



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:04 AM GMT

PDB ID : 3D91  
Title : Human renin in complex with remikiren  
Authors : Prade, L.; Bezencon, O.; Bur, D.; Weller, T.; Fischli, W.; Remen, L.  
Deposited on : 2008-05-26  
Resolution : 2.20 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

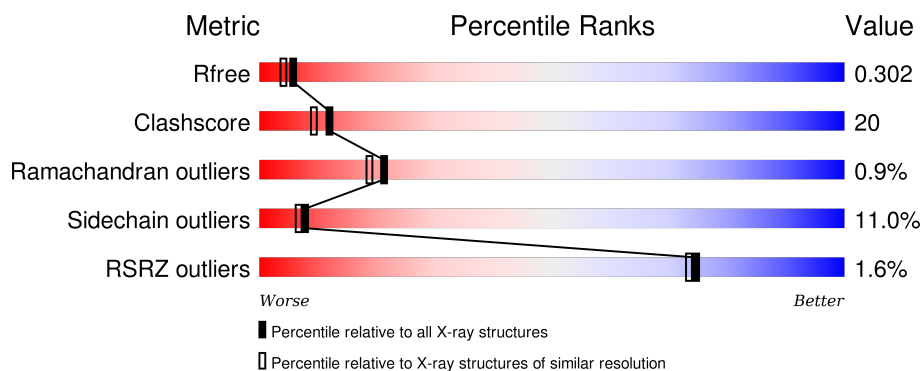
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	341	<div> <div> <div>61%</div> <div>31%</div> <div>5%</div> </div> </div>
1	B	341	<div> <div>3%</div> <div>61%</div> <div>34%</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
3	DMS	A	351	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5529 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.

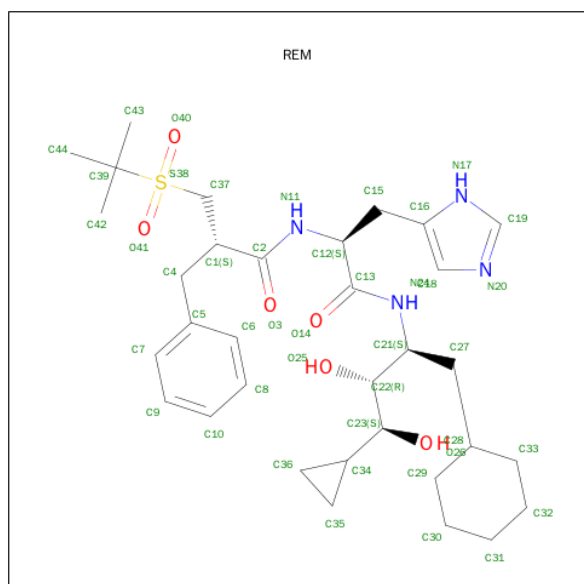
- Molecule 1 is a protein called Renin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2576	1645	418	499	14			
1	B	337	Total	C	N	O	S	0	0	0
			2599	1661	421	503	14			

There are 2 discrepancies between the modelled and reference sequences:

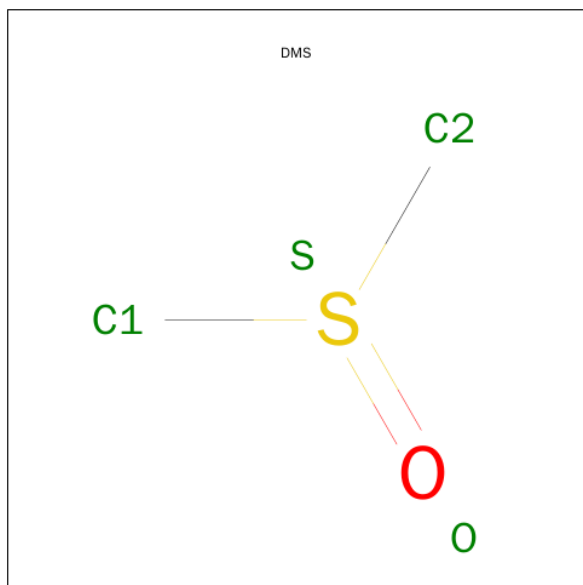
Chain	Residue	Modelled	Actual	Comment	Reference
A	341	HIS	-	EXPRESSION TAG	UNP P00797
B	341	HIS	-	EXPRESSION TAG	UNP P00797

