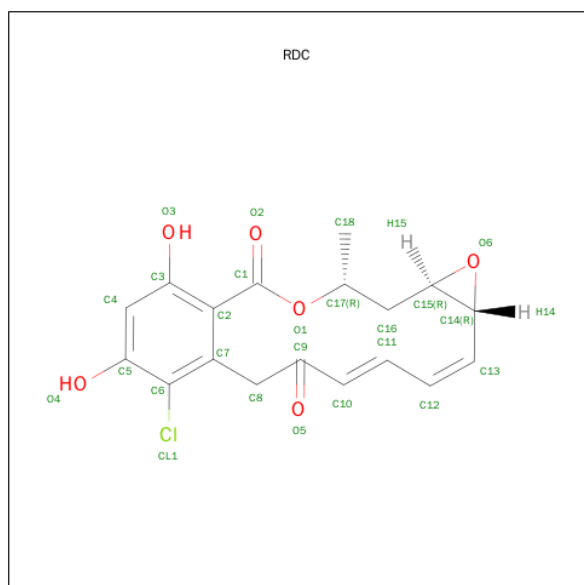
- Molecule 1 is a protein called Virulence sensor histidine kinase phoQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1026	646	176	199	5			
1	B	123	Total	C	N	O	S	0	0	0
			951	598	163	185	5			
1	C	122	Total	C	N	O	S	0	0	0
			941	592	160	184	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	SER	-	EXPRESSION TAG	UNP P14147
B	331	SER	-	EXPRESSION TAG	UNP P14147
C	331	SER	-	EXPRESSION TAG	UNP P14147

- Molecule 2 is RADICICOL (three-letter code: RDC) (formula: C<sub>18</sub>H<sub>17</sub>ClO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			25	18	1	6		
2	B	1	Total	C	Cl	O	0	0
			25	18	1	6		
2	C	1	Total	C	Cl	O	0	0
			25	18	1	6		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.92Å 63.76Å 87.77Å 90.00° 121.41° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 49.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.60) 96.8 (49.01-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.246 , 0.299 0.250 , 0.296	Depositor DCC
$R_{free}$ test set	1312 reflections (11.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.3	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 12655 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% 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 [i](#)

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

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

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	0.40	0/1042	0.71	2/1411 (0.1%)
1	B	0.41	0/967	0.64	0/1309
1	C	0.45	0/956	0.69	0/1294
All	All	0.42	0/2965	0.68	2/4014 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	GLY	N-CA-C	5.19	126.07	113.10
1	A	332	VAL	CB-CA-C	-5.16	101.60	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1026	0	1015	51	0
1	B	951	0	924	42	0
1	C	941	0	917	66	0
2	A	25	0	14	5	0
2	B	25	0	14	8	0
2	C	25	0	14	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2993	0	2898	164	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 28.

All (164) 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:386:ASN:HD21	1:C:447:LEU:HA	1.13	1.14
1:C:408:ASP:O	1:C:480:GLN:HB2	1.50	1.11
1:C:447:LEU:HD11	2:C:700:RDC:H161	1.06	1.06
1:A:338:LEU:HD22	1:A:374:VAL:HG22	1.40	1.00
1:C:390:ASN:HD22	1:C:447:LEU:CD2	1.77	0.97
1:C:447:LEU:HD21	2:C:700:RDC:H17	1.51	0.93
1:C:390:ASN:HD22	1:C:447:LEU:HD23	1.32	0.92
1:C:447:LEU:CD1	2:C:700:RDC:H161	1.99	0.88
