



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:20 pm GMT

PDB ID : 4ZPT  
Title : Structure of MERS-Coronavirus Spike Receptor-binding Domain (England1 Strain) in Complex with Vaccine-Elicited Murine Neutralizing Antibody D12 (Crystal Form 1)  
Authors : Joyce, M.G.; Mascola, J.R.; Graham, B.S.; Kwong, P.D.  
Deposited on : 2015-05-08  
Resolution : 2.59 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

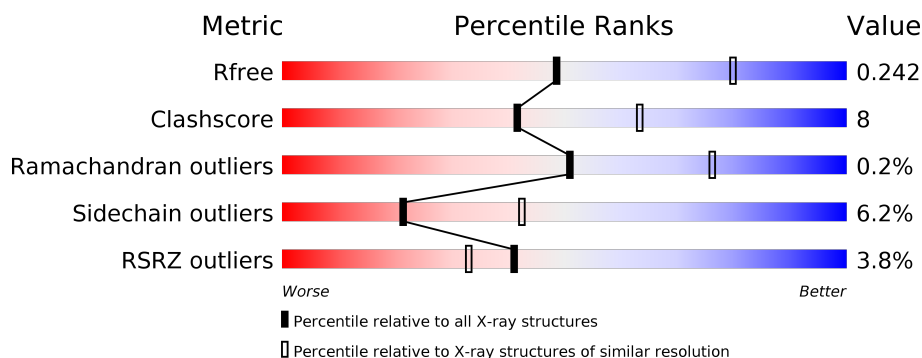
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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	216	<div> <div>85%</div> <div>13% ..</div> </div>
1	H	216	<div> <div>4%</div> <div>80%</div> <div>14% . ..</div> </div>
2	B	214	<div> <div>87%</div> <div>11% ..</div> </div>
2	L	214	<div> <div>84%</div> <div>13% ..</div> </div>
3	R	208	<div> <div>9%</div> <div>84%</div> <div>14% .</div> </div>
3	S	208	<div> <div>9%</div> <div>77%</div> <div>17% 6%</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
4	NAG	R	601	X	-	-	X
4	NAG	S	601	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10054 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 D12 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1602	1008	263	322	9			
1	H	214	Total	C	N	O	S	0	0	0
			1605	1010	263	323	9			

- Molecule 2 is a protein called D12 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1651	1023	282	340	6			
2	L	212	Total	C	N	O	S	0	0	0
			1651	1023	282	340	6			

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	208	Total	C	N	O	S	0	0	0
			1611	1029	256	315	11			
3	S	208	Total	C	N	O	S	0	0	0
			1611	1029	256	315	11			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	S	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

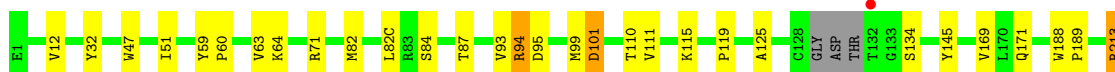
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		
5	B	55	Total	O	0	0
			55	55		
5	R	29	Total	O	0	0
			29	29		
5	H	57	Total	O	0	0
			57	57		
5	S	19	Total	O	0	0
			19	19		
5	L	60	Total	O	0	0
			60	60		

### 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 the various outlier classes 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.

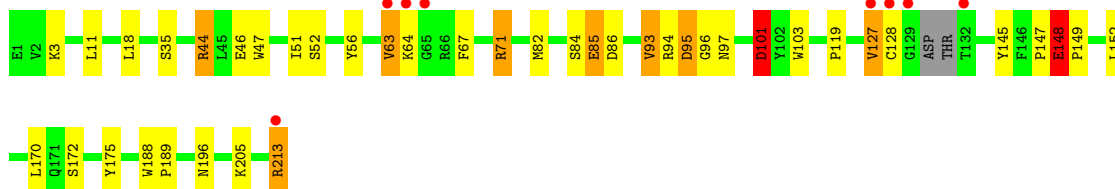
- Molecule 1: D12 Fab Heavy chain

Chain A: 




