



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 10:45 AM EDT

PDB ID : 7L4Z
Title : Structure of SARS-CoV-2 spike RBD in complex with cyclic peptide
Authors : Christie, M.; Mackay, J.P.; Passioura, T.; Payne, R.J.
Deposited on : 2020-12-21
Resolution : 3.96 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

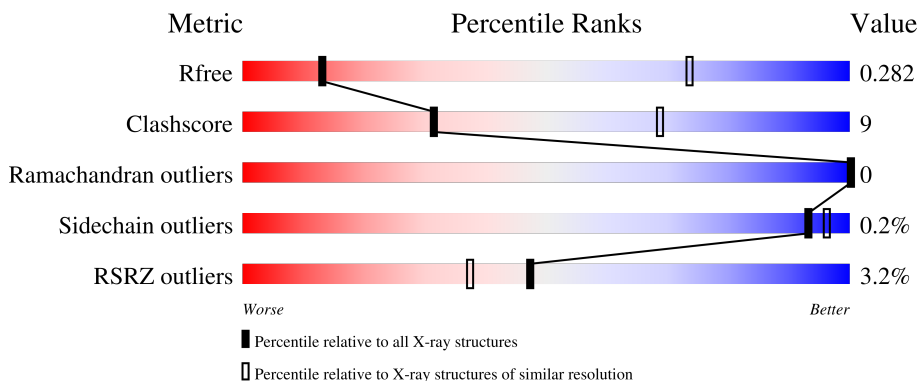
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	229	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">3% 66% 21% 13%</p>
1	B	229	<div style="display: flex; align-items: center;"> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">70% 17% 13%</p>
1	C	229	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">4% 70% 18% 12%</p>
1	D	229	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">2% 66% 22% 11%</p>
1	E	229	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">4% 69% 19% 12%</p>

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Mol	Chain	Length	Quality of chain
2	R	17	 59% 41%
2	S	17	 71% 29%
2	T	17	 71% 29%
2	U	17	 12% 71% 29%
2	V	17	 6% 59% 41%

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	DTY	T	1	-	-	-	X
2	DTY	V	1	-	-	-	X
3	NAG	E	601	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8694 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	199	1581	1014	265	294	8	0	0	0
1	D	203	1606	1028	269	301	8	0	0	0
1	A	199	1581	1014	265	294	8	0	0	0
1	C	202	1598	1022	268	300	8	0	0	0
1	E	201	1590	1018	266	298	8	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
D	542	HIS	-	expression tag	UNP P0DTC2
D	543	HIS	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2
D	546	HIS	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2
A	542	HIS	-	expression tag	UNP P0DTC2
A	543	HIS	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
C	542	HIS	-	expression tag	UNP P0DTC2

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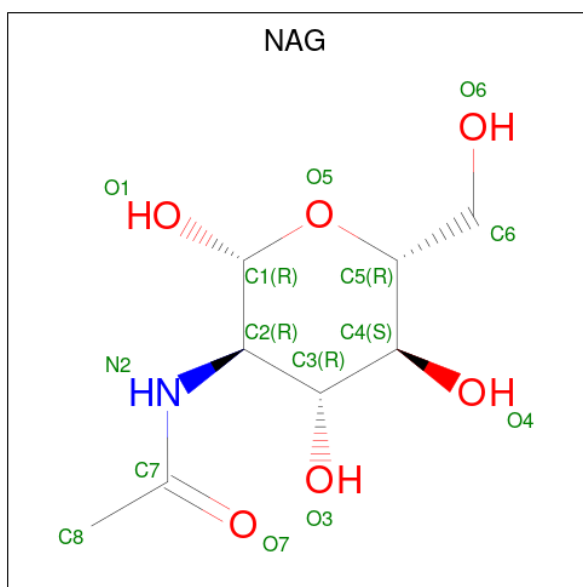
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Chain	Residue	Modelled	Actual	Comment	Reference
C	543	HIS	-	expression tag	UNP P0DTC2
C	544	HIS	-	expression tag	UNP P0DTC2
C	545	HIS	-	expression tag	UNP P0DTC2
C	546	HIS	-	expression tag	UNP P0DTC2
C	547	HIS	-	expression tag	UNP P0DTC2
E	542	HIS	-	expression tag	UNP P0DTC2
E	543	HIS	-	expression tag	UNP P0DTC2
E	544	HIS	-	expression tag	UNP P0DTC2
E	545	HIS	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	HIS	-	expression tag	UNP P0DTC2