1:A:374:VAL:H	1:A:480:GLN:HE22	1.21	0.84
1:C:386:ASN:ND2	1:C:447:LEU:HA	1.92	0.84
1:B:447:LEU:HD12	2:B:700:RDC:H161	1.60	0.84
1:B:450:ALA:O	1:B:454:THR:HG22	1.77	0.82
1:C:447:LEU:HD11	2:C:700:RDC:C16	2.01	0.82
1:C:345:LEU:HB2	1:C:365:MET:HE1	1.61	0.82
1:A:421:ILE:HD11	1:A:464:SER:N	1.96	0.81
1:A:421:ILE:O	1:A:421:ILE:HG13	1.82	0.80
1:C:406:THR:O	1:C:408:ASP:N	2.14	0.79
1:C:342:ALA:HB3	1:C:343:PRO:HD3	1.64	0.79
1:A:338:LEU:CD2	1:A:374:VAL:HG22	2.12	0.79
1:B:386:ASN:HD22	1:B:450:ALA:HB2	1.48	0.79
1:A:421:ILE:CD1	1:A:463:ALA:HB1	2.15	0.77
1:C:341:VAL:HG21	1:C:371:ILE:HG22	1.67	0.77
1:C:390:ASN:ND2	1:C:447:LEU:CD2	2.48	0.76
1:C:447:LEU:CD2	2:C:700:RDC:H17	2.16	0.75
1:A:374:VAL:H	1:A:480:GLN:NE2	1.82	0.75
2:C:700:RDC:O2	2:C:700:RDC:H81	1.87	0.74
1:A:342:ALA:HB3	1:A:343:PRO:HD3	1.70	0.73
1:C:341:VAL:CG2	1:C:371:ILE:HG22	2.18	0.73
1:C:386:ASN:HD21	1:C:447:LEU:CA	1.99	0.73
2:B:700:RDC:H81	2:B:700:RDC:O2	1.92	0.70
1:C:338:LEU:HD23	1:C:374:VAL:HG22	1.74	0.70
1:B:421:ILE:HG22	1:B:423:HIS:H	1.57	0.68
1:A:358:ARG:HB2	1:B:460:GLN:NE2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:LEU:HB2	1:C:365:MET:CE	2.25	0.67
2:A:700:RDC:O2	2:A:700:RDC:H81	1.93	0.67
1:C:364:SER:HB3	1:C:400:GLU:OE1	1.95	0.67
2:C:700:RDC:H11	2:C:700:RDC:O2	1.95	0.67
1:C:408:ASP:O	1:C:480:GLN:CB	2.36	0.66
1:C:398:PHE:N	1:C:417:ASP:OD2	2.26	0.65
1:A:421:ILE:HD12	1:A:463:ALA:HB1	1.79	0.65
1:B:415:GLU:OE1	1:B:466:SER:HB2	1.97	0.64
1:C:409:HIS:HD2	1:C:478:GLY:HA2	1.62	0.64
1:C:480:GLN:O	1:C:481:HIS:HB2	1.98	0.64
1:A:358:ARG:HB2	1:B:460:GLN:HE21	1.63	0.64
1:A:358:ARG:NH1	1:B:458:ALA:HA	2.13	0.63
1:B:396:LEU:HB3	1:B:417:ASP:OD2	1.98	0.63
1:A:400:GLU:OE1	1:A:400:GLU:HA	1.99	0.62
1:C:390:ASN:ND2	1:C:447:LEU:HD21	2.12	0.62
2:A:700:RDC:O2	2:A:700:RDC:H11	1.99	0.62
1:A:421:ILE:HG23	1:A:471:ALA:HB2	1.81	0.62
1:C:416:ASP:OD1	1:C:470:GLY:HA3	1.99	0.62
1:A:384:MET:CE	1:A:412:ILE:HG21	2.29	0.61
1:C:390:ASN:ND2	1:C:447:LEU:HD23	2.09	0.61
1:A:332:VAL:HG12	1:A:332:VAL:O	2.00	0.61
1:C:406:THR:O	1:C:407:ASP:C	2.39	0.61
1:B:421:ILE:HG23	1:B:422:PRO:HD2	1.83	0.60
1:C:447:LEU:HD21	2:C:700:RDC:C17	2.29	0.60
2:B:700:RDC:H11	2:B:700:RDC:O2	2.01	0.60
1:B:338:LEU:HD22	1:B:372:SER:CB	2.30	0.60
1:B:481:HIS:N	1:B:481:HIS:CD2	2.70	0.60
1:C:341:VAL:HA	1:C:344:LEU:HD12	1.84	0.58
1:A:333:LEU:CD2	1:A:483:THR:HB	2.34	0.58
1:B:419:PRO:HG2	2:B:700:RDC:CL1	2.42	0.57