- Molecule 2 is NALPHA-[(2S)-2-BENZYL-3-(TERT-BUTYLSULFONYL)PROPANOYL]-N-[(1S,2R,3S)-1-(CYCLOHEXYLMETHYL)-3-CYCLOPROPYL-2,3-DIHYDROXYPROPYL]-L-HISTIDINAMIDE (three-letter code: REM) (formula: C<sub>33</sub>H<sub>50</sub>N<sub>4</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			44	33	4	6	1		
2	B	1	Total	C	N	O	S	0	0
			44	33	4	6	1		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

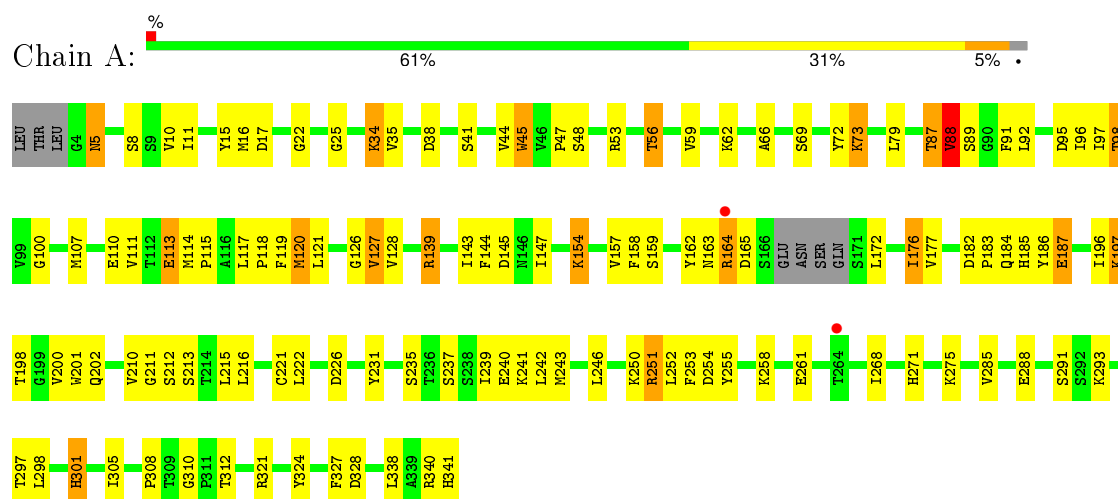
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	115	Total	O	0	0
			115	115		

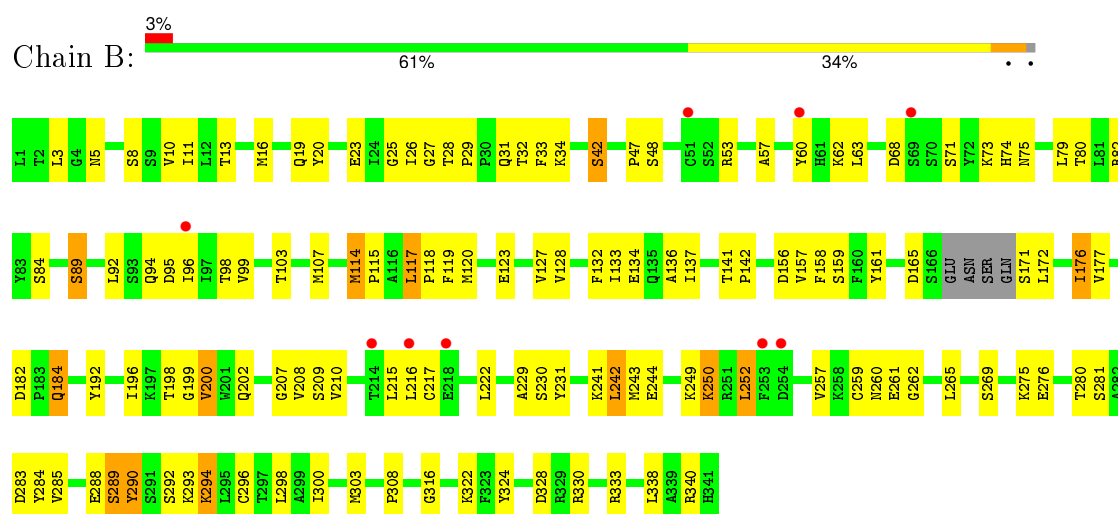
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Renin