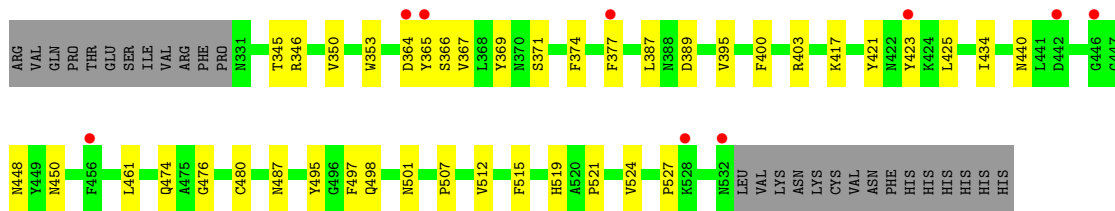
- Molecule 2 is a protein called ACE-DTY-LYS-ALA-GLY-VAL-VAL-TYR-GLY-TYR-ASN-ALA-TRP-ILE-ARG-CYS-NH₂.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	17	Total 128	C 85	N 22	O 20	S 1	0	0	1
2	T	17	Total 128	C 85	N 22	O 20	S 1	0	0	1
2	R	17	Total 128	C 85	N 22	O 20	S 1	0	0	1
2	U	17	Total 128	C 85	N 22	O 20	S 1	0	0	1
2	V	17	Total 128	C 85	N 22	O 20	S 1	0	0	1

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	Total 14	8	1	5	0	0
3	D	1	Total 14	8	1	5	0	0
3	D	1	Total 14	8	1	5	0	0
3	A	1	Total 14	8	1	5	0	0
3	A	1	Total 14	8	1	5	0	0
3	C	1	Total 14	8	1	5	0	0
3	E	1	Total 14	8	1	5	0	0



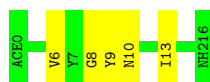
• Molecule 1: Spike protein S1



• Molecule 2: ACE-DTY-LYS-ALA-GLY-VAL-VAL-TYR-GLY-TYR-ASN-ALA-TRP-ILE-ARG-CYS-NH2



• Molecule 2: ACE-DTY-LYS-ALA-GLY-VAL-VAL-TYR-GLY-TYR-ASN-ALA-TRP-ILE-ARG-CYS-NH2

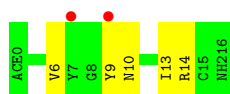


• Molecule 2: ACE-DTY-LYS-ALA-GLY-VAL-VAL-TYR-GLY-TYR-ASN-ALA-TRP-ILE-ARG-CYS-NH2

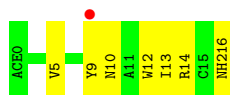


• Molecule 2: ACE-DTY-LYS-ALA-GLY-VAL-VAL-TYR-GLY-TYR-ASN-ALA-TRP-ILE-ARG-CYS-NH2





● Molecule 2: ACE-DTY-LYS-ALA-GLY-VAL-VAL-TYR-GLY-TYR-ASN-ALA-TRP-ILE-ARG-CYS-NH2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	284.92Å 284.92Å 156.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.39 – 3.96 48.85 – 3.96	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.39-3.96) 99.7 (48.85-3.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 4.00Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.257 , 0.282 0.257 , 0.282	Depositor DCC
R_{free} test set	1065 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	110.5	Xtrriage
Anisotropy	0.767	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 109.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8694	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, 0.333 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: DTY, ACE, NH2, 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	0.31	0/1626	0.49	0/2213
1	B	0.32	0/1626	0.49	0/2213
1	C	0.30	0/1642	0.47	0/2234
1	D	0.31	0/1650	0.48	0/2245
1	E	0.30	0/1634	0.47	0/2223
2	R	0.28	0/115	0.36	0/155
2	S	0.34	0/115	0.49	0/155
2	T	0.28	0/115	0.40	0/155
2	U	0.37	0/115	0.47	0/155
2	V	0.28	0/115	0.41	0/155
All	All	0.31	0/8753	0.48	0/11903