1:A:421:ILE:HD13	1:A:463:ALA:HB1	1.86	0.57
1:C:388:LEU:O	1:C:391:ALA:N	2.38	0.56
1:B:338:LEU:HD22	1:B:372:SER:HB2	1.85	0.56
1:A:386:ASN:HD22	1:A:450:ALA:H	1.51	0.56
1:A:364:SER:OG	1:A:400:GLU:OE1	2.20	0.56
1:B:386:ASN:HD22	1:B:450:ALA:CB	2.18	0.56
1:C:367:ILE:HG22	1:C:402:SER:HA	1.88	0.56
1:A:386:ASN:ND2	1:A:450:ALA:H	2.04	0.55
1:C:345:LEU:HD21	1:C:384:MET:HG3	1.88	0.55
1:B:365:MET:SD	1:B:367:ILE:HD12	2.46	0.55
1:B:342:ALA:HB3	1:B:343:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLU:HB2	1:C:379:ASP:OD2	2.07	0.55
1:A:358:ARG:HH11	1:B:458:ALA:HA	1.72	0.55
1:C:363:ILE:HD11	1:C:392:CYS:SG	2.47	0.54
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.73	0.54
1:C:386:ASN:HD22	1:C:450:ALA:HB2	1.72	0.54
1:A:388:LEU:HD21	1:A:401:ILE:CD1	2.38	0.53
1:B:454:THR:HG21	1:B:461:ILE:HG13	1.90	0.53
2:A:700:RDC:H11	2:A:700:RDC:C1	2.37	0.53
1:A:356:TYR:HA	1:B:460:GLN:HE22	1.74	0.53
1:C:446:GLY:O	1:C:447:LEU:C	2.48	0.52
1:B:373:PHE:CE2	1:B:380:PHE:HB2	2.44	0.52
1:C:341:VAL:O	1:C:344:LEU:HB2	2.10	0.52
1:C:409:HIS:CD2	1:C:478:GLY:HA2	2.42	0.52
1:A:384:MET:HE2	1:A:412:ILE:HG21	1.90	0.52
1:B:379:ASP:O	1:B:383:VAL:HG23	2.10	0.51
1:C:451:ARG:NH2	2:C:700:RDC:O6	2.41	0.51
2:A:700:RDC:O2	2:A:700:RDC:H182	2.10	0.51
1:B:345:LEU:O	1:B:349:ILE:HG13	2.11	0.51
1:B:365:MET:HB2	1:B:401:ILE:HB	1.92	0.51
1:A:393:LYS:HD3	1:B:464:SER:HB3	1.92	0.51
2:B:700:RDC:C1	2:B:700:RDC:H11	2.41	0.51
1:C:406:THR:O	1:C:409:HIS:N	2.42	0.51
1:B:342:ALA:HA	1:B:365:MET:HE3	1.93	0.50
1:C:421:ILE:HG23	1:C:422:PRO:HD2	1.93	0.50
1:A:421:ILE:HD11	1:A:464:SER:H	1.72	0.50
1:C:448:ALA:O	1:C:452:GLU:N	2.45	0.50
1:C:408:ASP:C	1:C:480:GLN:HB2	2.28	0.50
1:B:383:VAL:O	1:B:386:ASN:HB3	2.12	0.50
1:C:446:GLY:O	1:C:447:LEU:O	2.31	0.49
1:A:341:VAL:HG13	1:A:380:PHE:CZ	2.49	0.48
1:B:338:LEU:HD22	1:B:372:SER:HB3	1.96	0.47
2:C:700:RDC:H182	2:C:700:RDC:O2	2.15	0.47
1:B:422:PRO:O	1:B:423:HIS:HB2	2.14	0.47
1:A:388:LEU:CD2	1:A:401:ILE:HD11	2.44	0.47
1:C:377:GLN:HG3	1:C:378:ASN:N	2.30	0.47
1:A:421:ILE:HG22	2:A:700:RDC:C10	2.45	0.47
1:A:333:LEU:HD21	1:A:483:THR:HB	1.96	0.47
1:A:333:LEU:HD23	1:A:484:GLN:O	2.15	0.47
1:C:361:VAL:HG12	1:C:395:CYS:SG	2.55	0.47
1:A:388:LEU:HD21	1:A:401:ILE:HD11	1.98	0.46
1:B:480:GLN:C	1:B:481:HIS:CD2	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HD22	1:A:483:THR:HB	1.97	0.45
1:C:402:SER:OG	1:C:413:PHE:HB2	2.16	0.45
1:B:376:GLU:HA	1:B:376:GLU:OE1	2.17	0.45