#### • Molecule 1: Renin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.79 Å 93.55 Å 117.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 49.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	84.1 (20.00-2.20) 84.1 (49.73-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.301 0.216 , 0.302	Depositor DCC
$R_{free}$ test set	1605 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 87.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 32032 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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

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

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	0.91	5/2636 (0.2%)	0.93	5/3573 (0.1%)
1	B	0.71	1/2659 (0.0%)	0.78	1/3605 (0.0%)
All	All	0.81	6/5295 (0.1%)	0.86	6/7178 (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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	VAL	CB-CG1	-9.89	1.32	1.52
1	A	88	VAL	CA-CB	6.86	1.69	1.54
1	A	128	VAL	CB-CG2	-5.38	1.41	1.52
1	A	45	TRP	C-O	-5.21	1.13	1.23
1	A	72	TYR	CD2-CE2	5.13	1.47	1.39
1	B	296	CYS	CB-SG	5.12	1.91	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	VAL	CG1-CB-CG2	6.14	120.73	110.90
1	A	17	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	226	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	117	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	17	ASP	CB-CG-OD1	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	TYR	CB-CG-CD2	5.06	124.04	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	LYS	Peptide

## 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	2576	0	2505	114	0
1	B	2599	0	2537	98	0
2	A	44	0	50	2	0
2	B	44	0	50	3	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	143	0	0	20	0
4	B	115	0	0	18	0
All	All	5529	0	5154	208	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 20.

