



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:45 pm BST

PDB ID : 2VNU
Title : Crystal structure of Sc Rrp44
Authors : Lorentzen, E.; Basquin, J.; Conti, E.
Deposited on : 2008-02-07
Resolution : 2.30 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 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 : 2.11
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) : 2.11

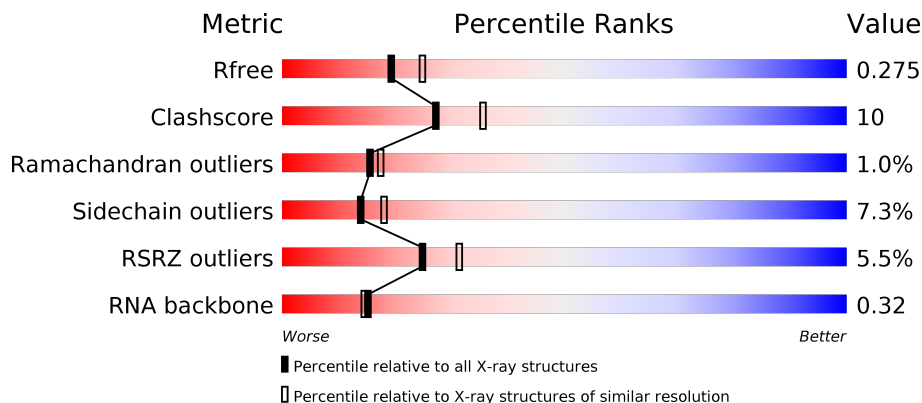
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	B	10	
2	D	760	

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
5	1PE	D	1502	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6091 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 RNA chain called 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	10	199	90	45	55	9	0	0	1

- Molecule 2 is a protein called EXOSOME COMPLEX EXONUCLEASE RRP44.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	D	694	5424	3453	937	1007	9	18	0	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	551	ASN	ASP	engineered mutation	UNP Q08162

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	C O	0	0
			16	10 6		

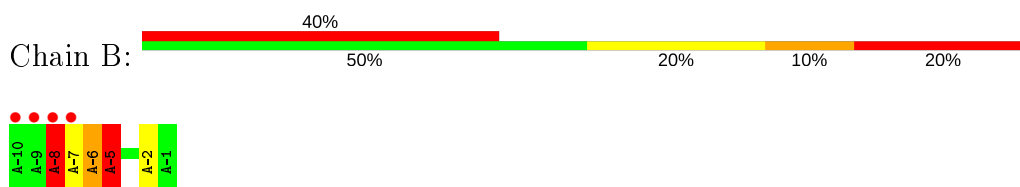
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	18	Total	O	0	0
			18	18		
6	D	432	Total	O	0	0
			432	432		

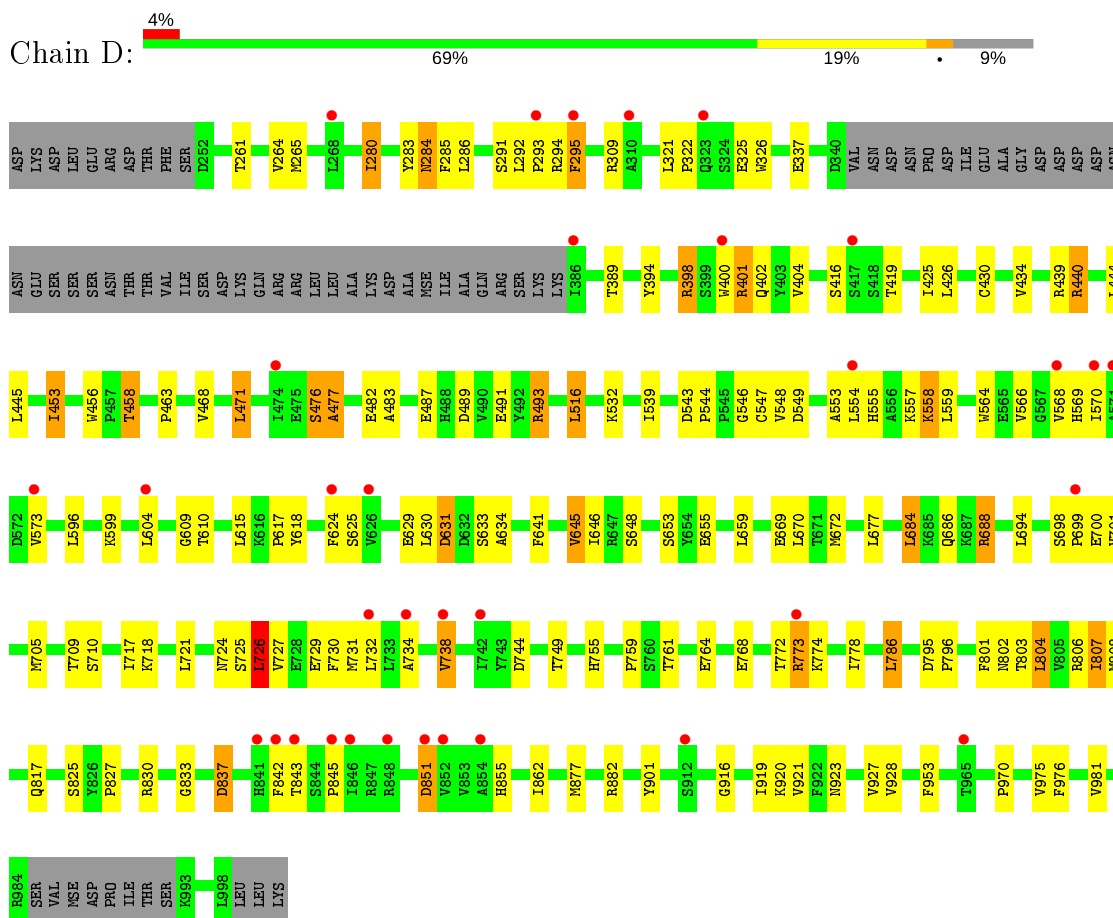
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 5'-R(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP)-3'