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1581	0	1497	36	1
1	B	1581	0	1498	26	1
1	C	1598	0	1520	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1606	0	1530	34	0
1	E	1590	0	1514	29	0
2	R	128	0	120	5	1
2	S	128	0	120	4	1
2	T	128	0	120	4	0
2	U	128	0	120	5	0
2	V	128	0	120	5	1
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	28	0	26	0	0
3	E	14	0	13	0	0
All	All	8694	0	8250	153	3

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 9.

All (153) 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:379:CYS:HB2	1:A:384:PRO:HD3	1.64	0.80
1:E:431:GLY:HA3	1:E:513:LEU:O	1.90	0.72
1:B:431:GLY:HA3	1:B:513:LEU:O	1.91	0.69
1:C:371:SER:HB2	1:C:374:PHE:HE2	1.56	0.69
1:D:418:ILE:HA	1:D:422:ASN:HD22	1.61	0.66
1:D:401:VAL:HG22	1:D:509:ARG:HG2	1.78	0.66
1:D:472:ILE:HG22	1:D:490:PHE:HA	1.78	0.63
1:E:389:ASP:HB3	2:V:10:ASN:HB2	1.80	0.62
1:C:395:VAL:HG21	2:U:6:VAL:HG11	1.81	0.62
1:E:524:VAL:HG23	2:V:14:ARG:HB2	1.82	0.61
1:A:359:SER:OG	1:A:360:ASN:OD1	2.17	0.60
1:A:331:ASN:H	2:R:0:ACE:H2	1.67	0.60
1:A:345:THR:O	1:A:509:ARG:NH2	2.34	0.59
1:A:473:TYR:CE2	1:A:475:ALA:HB2	2.38	0.59
1:D:365:TYR:HD2	1:D:388:ASN:HA	1.67	0.58
1:D:421:TYR:HA	1:D:461:LEU:HD13	1.85	0.58
1:D:472:ILE:HA	1:D:491:PRO:HD3	1.86	0.58
1:A:457:ARG:NE	1:A:467:ASP:OD2	2.34	0.58
1:A:473:TYR:HE2	1:A:475:ALA:HB2	1.68	0.57
1:C:474:GLN:HB3	1:C:480:CYS:SG	2.45	0.56
1:D:379:CYS:HB2	1:D:384:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TYR:CZ	1:D:455:LEU:HD21	2.40	0.56
1:D:457:ARG:NE	1:D:467:ASP:OD2	2.28	0.56
1:C:497:PHE:HB3	1:C:507:PRO:HD3	1.88	0.56
1:C:389:ASP:HA	2:U:10:ASN:HB2	1.89	0.55
1:B:521:PRO:HG2	1:B:524:VAL:HB	1.87	0.55
1:A:354:ASN:HD21	1:A:356:LYS:HE2	1.71	0.55
1:C:524:VAL:HG13	2:U:14:ARG:HB2	1.88	0.55
1:C:366:SER:HA	1:C:369:TYR:CZ	2.42	0.54
1:D:342:PHE:CE1	1:D:511:VAL:HG11	2.42	0.54
1:E:347:PHE:CE1	1:E:399:SER:HB2	2.42	0.54
1:D:342:PHE:HE1	1:D:511:VAL:HG11	1.72	0.54
1:E:438:SER:HB3	1:E:509:ARG:HG3	1.88	0.54
1:D:519:HIS:ND1	1:D:526:GLY:O	2.40	0.54
1:A:383:SER:HG	1:A:385:THR:HG1	1.54	0.54
1:A:449:TYR:CZ	1:E:455:LEU:HD21	2.42	0.53
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.89	0.53
1:A:342:PHE:CE1	1:A:511:VAL:HG21	2.42	0.53
1:E:403:ARG:HB2	1:E:495:TYR:HE1	1.73	0.53
1:B:377:PHE:CD1	1:B:434:ILE:HG12	2.44	0.53
1:A:472:ILE:HG13	1:A:489:TYR:O	2.08	0.53
1:D:457:ARG:HD3	1:D:461:LEU:HD11	1.91	0.53
1:D:353:TRP:CZ2	1:D:466:ARG:HB2	2.45	0.52
1:A:365:TYR:HA	1:A:368:LEU:HD13	1.91	0.52
1:E:401:VAL:HG22	1:E:509:ARG:HG2	1.92	0.52