All (208) 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:B:32:THR:HB	4:B:462:HOH:O	1.58	1.02
1:A:164:ARG:HH11	1:A:164:ARG:HG3	0.87	1.00
1:A:164:ARG:HH11	1:A:164:ARG:CG	1.77	0.97
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.28	0.96
1:B:132:PHE:HB3	1:B:134:GLU:OE1	1.65	0.95
1:A:154:LYS:HG3	4:A:474:HOH:O	1.68	0.93
1:A:196:ILE:CD1	1:A:222:LEU:HD22	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HG3	1:A:164:ARG:NH1	1.68	0.92
1:A:251:ARG:HB2	1:A:254:ASP:OD1	1.70	0.91
1:B:94:GLN:HB2	1:B:107:MET:SD	2.12	0.89
1:A:25:GLY:HA3	4:A:418:HOH:O	1.71	0.89
1:A:117:LEU:HD11	1:B:60:TYR:CG	2.08	0.88
1:B:171:SER:HB2	4:B:409:HOH:O	1.74	0.86
1:A:117:LEU:HD11	1:B:60:TYR:CD1	2.13	0.83
1:A:221:CYS:HB2	4:A:358:HOH:O	1.79	0.82
1:A:139:ARG:CG	1:A:139:ARG:HH11	1.91	0.82
1:B:182:ASP:OD1	1:B:184:GLN:HG3	1.80	0.81
1:A:196:ILE:HD11	1:A:222:LEU:HD22	1.64	0.78
1:A:143:ILE:O	1:A:147:ILE:HG13	1.84	0.78
1:B:276:GLU:HB3	4:B:465:HOH:O	1.85	0.77
1:B:209:SER:HB2	1:B:269:SER:HB2	1.67	0.76
1:B:285:VAL:HG22	1:B:298:LEU:HD22	1.69	0.74
1:B:269:SER:HB3	4:B:465:HOH:O	1.89	0.71
1:A:89:SER:OG	1:A:113:GLU:CG	2.39	0.71
1:A:5:ASN:HA	1:A:154:LYS:HB2	1.73	0.70
1:B:34:LYS:NZ	1:B:123:GLU:O	2.26	0.69
1:A:45:TRP:CE2	1:A:127:VAL:HG13	2.28	0.68
1:A:89:SER:OG	1:A:113:GLU:HG3	1.93	0.68
1:A:87:THR:HG22	4:A:466:HOH:O	1.93	0.67
1:A:308:PRO:HD2	4:A:485:HOH:O	1.94	0.67
1:B:11:ILE:HD12	1:B:172:LEU:HD11	1.77	0.67
1:B:157:VAL:HG12	1:B:328:ASP:HA	1.78	0.66
1:A:305:ILE:O	1:A:310:GLY:HA3	1.96	0.65
1:B:5:ASN:ND2	4:B:460:HOH:O	2.19	0.65
1:B:19:GLN:HE21	2:B:350:REM:H8	1.61	0.64
1:B:290:TYR:CD2	1:B:290:TYR:N	2.65	0.64
1:A:241:LYS:NZ	1:A:241:LYS:CB	2.61	0.63
1:A:139:ARG:HG2	1:A:139:ARG:NH1	2.06	0.63
1:A:250:LYS:HG2	1:A:251:ARG:O	1.98	0.62
1:B:96:ILE:HG22	1:B:103:THR:HG23	1.81	0.62
1:A:251:ARG:NH1	1:A:254:ASP:OD2	2.33	0.62
1:B:288:GLU:O	1:B:289:SER:HB3	2.00	0.61
1:A:197:LYS:CD	4:A:490:HOH:O	2.49	0.61
1:B:132:PHE:CB	1:B:134:GLU:OE1	2.44	0.61
1:B:290:TYR:HD2	1:B:290:TYR:N	1.99	0.61
1:A:200:VAL:HG13	1:A:202:GLN:HB3	1.80	0.61
1:A:182:ASP:OD2	1:A:184:GLN:HG2	2.01	0.61
4:A:470:HOH:O	1:B:34:LYS:HE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:SER:OG	1:A:95:ASP:OD2	2.19	0.60
1:B:19:GLN:NE2	2:B:350:REM:H8	2.16	0.60
1:B:79:LEU:HD22	1:B:92:LEU:HG	1.83	0.60
1:A:45:TRP:CZ2	1:A:127:VAL:HG13	2.36	0.60
1:A:196:ILE:HD13	1:A:222:LEU:HD22	1.82	0.60
1:A:35:VAL:HG12	1:A:126:GLY:HA3	1.84	0.59
1:A:56:THR:O	1:A:59:VAL:HG12	2.02	0.59
1:A:197:LYS:HD2	4:A:490:HOH:O	2.03	0.59
1:B:243:MET:SD	1:B:298:LEU:HD12	2.42	0.59
1:A:301:HIS:HB2	4:A:360:HOH:O	2.03	0.58
1:B:48:SER:O	1:B:63:LEU:HD22	2.03	0.58
1:B:11:ILE:HD11	4:B:422:HOH:O	2.03	0.58
1:A:5:ASN:CA	1:A:154:LYS:HB2	2.34	0.57
1:A:241:LYS:HG3	4:A:452:HOH:O	2.04	0.57
1:B:94:GLN:HB2	1:B:107:MET:CE	2.35	0.57
1:A:241:LYS:NZ	1:A:241:LYS:HB3	2.19	0.56
1:B:330:ARG:NE	4:B:463:HOH:O	2.37	0.56
1:A:11:ILE:HD12	1:A:172:LEU:HD11	1.86	0.56
1:B:182:ASP:OD1	1:B:184:GLN:CG	2.52	0.56
1:A:45:TRP:NE1	1:A:127:VAL:HG13	2.20	0.56
1:B:192:TYR:HB3	1:B:333:ARG:HD2	1.87	0.56
1:B:107:MET:HB2	4:B:464:HOH:O	2.04	0.56