- Molecule 1: D12 Fab Heavy chain

Chain H: 



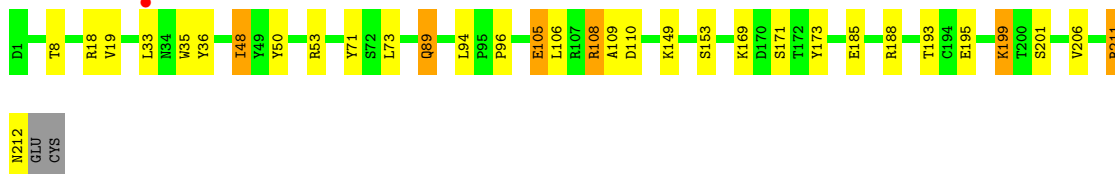
- Molecule 2: D12 Fab Light chain

Chain B: 




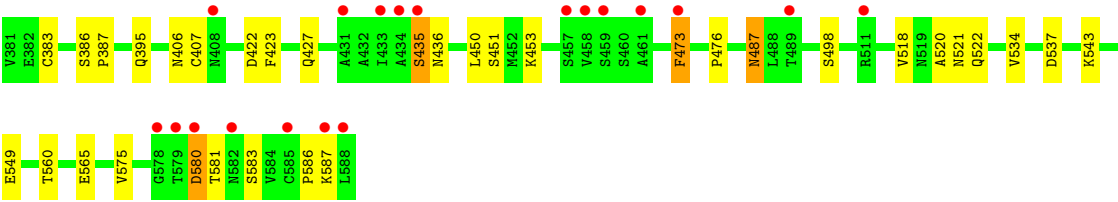
- Molecule 2: D12 Fab Light chain

Chain L: 

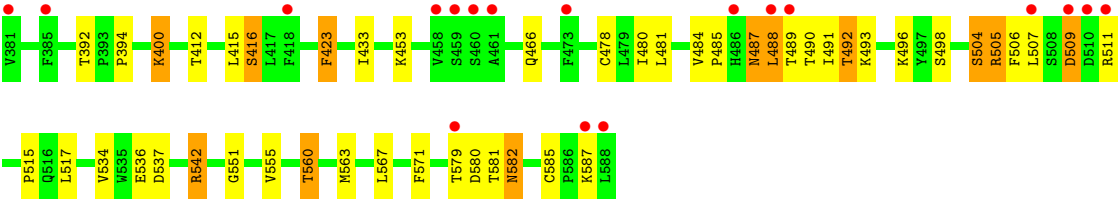
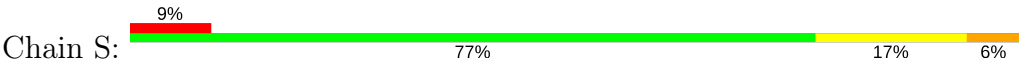


- Molecule 3: Spike glycoprotein

Chain R: 



● Molecule 3: Spike glycoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.45Å 128.79Å 170.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.05 – 2.59 37.05 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.05-2.59) 98.7 (37.05-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.204 , 0.244 0.209 , 0.242	Depositor DCC
$R_{free}$ test set	2529 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG

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	0.68	1/1640 (0.1%)	0.64	2/2236 (0.1%)
1	H	0.72	1/1643 (0.1%)	0.68	1/2239 (0.0%)
2	B	0.66	1/1685 (0.1%)	0.59	1/2290 (0.0%)
2	L	0.74	1/1685 (0.1%)	0.63	2/2290 (0.1%)
3	R	0.58	0/1651	0.54	0/2254
3	S	0.55	0/1651	0.59	0/2254
All	All	0.66	4/9955 (0.0%)	0.61	6/13563 (0.0%)