1:B:331:ASN:HB3	2:S:0:ACE:H2	1.91	0.52
1:B:422:ASN:HD21	1:B:454:ARG:H	1.56	0.52
1:C:448:ASN:OD1	1:C:450:ASN:ND2	2.43	0.51
1:C:350:VAL:HA	1:C:400:PHE:HB2	1.92	0.51
1:A:354:ASN:O	1:A:398:ASP:HA	2.11	0.51
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.76	0.51
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.91	0.50
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.46	0.50
1:A:354:ASN:ND2	1:A:356:LYS:HE2	2.27	0.50
1:A:421:TYR:HA	1:A:461:LEU:HD13	1.93	0.50
1:C:377:PHE:HD1	1:C:434:ILE:HG23	1.76	0.50
1:E:475:ALA:HB3	1:E:489:TYR:HE2	1.76	0.50
1:B:447:GLY:HA2	1:B:497:PHE:O	2.12	0.50
1:D:389:ASP:HB3	2:T:10:ASN:HB2	1.94	0.50
1:E:421:TYR:CD1	1:E:457:ARG:HB3	2.47	0.49
2:T:9:TYR:O	2:T:13:ILE:HG12	2.13	0.49
1:A:341:VAL:HG12	1:A:342:PHE:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:PRO:HA	1:D:387:LEU:HB2	1.95	0.48
1:A:360:ASN:OD1	2:R:4:GLY:HA2	2.13	0.48
2:U:6:VAL:O	2:U:6:VAL:HG13	2.11	0.48
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.96	0.48
1:D:341:VAL:HG12	1:D:342:PHE:HD1	1.78	0.48
1:D:350:VAL:HG22	1:D:422:ASN:HB3	1.95	0.48
1:A:403:ARG:HB2	1:A:495:TYR:HE1	1.79	0.48
1:C:498:GLN:H	1:C:501:ASN:ND2	2.12	0.48
1:E:421:TYR:HA	1:E:461:LEU:HD13	1.95	0.48
1:B:377:PHE:HD1	1:B:434:ILE:HG12	1.78	0.47
1:A:474:GLN:HB3	1:A:480:CYS:SG	2.53	0.47
1:B:389:ASP:HB3	2:S:10:ASN:HB2	1.96	0.47
1:B:364:ASP:O	1:B:367:VAL:HG12	2.14	0.47
1:D:366:SER:HA	1:D:369:TYR:CE2	2.50	0.47
1:D:377:PHE:CD1	1:D:434:ILE:HG12	2.50	0.47
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.25	0.47
1:E:418:ILE:HG23	1:E:422:ASN:HB2	1.97	0.47
1:D:403:ARG:HB2	1:D:495:TYR:HE1	1.78	0.47
1:D:532:ASN:O	1:D:533:LEU:HD12	2.14	0.47
2:U:9:TYR:O	2:U:13:ILE:HG12	2.15	0.47
1:B:456:PHE:CE2	1:B:491:PRO:HA	2.50	0.46
1:E:374:PHE:HA	1:E:436:TRP:HB3	1.97	0.46
1:B:490:PHE:CD1	1:B:491:PRO:HD2	2.51	0.46
1:C:345:THR:HG22	1:C:346:ARG:HG3	1.96	0.46
1:E:487:ASN:HA	1:E:489:TYR:CZ	2.50	0.46
1:C:353:TRP:CD1	1:C:423:TYR:HD1	2.34	0.46
1:A:453:TYR:HB3	1:A:495:TYR:CE2	2.51	0.46
1:E:532:ASN:O	1:E:533:LEU:HD23	2.16	0.46
1:E:457:ARG:NE	1:E:467:ASP:OD2	2.46	0.46
1:B:332:ILE:HD11	2:S:3:ALA:HA	1.97	0.46
1:E:418:ILE:O	1:E:422:ASN:N	2.45	0.45
1:C:395:VAL:HG22	1:C:515:PHE:HB3	1.98	0.45
1:A:389:ASP:HB3	2:R:10:ASN:HB2	1.98	0.45
1:B:418:ILE:HG23	1:B:422:ASN:HB2	1.97	0.45
1:B:472:ILE:HD12	1:B:482:GLY:HA2	1.99	0.45
1:D:521:PRO:HG2	1:D:524:VAL:HB	1.98	0.45
1:A:442:ASP:OD1	1:A:451:TYR:OH	2.21	0.45
1:A:365:TYR:CE2	1:A:392:PHE:HE2	2.35	0.45
1:C:521:PRO:HB2	1:C:524:VAL:HB	1.98	0.44