1:A:253:PHE:N	4:A:491:HOH:O	2.38	0.56
1:B:260:ASN:ND2	1:B:292:SER:HA	2.21	0.55
1:B:115:PRO:HD3	4:B:423:HOH:O	2.07	0.55
1:B:118:PRO:HD2	1:B:119:PHE:CD2	2.42	0.55
1:B:80:THR:HB	4:B:447:HOH:O	2.06	0.55
1:A:35:VAL:HG12	1:A:126:GLY:CA	2.37	0.55
1:B:31:GLN:O	1:B:33:PHE:CE2	2.60	0.55
1:B:171:SER:N	4:B:449:HOH:O	2.40	0.55
1:A:288:GLU:HG2	4:A:435:HOH:O	2.08	0.54
1:B:200:VAL:HG22	1:B:202:GLN:HB2	1.88	0.54
1:B:27:GLY:HA2	1:B:95:ASP:OD1	2.08	0.53
1:A:10:VAL:HB	1:A:176:ILE:HG23	1.90	0.53
1:A:241:LYS:HB3	1:A:241:LYS:HZ3	1.72	0.53
1:A:97:ILE:HG22	1:A:98:THR:N	2.23	0.53
1:A:164:ARG:NH1	1:A:341:HIS:CE1	2.77	0.52
1:A:35:VAL:HG12	1:A:126:GLY:C	2.29	0.52
1:B:23:GLU:HB2	4:B:462:HOH:O	2.08	0.52
1:B:118:PRO:HD2	1:B:119:PHE:CE2	2.45	0.52
1:B:79:LEU:HD12	1:B:137:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:OG	1:A:113:GLU:HG2	2.09	0.52
1:B:259:CYS:HB3	1:B:289:SER:O	2.10	0.52
1:A:163:ASN:OD1	1:A:341:HIS:HD2	1.93	0.51
1:B:47:PRO:HB2	1:B:63:LEU:HD23	1.92	0.51
1:A:144:PHE:CZ	1:A:158:PHE:HD2	2.28	0.51
1:A:246:LEU:HD11	1:A:268:ILE:HD11	1.92	0.51
1:B:25:GLY:HA3	4:B:431:HOH:O	2.09	0.51
1:A:95:ASP:OD1	1:A:96:ILE:N	2.37	0.51
1:A:288:GLU:HA	4:A:435:HOH:O	2.11	0.51
1:A:121:LEU:HD21	1:B:60:TYR:HE2	1.75	0.51
1:A:197:LYS:HZ3	1:A:202:GLN:HE21	1.59	0.51
1:A:187:GLU:HB3	1:A:340:ARG:NH1	2.26	0.50
1:A:47:PRO:HG2	1:A:62:LYS:O	2.12	0.50
1:B:13:THR:O	1:B:20:TYR:HA	2.11	0.50
1:A:35:VAL:HA	1:A:126:GLY:O	2.11	0.50
1:B:243:MET:O	1:B:244:GLU:C	2.49	0.50
1:A:182:ASP:CG	1:A:184:GLN:HG2	2.32	0.50
1:B:265:LEU:HB2	1:B:281:SER:HB3	1.93	0.50
1:B:96:ILE:CG2	1:B:103:THR:CG2	2.90	0.50
1:B:10:VAL:HB	1:B:176:ILE:HG23	1.93	0.50
1:B:249:LYS:HA	4:B:427:HOH:O	2.12	0.49
1:A:79:LEU:N	1:A:79:LEU:HD23	2.26	0.49
1:A:196:ILE:CD1	1:A:222:LEU:CD2	2.83	0.49
1:A:241:LYS:HZ2	1:A:241:LYS:HB2	1.77	0.49
2:A:350:REM:H37A	2:A:350:REM:C6	2.43	0.48
1:B:182:ASP:CG	1:B:184:GLN:HG3	2.34	0.48
1:B:208:VAL:HB	1:B:216:LEU:HB2	1.94	0.48
1:A:120:MET:CE	4:A:460:HOH:O	2.62	0.48
1:A:8:SER:OG	1:A:100:GLY:HA3	2.14	0.48
1:A:117:LEU:HD21	1:B:60:TYR:CE2	2.48	0.48
1:A:118:PRO:HD2	1:A:119:PHE:CD2	2.48	0.48
1:A:89:SER:HG	1:A:113:GLU:CG	2.26	0.48
1:B:294:LYS:HA	1:B:294:LYS:HE3	1.97	0.47
1:A:164:ARG:HH12	1:A:341:HIS:CE1	2.32	0.47
1:A:196:ILE:HD13	1:A:222:LEU:CD2	2.44	0.47
1:B:275:LYS:NZ	1:B:276:GLU:O	2.47	0.47
1:A:243:MET:HG3	1:A:255:TYR:CD1	2.49	0.47
1:B:217:CYS:O	1:B:217:CYS:SG	2.73	0.46
1:B:196:ILE:HD13	1:B:222:LEU:CD2	2.44	0.46
1:B:96:ILE:HG22	1:B:103:THR:CG2	2.44	0.46
1:A:328:ASP:C	1:A:328:ASP:OD1	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:HZ3	1:A:200:VAL:HG11	1.81	0.46
1:A:158:PHE:HA	1:A:177:VAL:O	2.15	0.46
1:A:164:ARG:CG	1:A:164:ARG:NH1	2.50	0.46
2:A:350:REM:H34	4:A:450:HOH:O	2.15	0.46
1:B:210:VAL:CG2	1:B:242:LEU:HD12	2.46	0.46
1:A:139:ARG:CG	1:A:139:ARG:NH1	2.62	0.45
1:A:183:PRO:HA	1:A:186:TYR:CE1	2.51	0.45
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.44	0.45
1:A:241:LYS:HZ2	1:A:241:LYS:CB	2.28	0.45
1:B:280:THR:O	1:B:283:ASP:N	2.38	0.45
1:A:44:VAL:HG12	1:A:45:TRP:N	2.30	0.45
1:A:200:VAL:CG1	1:A:202:GLN:HB3	2.47	0.45