1:A:386:ASN:HD22	1:A:450:ALA:N	2.15	0.45
1:B:368:SER:OG	1:B:370:GLU:HG2	2.16	0.45
1:C:398:PHE:HB2	1:C:417:ASP:OD2	2.16	0.45
1:C:447:LEU:HD23	1:C:447:LEU:H	1.82	0.45
2:B:700:RDC:H182	2:B:700:RDC:O2	2.17	0.45
1:B:342:ALA:HA	1:B:365:MET:CE	2.47	0.45
1:A:344:LEU:HD11	1:A:377:GLN:HG3	1.99	0.44
2:C:700:RDC:H11	2:C:700:RDC:C1	2.46	0.44
1:C:369:PRO:C	1:C:371:ILE:N	2.69	0.44
1:A:450:ALA:O	1:A:454:THR:HG23	2.18	0.44
1:A:413:PHE:CE2	1:A:474:GLU:HG3	2.52	0.44
1:B:466:SER:HB3	1:B:472:ARG:HB2	1.99	0.44
1:C:342:ALA:HB3	1:C:343:PRO:CD	2.41	0.44
1:A:382:GLU:OE1	1:A:453:ILE:HD11	2.18	0.44
1:A:421:ILE:HD11	1:A:464:SER:CA	2.48	0.43
1:B:422:PRO:HD3	2:B:700:RDC:H10	1.99	0.43
1:A:403:ALA:O	1:A:404:ARG:HD2	2.17	0.43
1:C:454:THR:HG23	1:C:455:GLU:N	2.33	0.43
1:C:410:LEU:HB3	1:C:477:PHE:HB2	2.00	0.43
1:C:396:LEU:HA	1:C:396:LEU:HD12	1.79	0.43
1:C:447:LEU:CG	2:C:700:RDC:H17	2.48	0.43
1:B:339:HIS:CD2	1:B:377:GLN:HB2	2.53	0.43
1:B:349:ILE:HG23	1:B:363:ILE:HB	2.00	0.43
1:A:394:TYR:O	1:A:418:GLY:HA3	2.19	0.43
1:C:415:GLU:OE1	1:C:466:SER:HB2	2.19	0.43
1:B:421:ILE:HG22	1:B:423:HIS:N	2.30	0.42
1:A:352:LEU:HD12	1:A:356:TYR:HE1	1.84	0.42
1:B:366:ASP:C	1:B:367:ILE:HG13	2.39	0.42
1:C:451:ARG:NH1	1:C:451:ARG:HG2	2.33	0.42
1:A:384:MET:HE1	1:A:412:ILE:HG21	2.00	0.42
1:C:367:ILE:O	1:C:367:ILE:HG13	2.20	0.42
1:A:448:ALA:O	1:A:452:GLU:HG2	2.19	0.42
1:A:370:GLU:HG3	1:A:370:GLU:H	1.45	0.42
1:A:374:VAL:N	1:A:480:GLN:HE22	2.03	0.42
1:A:421:ILE:HD11	1:A:464:SER:O	2.20	0.42
1:C:390:ASN:OD1	1:C:394:TYR:CE1	2.73	0.42
1:C:480:GLN:O	1:C:481:HIS:CB	2.66	0.41
1:A:418:GLY:O	1:A:419:PRO:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLU:OE1	1:A:455:GLU:HA	2.20	0.41
1:B:376:GLU:HB2	1:B:379:ASP:OD2	2.20	0.41
1:C:369:PRO:C	1:C:371:ILE:H	2.24	0.41
1:A:358:ARG:NH2	1:B:455:GLU:HG3	2.35	0.41
1:B:447:LEU:HG	2:B:700:RDC:H17	2.03	0.41
1:C:451:ARG:C	1:C:454:THR:HG22	2.42	0.40
1:C:349:ILE:HD12	1:C:365:MET:HE3	2.04	0.40
1:C:418:GLY:O	1:C:419:PRO:O	2.39	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	129/157 (82%)	115 (89%)	12 (9%)	2 (2%)	12	24
1	B	119/157 (76%)	106 (89%)	11 (9%)	2 (2%)	11	22
1	C	118/157 (75%)	103 (87%)	9 (8%)	6 (5%)	2	3
All	All	366/471 (78%)	324 (88%)	32 (9%)	10 (3%)	6	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	ASP
1	C	419	PRO
1	B	479	ARG
1	C	447	LEU
1	C	448	ALA
1	B	397	GLU
1	A	377	GLN
1	C	421	ILE
1	C	418	GLY