1:D:409:GLN:HB3	1:D:419:ALA:HB2	2.00	0.44
1:A:457:ARG:HD3	1:A:461:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:GLY:HA2	1:D:515:PHE:CE2	2.52	0.44
1:A:472:ILE:HD11	1:A:488:CYS:HB3	2.00	0.44
1:B:449:TYR:CE2	1:D:456:PHE:HZ	2.36	0.44
1:A:403:ARG:HB2	1:A:495:TYR:CE1	2.53	0.44
1:E:353:TRP:CZ2	1:E:466:ARG:HB2	2.52	0.44
2:S:9:TYR:O	2:S:13:ILE:HG12	2.17	0.44
1:C:440:ASN:OD1	1:C:440:ASN:N	2.50	0.44
1:E:425:LEU:HD21	1:E:512:VAL:HG11	2.00	0.44
1:A:384:PRO:HA	1:A:387:LEU:HB2	1.99	0.43
1:E:366:SER:HA	1:E:369:TYR:CE2	2.52	0.43
1:D:457:ARG:HD3	1:D:461:LEU:CD1	2.48	0.43
1:C:403:ARG:HG3	1:C:495:TYR:CD1	2.53	0.43
1:E:447:GLY:HA2	1:E:497:PHE:O	2.18	0.43
2:R:12:TRP:O	2:R:16:NH2:N	2.52	0.43
2:V:9:TYR:O	2:V:13:ILE:HG12	2.19	0.43
2:V:12:TRP:O	2:V:16:NH2:N	2.52	0.43
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.00	0.43
1:D:414:GLN:O	1:D:424:LYS:NZ	2.52	0.43
1:C:421:TYR:HA	1:C:461:LEU:HD13	2.01	0.42
1:B:374:PHE:HA	1:B:436:TRP:HB3	2.01	0.42
1:D:388:ASN:O	2:T:8:GLY:HA3	2.19	0.42
1:D:355:ARG:NE	1:D:398:ASP:OD1	2.45	0.42
1:A:362:VAL:HA	2:R:7:TYR:O	2.20	0.42
1:E:392:PHE:O	2:V:5:VAL:HG23	2.20	0.42
1:C:425:LEU:HD21	1:C:512:VAL:HG11	2.00	0.42
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.81	0.42
1:D:474:GLN:HB3	1:D:480:CYS:SG	2.60	0.42
1:C:417:LYS:H	1:C:417:LYS:HG3	1.53	0.42
1:C:365:TYR:CD2	1:C:387:LEU:HG	2.55	0.42
1:C:519:HIS:CG	1:C:527:PRO:HG3	2.54	0.42
1:E:524:VAL:HG13	1:E:525:CYS:SG	2.59	0.42
1:C:364:ASP:O	1:C:367:VAL:HG12	2.20	0.41
1:B:334:ASN:O	1:B:362:VAL:HG12	2.19	0.41
1:A:449:TYR:CE1	1:E:455:LEU:HD21	2.55	0.41
1:B:473:TYR:CZ	1:B:475:ALA:HB2	2.55	0.41
1:B:400:PHE:CE1	1:B:510:VAL:HB	2.55	0.41
1:E:411:ALA:HB3	1:E:414:GLN:HG3	2.01	0.41
1:C:498:GLN:H	1:C:501:ASN:HD21	1.67	0.41
1:E:455:LEU:HD22	1:E:493:GLN:NE2	2.35	0.41
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.56	0.41
1:B:474:GLN:O	1:B:476:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:ILE:HD12	1:D:480:CYS:HB3	2.03	0.41
1:E:337:PRO:HB2	1:E:340:GLU:HG2	2.02	0.41
1:D:392:PHE:O	2:T:6:VAL:N	2.48	0.40
1:A:398:ASP:O	1:A:511:VAL:HA	2.21	0.40
1:C:476:GLY:H	1:C:487:ASN:HB3	1.86	0.40
1:E:398:ASP:OD2	1:E:423:TYR:OH	2.26	0.40
1:E:398:ASP:O	1:E:511:VAL:HA	2.21	0.40
1:B:454:ARG:HA	1:B:492:LEU:HD23	2.04	0.40
1:D:393:THR:HG23	1:D:516:GLU:HB3	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:OD2	2:S:9:TYR:OH[11_444]	2.09	0.11
1:B:364:ASP:OD2	2:R:9:TYR:OH[11_444]	2.15	0.05
1:C:364:ASP:OD2	2:V:9:TYR:OH[11_443]	2.19	0.01