1:A:73:LYS:HE3	4:A:363:HOH:O	2.16	0.45
1:B:94:GLN:OE1	1:B:107:MET:CE	2.64	0.45
1:B:74:HIS:CE1	1:B:75:ASN:O	2.70	0.45
1:A:241:LYS:CG	4:A:452:HOH:O	2.62	0.44
1:B:229:ALA:O	1:B:316:GLY:HA3	2.18	0.44
1:B:132:PHE:HD1	4:B:461:HOH:O	1.99	0.44
1:A:38:ASP:OD2	1:A:41:SER:HB3	2.16	0.44
1:B:80:THR:OG1	1:B:89:SER:HB3	2.17	0.44
1:A:15:TYR:CE2	1:A:16:MET:HG3	2.52	0.44
1:B:207:GLY:HA2	1:B:217:CYS:O	2.17	0.44
1:A:197:LYS:NZ	1:A:202:GLN:HE21	2.15	0.44
1:A:22:GLY:O	1:A:34:LYS:HA	2.17	0.44
1:B:73:LYS:HE3	1:B:94:GLN:NE2	2.32	0.44
1:B:298:LEU:C	1:B:300:ILE:H	2.21	0.44
1:A:73:LYS:CE	4:A:363:HOH:O	2.66	0.44
1:A:285:VAL:HG22	1:A:298:LEU:CD2	2.48	0.43
1:B:114:MET:O	1:B:114:MET:HG2	2.17	0.43
1:A:297:THR:HG22	1:A:298:LEU:N	2.34	0.43
1:B:25:GLY:O	1:B:26:ILE:HG12	2.18	0.43
1:A:183:PRO:C	1:A:185:HIS:H	2.21	0.43
1:B:192:TYR:CD2	1:B:333:ARG:NH1	2.87	0.43
1:A:97:ILE:CG2	1:A:98:THR:N	2.82	0.43
1:B:262:GLY:O	1:B:265:LEU:HG	2.19	0.43
1:B:42:SER:HB2	1:B:136:ALA:HB2	2.00	0.42
1:A:210:VAL:HG21	1:A:242:LEU:HD12	2.00	0.42
1:B:128:VAL:HG12	1:B:128:VAL:O	2.17	0.42
1:B:57:ALA:HB3	1:B:114:MET:HG2	2.01	0.42
1:A:45:TRP:N	1:A:45:TRP:CD1	2.87	0.42
1:A:271:HIS:HD2	1:A:275:LYS:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PHE:HA	1:B:177:VAL:O	2.20	0.42
1:B:141:THR:HA	1:B:142:PRO:HD3	1.78	0.42
1:B:289:SER:C	1:B:290:TYR:CD2	2.93	0.42
1:B:28:THR:HA	1:B:29:PRO:HA	1.79	0.42
1:B:134:GLU:OE1	1:B:199:GLY:HA2	2.19	0.41
1:A:113:GLU:HG3	1:B:16:MET:HE3	2.02	0.41
1:A:120:MET:SD	1:B:60:TYR:HD2	2.43	0.41
1:B:127:VAL:HG21	2:B:350:REM:H30A	2.02	0.41
1:B:257:VAL:HG11	1:B:265:LEU:HD11	2.02	0.41
1:A:88:VAL:HG22	1:A:111:VAL:HG11	2.02	0.41
1:A:242:LEU:HA	1:A:242:LEU:HD12	1.88	0.41
1:A:48:SER:HB2	1:A:110:GLU:HB3	2.01	0.41
1:A:258:LYS:O	1:A:261:GLU:HG2	2.20	0.41
1:B:133:ILE:HD12	1:B:142:PRO:CD	2.51	0.41
1:A:162:TYR:O	1:A:321:ARG:HA	2.20	0.41
1:A:114:MET:HA	1:A:115:PRO:HD2	1.88	0.41
1:A:197:LYS:HZ3	1:A:200:VAL:CG1	2.34	0.41
1:A:11:ILE:HG23	1:A:172:LEU:CD1	2.51	0.41
1:B:114:MET:HA	1:B:115:PRO:HD2	1.82	0.41
1:B:281:SER:HA	1:B:284:TYR:CE2	2.56	0.41
1:A:235:SER:O	1:A:239:ILE:HG12	2.21	0.41
1:A:211:GLY:O	1:A:213:SER:N	2.54	0.41
1:B:308:PRO:HG2	4:B:396:HOH:O	2.21	0.41
1:A:117:LEU:HA	1:A:118:PRO:HA	1.82	0.41
1:B:288:GLU:O	1:B:289:SER:CB	2.68	0.41
1:A:92:LEU:HD13	1:A:107:MET:CE	2.50	0.41
1:A:66:ALA:HB3	4:A:448:HOH:O	2.19	0.41
1:B:32:THR:CB	4:B:462:HOH:O	2.40	0.40
1:A:159:SER:HB3	1:A:324:TYR:CE1	2.56	0.40
1:B:230:SER:N	4:B:467:HOH:O	2.54	0.40
1:A:201:TRP:CH2	1:A:327:PHE:HB3	2.55	0.40
1:A:79:LEU:HA	4:A:367:HOH:O	2.21	0.40
1:A:324:TYR:CD1	1:A:324:TYR:C	2.95	0.40
1:A:91:PHE:C	1:A:91:PHE:CD1	2.94	0.40
1:B:115:PRO:HB2	1:B:117:LEU:O	2.21	0.40
1:B:231:TYR:O	1:B:316:GLY:HA3	2.22	0.40
1:B:161:TYR:HB2	1:B:324:TYR:CE2	2.56	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	330/341 (97%)	310 (94%)	17 (5%)	3 (1%)	21	19
1	B	333/341 (98%)	303 (91%)	27 (8%)	3 (1%)	21	19
All	All	663/682 (97%)	613 (92%)	44 (7%)	6 (1%)	21	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	A	212	SER
1	B	289	SER
1	A	252	LEU
1	B	252	LEU
1	B	165	ASP