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Mol	Chain	Res	Type
1	A	332	VAL

### 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	114/134 (85%)	106 (93%)	8 (7%)	19	37
1	B	104/134 (78%)	99 (95%)	5 (5%)	31	58
1	C	103/134 (77%)	101 (98%)	2 (2%)	65	86
All	All	321/402 (80%)	306 (95%)	15 (5%)	32	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	LEU
1	A	352	LEU
1	A	353	ASN
1	A	370	GLU
1	A	390	ASN
1	A	405	GLN
1	A	419	PRO
1	A	451	ARG
1	B	362	ASN
1	B	366	ASP
1	B	390	ASN
1	B	402	SER
1	B	481	HIS
1	C	372	SER
1	C	447	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	ASN

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Mol	Chain	Res	Type
1	A	460	GLN
1	A	480	GLN
1	B	362	ASN
1	B	386	ASN
1	B	423	HIS
1	B	460	GLN
1	B	481	HIS
1	C	386	ASN
1	C	390	ASN
1	C	409	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	RDC	A	700	-	27,27,27	2.16	9 (33%)	33,39,39	2.79	14 (42%)
2	RDC	B	700	-	27,27,27	2.26	10 (37%)	33,39,39	2.74	14 (42%)
2	RDC	C	700	-	27,27,27	2.02	8 (29%)	33,39,39	2.72	13 (39%)

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	RDC	A	700	-	-	0/23/28/28	0/1/3/3
2	RDC	B	700	-	-	0/23/28/28	0/1/3/3
2	RDC	C	700	-	-	0/23/28/28	0/1/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	RDC	O6-C14	-2.17	1.39	1.44
2	C	700	RDC	O6-C14	-2.02	1.39	1.44
2	C	700	RDC	C14-C13	2.05	1.58	1.50
2	B	700	RDC	O1-C17	2.11	1.50	1.47
2	A	700	RDC	C8-C7	2.13	1.56	1.52
2	C	700	RDC	O5-C9	2.15	1.26	1.23
2	B	700	RDC	C5-C6	2.17	1.43	1.40
2	B	700	RDC	C14-C13	2.17	1.58	1.50
2	C	700	RDC	C8-C7	2.30	1.56	1.52
2	A	700	RDC	O5-C9	2.32	1.26	1.23
2	B	700	RDC	C11-C10	2.34	1.40	1.34
2	A	700	RDC	C2-C3	2.35	1.45	1.41
2	B	700	RDC	O5-C9	2.37	1.26	1.23
2	A	700	RDC	O1-C1	2.46	1.39	1.34
2	A	700	RDC	C11-C10	2.51	1.41	1.34
2	B	700	RDC	C8-C7	2.53	1.57	1.52
2	C	700	RDC	C16-C17	2.79	1.58	1.51
2	A	700	RDC	C16-C17	3.00	1.59	1.51
2	B	700	RDC	C16-C17	3.03	1.59	1.51
2	C	700	RDC	C2-C3	3.08	1.46	1.41
2	B	700	RDC	C2-C3	3.20	1.47	1.41
2	A	700	RDC	C2-C7	4.96	1.49	1.40
2	C	700	RDC	C15-C14	4.98	1.58	1.47
2	C	700	RDC	C2-C7	5.03	1.49	1.40
2	A	700	RDC	C15-C14	5.23	1.59	1.47
2	B	700	RDC	C15-C14	5.25	1.59	1.47
2	B	700	RDC	C2-C7	5.57	1.50	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	RDC	C12-C11-C10	-4.07	115.62	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	RDC	C12-C11-C10	-3.97	115.84	124.66
2	A	700	RDC	C12-C11-C10	-3.85	116.11	124.66
2	A	700	RDC	O6-C15-C14	-3.39	54.03	59.47