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	H	0	1
2	L	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ASP	CB-CG	-6.48	1.38	1.51
1	H	103	TRP	NE1-CE2	-5.82	1.29	1.37
2	L	50	TYR	CE1-CZ	-5.32	1.31	1.38
2	B	35	TRP	NE1-CE2	-5.28	1.30	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	148	GLU	C-N-CD	-10.23	98.09	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	CB-CG-OD1	-9.23	109.99	118.30
1	A	101	ASP	CB-CA-C	-6.83	96.75	110.40
2	L	48	ILE	CG1-CB-CG2	-5.42	99.48	111.40
2	L	18	ARG	NE-CZ-NH2	5.33	122.97	120.30
2	B	104	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	148	GLU	Peptide
2	L	211	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	1602	0	1564	15	0
1	H	1605	0	1563	31	0
2	B	1651	0	1584	12	0
2	L	1651	0	1584	29	0
3	R	1611	0	1572	22	0
3	S	1611	0	1570	51	0
4	R	14	0	13	4	0
4	S	14	0	13	2	0
5	A	75	0	0	0	0
5	B	55	0	0	0	0
5	H	57	0	0	1	0
5	L	60	0	0	0	0
5	R	29	0	0	1	0
5	S	19	0	0	0	0
All	All	10054	0	9463	154	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 8.