### 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	284/291 (98%)	254 (89%)	30 (11%)	8	7
1	B	287/291 (99%)	254 (88%)	33 (12%)	7	6
All	All	571/582 (98%)	508 (89%)	63 (11%)	8	7

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	34	LYS
1	A	53	ARG
1	A	56	THR
1	A	73	LYS
1	A	87	THR
1	A	88	VAL
1	A	98	THR
1	A	113	GLU
1	A	120	MET
1	A	127	VAL
1	A	139	ARG
1	A	145	ASP
1	A	154	LYS
1	A	157	VAL
1	A	164	ARG
1	A	176	ILE
1	A	187	GLU
1	A	197	LYS
1	A	198	THR
1	A	215	LEU
1	A	216	LEU
1	A	237	SER
1	A	240	GLU
1	A	251	ARG
1	A	291	SER
1	A	293	LYS
1	A	301	HIS
1	A	312	THR
1	A	338	LEU
1	B	3	LEU
1	B	8	SER
1	B	42	SER
1	B	53	ARG
1	B	62	LYS
1	B	68	ASP
1	B	71	SER
1	B	82	ARG
1	B	84	SER
1	B	89	SER
1	B	98	THR
1	B	99	VAL
1	B	114	MET

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Mol	Chain	Res	Type
1	B	120	MET
1	B	156	ASP
1	B	159	SER
1	B	176	ILE
1	B	184	GLN
1	B	198	THR
1	B	200	VAL
1	B	215	LEU
1	B	241	LYS
1	B	242	LEU
1	B	250	LYS
1	B	252	LEU
1	B	261	GLU
1	B	290	TYR
1	B	293	LYS
1	B	294	LYS
1	B	303	MET
1	B	322	LYS
1	B	338	LEU
1	B	340	ARG