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	197/229 (86%)	187 (95%)	10 (5%)	0	100	100
1	B	197/229 (86%)	183 (93%)	14 (7%)	0	100	100
1	C	200/229 (87%)	194 (97%)	6 (3%)	0	100	100
1	D	201/229 (88%)	195 (97%)	6 (3%)	0	100	100
1	E	199/229 (87%)	185 (93%)	14 (7%)	0	100	100
2	R	14/17 (82%)	14 (100%)	0	0	100	100
2	S	14/17 (82%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	14/17 (82%)	14 (100%)	0	0	100	100
2	U	14/17 (82%)	14 (100%)	0	0	100	100
2	V	14/17 (82%)	14 (100%)	0	0	100	100
All	All	1064/1230 (86%)	1014 (95%)	50 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	172/202 (85%)	172 (100%)	0	100	100
1	B	172/202 (85%)	172 (100%)	0	100	100
1	C	175/202 (87%)	175 (100%)	0	100	100
1	D	176/202 (87%)	175 (99%)	1 (1%)	86	91
1	E	174/202 (86%)	173 (99%)	1 (1%)	86	91
2	R	10/10 (100%)	10 (100%)	0	100	100
2	S	10/10 (100%)	10 (100%)	0	100	100
2	T	10/10 (100%)	10 (100%)	0	100	100
2	U	10/10 (100%)	10 (100%)	0	100	100
2	V	10/10 (100%)	10 (100%)	0	100	100
All	All	919/1060 (87%)	917 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	518	LEU
1	E	531	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTY	U	1	2	11,12,13	0.39	0	12,15,17	0.45	0
2	DTY	T	1	2	11,12,13	0.39	0	12,15,17	0.53	0
2	DTY	S	1	2	11,12,13	0.39	0	12,15,17	0.32	0
2	DTY	R	1	2	11,12,13	0.39	0	12,15,17	0.45	0
2	DTY	V	1	2	11,12,13	0.37	0	12,15,17	0.38	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	DTY	U	1	2	-	2/5/6/8	0/1/1/1
2	DTY	T	1	2	-	2/5/6/8	0/1/1/1
2	DTY	S	1	2	-	2/5/6/8	0/1/1/1
2	DTY	R	1	2	-	2/5/6/8	0/1/1/1
2	DTY	V	1	2	-	4/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	1	DTY	N-CA-CB-CG
2	S	1	DTY	C-CA-CB-CG
2	T	1	DTY	N-CA-CB-CG
2	T	1	DTY	C-CA-CB-CG
2	R	1	DTY	N-CA-CB-CG
2	R	1	DTY	C-CA-CB-CG
2	U	1	DTY	N-CA-CB-CG
2	U	1	DTY	C-CA-CB-CG
2	V	1	DTY	N-CA-CB-CG
2	V	1	DTY	C-CA-CB-CG
2	V	1	DTY	CA-CB-CG-CD2
2	V	1	DTY	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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
3	NAG	B	601	1	14,14,15	0.56	0	17,19,21	0.51	0
3	NAG	D	601	1	14,14,15	0.97	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	E	601	1	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	D	602	1	14,14,15	0.72	0	17,19,21	0.68	0
3	NAG	A	601	1	14,14,15	0.42	0	17,19,21	0.40	0
3	NAG	C	601	1	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	A	602	1	14,14,15	0.42	0	17,19,21	0.68	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
3	NAG	B	601	1	-	3/6/23/26	0/1/1/1
3	NAG	D	601	1	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	2/6/23/26	0/1/1/1