All (154) 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)
3:R:587:LYS:HE3	4:R:601:NAG:O6	1.10	1.22
3:R:587:LYS:CE	4:R:601:NAG:O6	1.89	1.21
3:S:412:THR:O	3:S:416:SER:OG	1.62	1.17
1:H:213:ARG:CG	1:H:213:ARG:HH21	1.58	1.12
3:R:383:CYS:SG	3:R:407:CYS:CB	2.38	1.11
1:H:213:ARG:HG2	1:H:213:ARG:HH21	1.09	1.09
3:R:383:CYS:SG	3:R:407:CYS:SG	1.06	1.06
3:S:493:LYS:HD2	3:S:563:MET:HE2	1.44	1.00
3:S:493:LYS:HD2	3:S:563:MET:CE	1.91	0.99
2:L:33:LEU:CD2	2:L:71:TYR:CB	2.42	0.97
1:A:125:ALA:O	1:A:213:ARG:NH2	1.97	0.96
2:L:33:LEU:HD22	2:L:71:TYR:CG	2.01	0.95
1:H:95:ASP:HB3	1:H:96:GLY:HA2	1.49	0.94
3:S:466:GLN:HG2	3:S:517:LEU:CD2	1.98	0.93
2:L:33:LEU:CD2	2:L:71:TYR:CG	2.52	0.93
3:S:466:GLN:HG2	3:S:517:LEU:HD22	1.52	0.92
2:L:108:ARG:HH11	2:L:108:ARG:HG3	1.34	0.92
1:H:213:ARG:NH2	1:H:213:ARG:HG2	1.70	0.89
1:H:95:ASP:CB	1:H:96:GLY:HA2	2.03	0.88
3:S:542:ARG:HG3	3:S:555:VAL:HG22	1.53	0.87
1:H:51:ILE:HD13	1:H:71:ARG:HG2	1.57	0.87
1:H:56:TYR:CD1	3:S:536:GLU:HG3	2.10	0.86
3:S:506:PHE:CD1	3:S:511:ARG:HG3	2.11	0.85
1:H:56:TYR:HD1	3:S:536:GLU:HG3	1.42	0.85
1:H:213:ARG:CG	1:H:213:ARG:NH2	2.30	0.84
3:S:506:PHE:HD1	3:S:511:ARG:HG3	1.39	0.84
2:L:211:ARG:O	2:L:212:ASN:HB2	1.78	0.83
3:S:582:ASN:H	3:S:582:ASN:HD22	1.27	0.82
2:L:33:LEU:HD23	2:L:71:TYR:CB	2.10	0.81
2:L:33:LEU:HD22	2:L:71:TYR:CD2	2.14	0.81
3:R:383:CYS:CB	3:R:407:CYS:HG	1.93	0.81
2:L:211:ARG:O	2:L:212:ASN:CB	2.30	0.79
3:S:392:THR:OG1	3:S:492:THR:OG1	1.98	0.79
1:H:95:ASP:HB3	1:H:96:GLY:CA	2.14	0.78
3:S:493:LYS:HB3	3:S:563:MET:CE	2.13	0.78
3:S:582:ASN:N	3:S:582:ASN:ND2	2.30	0.77
2:L:33:LEU:HD23	2:L:71:TYR:HB3	1.66	0.76
3:R:487:ASN:ND2	5:R:701:HOH:O	2.19	0.75
3:S:582:ASN:H	3:S:582:ASN:ND2	1.85	0.75
4:S:601:NAG:H82	4:S:601:NAG:O3	1.86	0.75
2:L:33:LEU:CD2	2:L:71:TYR:HB2	2.15	0.75
3:R:587:LYS:HE3	4:R:601:NAG:HO6	0.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:493:LYS:HD2	3:S:563:MET:HE3	1.70	0.73
3:S:537:ASP:HB2	3:S:560:THR:OG1	1.88	0.73
3:S:493:LYS:HB3	3:S:563:MET:HE1	1.70	0.72
3:S:392:THR:HG1	3:S:492:THR:HG1	1.37	0.71
3:S:582:ASN:HD22	3:S:582:ASN:N	1.89	0.69
2:B:53:ARG:NH1	3:R:549:GLU:OE1	2.24	0.69
2:L:33:LEU:HD23	2:L:71:TYR:CG	2.29	0.68
1:H:213:ARG:HG3	1:H:213:ARG:HH21	1.56	0.68
1:H:51:ILE:HD13	1:H:71:ARG:CG	2.24	0.67
2:L:108:ARG:HG3	2:L:108:ARG:NH1	2.01	0.67
3:R:520:ALA:O	3:R:521:ASN:HB2	1.95	0.67
3:S:493:LYS:CD	3:S:563:MET:HE2	2.23	0.66
3:S:505:ARG:NH2	3:S:551:GLY:O	2.30	0.65
3:S:487:ASN:N	3:S:487:ASN:OD1	2.29	0.65
3:R:487:ASN:N	3:R:487:ASN:OD1	2.31	0.63
2:L:33:LEU:HD21	2:L:71:TYR:HB2	1.81	0.62
2:B:80:GLN:NE2	2:B:168:SER:O	2.32	0.62
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.80	0.62
2:L:110:ASP:OD2	2:L:199:LYS:NZ	2.31	0.62
1:A:59:TYR:HB2	1:A:64:LYS:HD2	1.81	0.61
2:L:108:ARG:NH1	2:L:109:ALA:O	2.32	0.61
1:H:148:GLU:OE1	5:H:301:HOH:O	2.16	0.61
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.85	0.59
3:S:485:PRO:HD2	3:S:488:LEU:HB2	1.83	0.59
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.86	0.58
3:S:579:THR:HG22	3:S:580:ASP:N	2.20	0.56
3:R:427:GLN:NE2	3:R:473:PHE:O	2.38	0.56
3:S:496:LYS:HD2	3:S:560:THR:HG21	1.88	0.56
3:S:493:LYS:CD	3:S:563:MET:CE	2.76	0.56
3:S:415:LEU:HD21	3:S:480:ILE:HD13	1.87	0.56
3:S:509:ASP:N	3:S:509:ASP:OD2	2.38	0.56
3:S:493:LYS:HB3	3:S:563:MET:HE2	1.87	0.55
3:S:466:GLN:HG2	3:S:517:LEU:HD21	1.88	0.55
4:S:601:NAG:O3	4:S:601:NAG:C8	2.55	0.55
3:S:488:LEU:HD13	3:S:491:ILE:HD12	1.87	0.54
2:L:36:TYR:HE2	2:L:89:GLN:HE21	1.54	0.54
3:S:582:ASN:CB	3:S:585:CYS:SG	2.96	0.54
1:H:56:TYR:CE1	3:S:536:GLU:HG3	2.42	0.54
1:H:47:TRP:CE3	2:L:96:PRO:HD2	2.43	0.53
2:B:108:ARG:NH1	2:B:109:ALA:O	2.40	0.53