2	A	700	RDC	O1-C17-C16	-3.26	98.47	106.74
2	B	700	RDC	O1-C17-C16	-3.21	98.61	106.74
2	C	700	RDC	O6-C15-C14	-3.17	54.39	59.47
2	B	700	RDC	O6-C15-C14	-3.09	54.51	59.47
2	C	700	RDC	O1-C17-C16	-2.81	99.62	106.74
2	A	700	RDC	C5-C6-C7	-2.69	119.52	122.13
2	C	700	RDC	O1-C1-O2	-2.43	119.47	123.53
2	B	700	RDC	O1-C1-O2	-2.15	119.93	123.53
2	B	700	RDC	C5-C6-C7	-2.15	120.05	122.13
2	C	700	RDC	C5-C6-C7	-2.12	120.07	122.13
2	A	700	RDC	O1-C1-O2	-2.09	120.04	123.53
2	B	700	RDC	C17-C16-C15	2.06	118.85	114.11
2	A	700	RDC	C5-C4-C3	2.17	122.24	120.05
2	A	700	RDC	O1-C17-C18	2.82	114.25	107.88
2	A	700	RDC	C4-C5-C6	2.87	120.79	118.53
2	B	700	RDC	O1-C1-C2	3.37	121.23	113.03
2	B	700	RDC	C4-C5-C6	3.42	121.22	118.53
2	C	700	RDC	O1-C17-C18	3.45	115.68	107.88
2	C	700	RDC	O1-C1-C2	3.55	121.65	113.03
2	B	700	RDC	O1-C17-C18	3.56	115.92	107.88
2	A	700	RDC	O1-C1-C2	3.61	121.81	113.03
2	C	700	RDC	C17-O1-C1	3.78	125.45	117.80
2	C	700	RDC	C4-C5-C6	3.99	121.66	118.53
2	B	700	RDC	C17-O1-C1	4.18	126.27	117.80
2	A	700	RDC	C17-O1-C1	4.25	126.42	117.80
2	C	700	RDC	C14-C13-C12	4.46	136.00	125.66
2	B	700	RDC	C14-C13-C12	4.55	136.21	125.66
2	C	700	RDC	O6-C15-C16	4.67	127.20	116.36
2	B	700	RDC	O6-C15-C16	4.69	127.25	116.36
2	A	700	RDC	O6-C15-C16	5.02	128.02	116.36
2	A	700	RDC	C14-C13-C12	5.07	137.42	125.66
2	A	700	RDC	O6-C14-C13	5.83	130.16	115.28
2	B	700	RDC	O6-C14-C13	5.89	130.34	115.28
2	C	700	RDC	O6-C14-C13	5.95	130.48	115.28
2	C	700	RDC	C15-O6-C14	7.26	67.34	61.04
2	B	700	RDC	C15-O6-C14	7.39	67.45	61.04
2	A	700	RDC	C15-O6-C14	7.56	67.60	61.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	RDC	5	0
2	B	700	RDC	8	0
2	C	700	RDC	12	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	133/157 (84%)	0.06	3 (2%) 64 57	35, 58, 91, 102	0
1	B	123/157 (78%)	0.12	1 (0%) 87 85	34, 63, 95, 127	0
1	C	122/157 (77%)	0.23	7 (5%) 27 20	38, 65, 97, 116	0
All	All	378/471 (80%)	0.13	11 (2%) 55 48	34, 62, 96, 127	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	GLU	5.2
1	A	421	ILE	5.1
1	A	422	PRO	3.2
1	C	421	ILE	3.1
1	C	400	GLU	2.6
1	C	366	ASP	2.5
1	A	408	ASP	2.3
1	C	422	PRO	2.2
1	C	397	GLU	2.1
1	C	337	GLU	2.1
1	C	446	GLY	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RDC	B	700	25/25	0.67	0.29	2.26	61,65,67,69	0
2	RDC	C	700	25/25	0.73	0.33	1.48	61,64,68,69	0
2	RDC	A	700	25/25	0.69	0.33	0.91	61,66,68,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.