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	194	ASN
1	A	202	GLN
1	A	271	HIS
1	A	331	ASN
1	A	341	HIS
1	B	150	GLN
1	B	184	GLN
1	B	194	ASN
1	B	331	ASN
1	B	341	HIS

### 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 ⓘ

4 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	REM	A	350	-	42,47,47	2.46	2 (4%)	52,67,67	2.25	11 (21%)
3	DMS	A	351	-	3,3,3	2.33	1 (33%)	3,3,3	0.92	0
2	REM	B	350	-	42,47,47	2.60	3 (7%)	52,67,67	2.02	10 (19%)
3	DMS	B	351	-	3,3,3	2.81	1 (33%)	3,3,3	0.37	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	REM	A	350	-	-	0/54/64/64	0/3/4/4
3	DMS	A	351	-	-	0/0/0/0	0/0/0/0
2	REM	B	350	-	-	0/54/64/64	0/3/4/4
3	DMS	B	351	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	REM	C39-S38	-14.27	1.67	1.82
2	A	350	REM	C39-S38	-13.61	1.68	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	REM	C37-S38	-7.57	1.66	1.78
2	A	350	REM	C37-S38	-6.55	1.67	1.78
2	B	350	REM	C18-N20	-2.17	1.28	1.35
3	A	351	DMS	O-S	3.88	1.76	1.50
3	B	351	DMS	O-S	4.82	1.83	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	REM	C27-C21-N24	-7.89	99.54	110.15
2	A	350	REM	C27-C21-N24	-7.11	100.59	110.15
2	A	350	REM	O40-S38-O41	-6.63	108.51	118.06
2	B	350	REM	C15-C12-N11	-5.30	99.70	110.80
2	B	350	REM	O40-S38-O41	-5.07	110.76	118.06
2	A	350	REM	O26-C23-C22	-3.81	100.30	109.45
2	A	350	REM	C32-C33-C28	-3.54	106.50	112.22
2	B	350	REM	C27-C28-C29	-3.18	104.12	111.67
2	A	350	REM	O41-S38-C37	-3.06	105.43	108.26
2	A	350	REM	O26-C23-C34	-3.04	105.43	110.80
2	B	350	REM	O25-C22-C23	-3.01	102.21	109.45
2	B	350	REM	O41-S38-C39	-2.09	105.65	107.72
2	A	350	REM	C13-C12-N11	-2.07	105.43	111.26
2	B	350	REM	C31-C32-C33	2.09	115.83	111.44
2	B	350	REM	C16-C18-N20	2.55	113.64	108.71
2	B	350	REM	O40-S38-C39	2.72	110.41	107.72
2	A	350	REM	C37-C1-C2	2.98	114.80	109.71
2	A	350	REM	C16-C18-N20	3.04	114.59	108.71
2	B	350	REM	O40-S38-C37	4.34	112.28	108.26
2	A	350	REM	O41-S38-C39	4.90	112.58	107.72
2	A	350	REM	O40-S38-C37	5.21	113.08	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	REM	2	0
2	B	350	REM	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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	334/341 (97%)	-0.01	2 (0%) 90 90	21, 57, 77, 86	0
1	B	337/341 (98%)	0.23	9 (2%) 58 57	43, 68, 90, 96	0
All	All	671/682 (98%)	0.11	11 (1%) 74 73	21, 61, 85, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	PHE	4.4
1	B	254	ASP	3.1
1	B	96	ILE	2.9
1	B	214	THR	2.7
1	B	60	TYR	2.6
1	B	69	SER	2.6
1	B	218	GLU	2.3
1	B	216	LEU	2.3
1	A	164	ARG	2.2
1	A	264	THR	2.2
1	B	51	CYS	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( $\text{\AA}^2$ )	Q<0.9
3	DMS	A	351	4/4	0.99	0.17	2.62	47,48,48,49	0
3	DMS	B	351	4/4	0.99	0.17	1.33	44,45,48,48	0
2	REM	A	350	44/44	0.95	0.14	0.92	26,44,57,60	0
2	REM	B	350	44/44	0.95	0.14	0.23	47,60,63,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.