3:R:406:ASN:HA	3:R:583:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:580:ASP:N	3:R:580:ASP:OD1	2.42	0.53
1:A:94:ARG:HD2	1:A:101:ASP:OD1	2.09	0.52
1:H:128:CYS:SG	1:H:213:ARG:HB2	2.50	0.52
1:A:32:TYR:CD2	1:A:94:ARG:HD3	2.45	0.52
3:R:435:SER:HA	3:R:586:PRO:HG3	1.91	0.52
1:H:170:LEU:HB2	1:H:175:TYR:CE1	2.46	0.51
1:H:18:LEU:HB3	1:H:82:MET:HE3	1.93	0.51
3:S:394:PRO:HG3	3:S:400:LYS:HB2	1.94	0.50
3:S:504:SER:HB3	3:S:515:PRO:HA	1.93	0.50
2:L:105:GLU:HG2	2:L:173:TYR:OH	2.12	0.50
1:H:85:GLU:OE2	1:H:86:ASP:OD2	2.30	0.49
3:S:511:ARG:NH2	3:S:542:ARG:HE	2.10	0.49
1:H:52:SER:HB2	3:S:536:GLU:HB2	1.94	0.49
3:S:582:ASN:HB2	3:S:585:CYS:SG	2.52	0.49
1:A:82:MET:HE2	1:A:82(C):LEU:HD21	1.95	0.49
2:B:195:GLU:HG2	2:B:206:VAL:HG22	1.95	0.49
1:A:51:ILE:HD13	1:A:71:ARG:HG2	1.94	0.48
1:H:188:TRP:CG	1:H:189:PRO:HA	2.48	0.48
3:S:493:LYS:HG2	3:S:567:LEU:HB2	1.94	0.48
2:B:150:ILE:HD11	2:B:179:LEU:HD21	1.95	0.48
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.48	0.48
1:A:47:TRP:CE3	2:B:96:PRO:HD2	2.49	0.48
3:S:453:LYS:HB2	3:S:481:LEU:CD1	2.44	0.47
2:L:108:ARG:HH11	2:L:108:ARG:CG	2.13	0.47
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.50	0.47
3:S:498:SER:HB3	3:S:534:VAL:HG23	1.96	0.47
1:A:87:THR:HG23	1:A:110:THR:HA	1.97	0.47
1:A:84:SER:HA	1:A:111:VAL:HB	1.96	0.47
3:R:587:LYS:HE2	4:R:601:NAG:O6	2.00	0.46
1:H:63:VAL:HG13	1:H:67:PHE:HB2	1.97	0.46
1:H:95:ASP:OD1	1:H:96:GLY:HA2	2.16	0.46
3:S:493:LYS:CB	3:S:563:MET:CE	2.91	0.46
3:R:383:CYS:SG	3:R:407:CYS:HB2	2.49	0.45
1:A:60:PRO:HG2	1:A:63:VAL:HG22	1.97	0.45
3:R:436:ASN:O	3:R:586:PRO:HD3	2.16	0.45
3:S:582:ASN:HB3	3:S:585:CYS:SG	2.56	0.45
2:B:167:ASP:OD1	2:B:169:LYS:HG2	2.17	0.45
3:S:484:VAL:HA	3:S:485:PRO:HD3	1.80	0.45
2:L:185:GLU:OE1	2:L:188:ARG:NH1	2.50	0.44
2:L:94:LEU:CD2	2:L:96:PRO:HD3	2.48	0.44
3:S:579:THR:HG22	3:S:580:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:VAL:CG2	1:H:128:CYS:N	2.80	0.44
1:A:12:VAL:HG11	1:A:82(C):LEU:HD13	2.00	0.44
3:S:480:ILE:HB	3:S:571:PHE:HB2	1.99	0.43
3:R:386:SER:N	3:R:387:PRO:CD	2.81	0.43
1:H:44:ARG:HA	1:H:44:ARG:HD2	1.77	0.43
2:L:195:GLU:HG2	2:L:206:VAL:HG22	2.01	0.43
2:L:33:LEU:CD2	2:L:71:TYR:HB3	2.29	0.43
3:R:476:PRO:HG2	3:R:575:VAL:CG2	2.48	0.43
2:L:149:LYS:HB2	2:L:193:THR:HB	2.01	0.43
2:B:108:ARG:HG3	2:B:109:ALA:O	2.19	0.43
3:R:498:SER:HB3	3:R:534:VAL:HG23	2.00	0.43
2:B:155:ARG:HD2	2:B:157:ASN:O	2.19	0.42
3:S:423:PHE:C	3:S:423:PHE:CD1	2.91	0.42
1:H:152:LEU:HA	1:H:196:ASN:O	2.19	0.42
3:R:395:GLN:HG3	3:R:498:SER:HB2	2.00	0.42
1:A:188:TRP:CG	1:A:189:PRO:HA	2.54	0.42
2:L:108:ARG:HD2	2:L:171:SER:HB2	2.00	0.42
2:L:36:TYR:OH	2:L:89:GLN:NE2	2.52	0.42
1:H:35:SER:HB2	1:H:93:VAL:HG12	2.02	0.42
1:H:95:ASP:CG	1:H:96:GLY:HA2	2.39	0.42
1:A:93:VAL:CG1	1:A:99:MET:HB3	2.49	0.42
3:S:496:LYS:HD2	3:S:560:THR:CG2	2.51	0.41
1:H:94:ARG:O	1:H:101:ASP:HB2	2.20	0.41
3:S:433:ILE:HG21	3:S:478:CYS:SG	2.60	0.41
3:S:579:THR:CG2	3:S:580:ASP:N	2.82	0.41
3:R:537:ASP:HB2	3:R:560:THR:OG1	2.21	0.41
2:L:169:LYS:HB2	2:L:169:LYS:HE3	1.89	0.40
2:B:15:LEU:HD11	2:B:106:LEU:HD21	2.04	0.40
1:A:169:VAL:HG11	2:B:160:LEU:HD22	2.04	0.40
2:L:94:LEU:HD23	2:L:96:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	209/216 (97%)	205 (98%)	4 (2%)	0	100	100
1	H	210/216 (97%)	206 (98%)	2 (1%)	2 (1%)	18	37
2	B	210/214 (98%)	205 (98%)	5 (2%)	0	100	100
2	L	210/214 (98%)	205 (98%)	4 (2%)	1 (0%)	32	58
3	R	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
3	S	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
All	All	1251/1276 (98%)	1216 (97%)	32 (3%)	3 (0%)	51	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	101	ASP
1	H	149	PRO
2	L	199	LYS