3	NAG	D	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	1/6/23/26	0/1/1/1
3	NAG	C	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	602	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	NAG	O5-C1	3.51	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	NAG	C1-O5-C5	2.48	115.55	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	NAG	C4-C5-C6-O6
3	E	601	NAG	C4-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	C	601	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	B	601	NAG	C1-C2-N2-C7
3	A	602	NAG	C3-C2-N2-C7
3	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	199/229 (86%)	0.39	8 (4%) 38 31	109, 154, 199, 263	0
1	B	199/229 (86%)	0.09	0 100 100	94, 130, 156, 178	0
1	C	202/229 (88%)	0.32	9 (4%) 33 27	119, 157, 196, 319	0
1	D	203/229 (88%)	0.17	4 (1%) 65 56	108, 153, 188, 332	0
1	E	201/229 (87%)	0.41	10 (4%) 28 25	138, 174, 205, 290	0
2	R	14/17 (82%)	0.02	0 100 100	133, 145, 165, 166	0
2	S	14/17 (82%)	0.39	0 100 100	121, 132, 152, 156	0
2	T	14/17 (82%)	-0.01	0 100 100	165, 178, 191, 191	0
2	U	14/17 (82%)	0.73	2 (14%) 2 3	167, 187, 198, 200	0
2	V	14/17 (82%)	0.62	1 (7%) 16 13	194, 205, 219, 227	0
All	All	1074/1230 (87%)	0.28	34 (3%) 47 37	94, 156, 198, 332	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	9	TYR	3.9
1	E	370	ASN	3.8
1	C	364	ASP	3.2
1	A	423	TYR	3.2
1	C	377	PHE	3.1
1	C	442	ASP	2.8
1	E	520	ALA	2.8
1	C	365	TYR	2.6
1	A	369	TYR	2.6
1	E	374	PHE	2.5
2	U	7	TYR	2.5
1	E	410	ILE	2.5
1	E	406	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	365	TYR	2.4
1	A	377	PHE	2.4
1	A	401	VAL	2.3
1	E	377	PHE	2.3
1	C	532	ASN	2.3
1	E	505	TYR	2.2
1	C	528	LYS	2.2
1	D	423	TYR	2.2
1	D	358	ILE	2.2
1	C	446	GLY	2.1
1	C	423	TYR	2.1
1	A	476	GLY	2.1
1	A	374	PHE	2.1
1	E	372	ALA	2.1
1	D	434	ILE	2.1
1	C	456	PHE	2.1
1	A	402	ILE	2.1
1	A	358	ILE	2.1
1	E	397	ALA	2.0
1	D	377	PHE	2.0
2	U	9	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
2	DTY	V	1	12/13	0.73	0.60	216,236,241,241	0
2	DTY	T	1	12/13	0.76	0.58	178,217,237,244	0
2	DTY	U	1	12/13	0.77	0.31	181,193,205,205	0
2	DTY	R	1	12/13	0.81	0.49	154,180,204,217	0
2	DTY	S	1	12/13	0.89	0.45	138,168,194,215	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
3	NAG	E	601	14/15	0.51	0.42	157,157,157,157	0
3	NAG	A	602	14/15	0.57	0.31	176,176,176,176	0
3	NAG	C	601	14/15	0.58	0.35	176,176,176,176	0
3	NAG	A	601	14/15	0.68	0.25	154,185,205,211	0
3	NAG	D	602	14/15	0.68	0.32	194,194,194,194	0
3	NAG	D	601	14/15	0.71	0.38	163,163,163,163	0
3	NAG	B	601	14/15	0.73	0.22	156,156,156,156	0

6.5 Other polymers [i](#)

There are no such residues in this entry.