### 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	184/186 (99%)	178 (97%)	6 (3%)	43	70
1	H	183/186 (98%)	167 (91%)	16 (9%)	12	23
2	B	190/192 (99%)	183 (96%)	7 (4%)	39	66
2	L	190/192 (99%)	180 (95%)	10 (5%)	26	50
3	R	190/190 (100%)	176 (93%)	14 (7%)	16	32
3	S	190/190 (100%)	173 (91%)	17 (9%)	11	22
All	All	1127/1136 (99%)	1057 (94%)	70 (6%)	21	42

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ARG
1	A	95	ASP
1	A	115	LYS
1	A	134	SER
1	A	171	GLN
1	A	213	ARG
2	B	8	THR
2	B	48	ILE
2	B	81	GLU
2	B	105	GLU
2	B	155	ARG
2	B	183	LYS
2	B	185	GLU
3	R	422	ASP
3	R	423	PHE
3	R	435	SER
3	R	450	LEU
3	R	451	SER
3	R	453	LYS
3	R	473	PHE
3	R	487	ASN
3	R	518	VAL
3	R	522	GLN
3	R	543	LYS
3	R	565	GLU
3	R	580	ASP
3	R	581	THR
1	H	3	LYS
1	H	44	ARG
1	H	46	GLU
1	H	63	VAL
1	H	64	LYS
1	H	71	ARG
1	H	84	SER
1	H	85	GLU
1	H	93	VAL
1	H	95	ASP
1	H	97	ASN
1	H	101	ASP
1	H	127	VAL
1	H	172	SER
1	H	205	LYS
1	H	213	ARG

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Mol	Chain	Res	Type
3	S	400	LYS
3	S	416	SER
3	S	423	PHE
3	S	487	ASN
3	S	488	LEU
3	S	489	THR
3	S	490	THR
3	S	492	THR
3	S	504	SER
3	S	505	ARG
3	S	507	LEU
3	S	509	ASP
3	S	542	ARG
3	S	560	THR
3	S	581	THR
3	S	582	ASN
3	S	587	LYS
2	L	8	THR
2	L	19	VAL
2	L	48	ILE
2	L	53	ARG
2	L	89	GLN
2	L	105	GLU
2	L	106	LEU
2	L	108	ARG
2	L	153	SER
2	L	201	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	S	486	HIS
3	S	566	GLN
3	S	582	ASN
2	L	37	GLN
2	L	89	GLN

### 5.3.3 RNA ⓘ

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](#)

2 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	$\# Z  > 2$
4	NAG	R	601	3	14,14,15	0.27	0	15,19,21	0.58	0
4	NAG	S	601	3	14,14,15	0.28	0	15,19,21	0.58	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
4	NAG	R	601	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	S	601	3	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	R	601	NAG	C1
4	S	601	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	601	NAG	4	0
4	S	601	NAG	2	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, 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	213/216 (98%)	-0.24	1 (0%) 90 89	26, 31, 45, 62	0
1	H	214/216 (99%)	0.16	8 (3%) 42 34	29, 39, 56, 80	0
2	B	212/214 (99%)	-0.01	1 (0%) 90 89	24, 32, 53, 77	0
2	L	212/214 (99%)	0.04	1 (0%) 90 89	24, 33, 46, 81	0
3	R	208/208 (100%)	0.36	19 (9%) 10 6	28, 42, 87, 142	0
3	S	208/208 (100%)	0.52	18 (8%) 11 7	39, 55, 93, 119	0
All	All	1267/1276 (99%)	0.14	48 (3%) 41 33	24, 37, 73, 142	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	580	ASP	6.5
3	R	578	GLY	5.8
3	R	579	THR	4.7
3	S	459	SER	4.5
3	R	588	LEU	4.3
3	S	510	ASP	4.3
1	H	132	THR	4.2
3	S	511	ARG	4.2
3	S	458	VAL	3.9
1	H	65	GLY	3.7
3	S	461	ALA	3.7
3	S	509	ASP	3.5
3	S	507	LEU	3.5
2	B	200	THR	3.4
3	S	486	HIS	3.3
3	S	588	LEU	3.2
3	R	434	ALA	3.1
1	H	128	CYS	3.1
1	H	129	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	R	459	SER	2.8
3	S	473	PHE	2.7
3	R	458	VAL	2.6
3	R	433	ILE	2.5
3	R	435	SER	2.5
3	R	408	ASN	2.5
3	R	511	ARG	2.5
1	H	213	ARG	2.4
3	R	587	LYS	2.4
3	S	579	THR	2.3
2	L	33	LEU	2.3
3	R	582	ASN	2.3
3	R	489	THR	2.3
3	R	585	CYS	2.3
3	R	461	ALA	2.3
3	S	489	THR	2.3
3	S	460	SER	2.3
3	S	587	LYS	2.2
3	R	457	SER	2.2
1	H	64	LYS	2.2
3	S	381	VAL	2.1
3	S	385	PHE	2.1
3	S	488	LEU	2.1
1	A	132	THR	2.1
3	S	418	PHE	2.1
1	H	63	VAL	2.0
3	R	473	PHE	2.0
3	R	431	ALA	2.0
1	H	127	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

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
4	NAG	R	601	14/15	0.48	0.44	1.47	124,129,132,132	0
4	NAG	S	601	14/15	0.63	0.40	-	127,133,136,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.