- Molecule 2: EXOSOME COMPLEX EXONUCLEASE RRP44



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.35Å 87.25Å 136.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.06 – 2.30 29.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.06-2.30) 99.8 (29.06-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.278 0.216 , 0.275	Depositor DCC
R_{free} test set	1168 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtrriage
Anisotropy	0.227	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6091	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, 1PE

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	B	0.88	0/225	1.84	8/350 (2.3%)
2	D	0.53	1/5540 (0.0%)	0.69	2/7499 (0.0%)
All	All	0.54	1/5765 (0.0%)	0.78	10/7849 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	322	PRO	C-N	-6.68	1.18	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-8	A	P-O3'-C3'	11.78	133.83	119.70
1	B	-6	A	OP2-P-O3'	-9.80	83.63	105.20
1	B	-6	A	O3'-P-O5'	-8.63	87.61	104.00
1	B	-5	A	O5'-P-OP2	8.39	120.77	110.70
2	D	726	LEU	CA-CB-CG	6.98	131.35	115.30
1	B	-5	A	C5'-C4'-O4'	-6.60	101.18	109.10
1	B	-5	A	O4'-C1'-N9	6.26	113.21	108.20
2	D	688	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	B	-6	A	OP1-P-O3'	-5.54	93.00	105.20
1	B	-5	A	OP1-P-OP2	5.14	127.31	119.60

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	B	199	0	100	4	0
2	D	5424	0	5329	110	0
3	D	1	0	0	0	0
4	D	1	0	0	0	0
5	D	16	0	22	9	0
6	B	18	0	0	0	0
6	D	432	0	0	18	0
All	All	6091	0	5451	112	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 10.

All (112) 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)
2:D:928:VAL:HB	6:D:2396:HOH:O	1.69	0.91
2:D:688:ARG:NH1	6:D:2256:HOH:O	2.02	0.89
2:D:837:ASP:HB3	6:D:2346:HOH:O	1.72	0.89
2:D:280:ILE:HD13	2:D:285:PHE:HA	1.65	0.79
2:D:634:ALA:HB1	2:D:684:LEU:HD13	1.65	0.78
2:D:453[A]:ILE:HD12	2:D:463:PRO:HB2	1.65	0.77
2:D:802:ASN:OD1	2:D:806:ARG:NH2	2.16	0.77
2:D:458:THR:HG21	6:D:2084:HOH:O	1.84	0.76
1:B:-5:A:H5'	1:B:-5:A:H8	1.51	0.76
2:D:292:LEU:O	2:D:294:ARG:O	2.06	0.74
2:D:734:ALA:O	2:D:738:VAL:HG13	1.88	0.72
2:D:755:HIS:HD2	2:D:833:GLY:H	1.36	0.72
2:D:804:LEU:HD21	2:D:919:ILE:HG22	1.72	0.71
2:D:564:TRP:CZ2	5:D:1502:1PE:H242	2.28	0.68
1:B:-5:A:H5'	1:B:-5:A:C8	2.29	0.68
2:D:916:GLY:HA3	6:D:2396:HOH:O	1.93	0.67
2:D:699:PRO:HB2	2:D:717:ILE:HG22	1.76	0.66
2:D:755:HIS:CD2	2:D:833:GLY:H	2.13	0.65
2:D:672:MSE:HE2	5:D:1502:1PE:H221	1.79	0.64
2:D:901:TYR:O	6:D:2393:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:773[A]:ARG:NH2	6:D:2313:HOH:O	2.32	0.62
2:D:718:LYS:NZ	6:D:2276:HOH:O	2.32	0.62
2:D:609:GLY:HA3	6:D:2211:HOH:O	2.01	0.60
2:D:721:LEU:H	2:D:724:ASN:HD22	1.49	0.59
2:D:882:ARG:HD3	6:D:2374:HOH:O	2.02	0.58
2:D:768:GLU:O	2:D:772:THR:HG22	2.04	0.58
2:D:803:THR:O	2:D:807:ILE:HG23	2.04	0.58
2:D:564:TRP:CZ3	5:D:1502:1PE:H122	2.38	0.57
2:D:694:LEU:HD22	2:D:833:GLY:HA2	1.87	0.57
2:D:759:PRO:HB2	2:D:761:THR:HG22	1.85	0.56
2:D:705:MSE:HG2	2:D:709:THR:O	2.05	0.56
2:D:491:GLU:OE2	2:D:493:ARG:HB2	2.05	0.56
2:D:539:ILE:HD13	2:D:646[A]:ILE:HG23	1.88	0.55
2:D:837:ASP:N	2:D:837:ASP:OD1	2.32	0.55
2:D:634:ALA:CB	2:D:684:LEU:HD13	2.35	0.55
2:D:804:LEU:HD21	2:D:919:ILE:CG2	2.37	0.54
2:D:558:LYS:HZ1	5:D:1502:1PE:H261	1.71	0.54
2:D:564:TRP:HZ2	5:D:1502:1PE:H242	1.70	0.54
2:D:280:ILE:HD11	2:D:430:CYS:HA	1.89	0.54
2:D:261:THR:O	2:D:265:MSE:HG2	2.09	0.53
2:D:555:HIS:ND1	2:D:569:HIS:HE1	2.07	0.52
2:D:921:VAL:HG12	2:D:953:PHE:CE1	2.44	0.52
2:D:284:ASN:HD22	2:D:286:LEU:H	1.57	0.52
2:D:476:SER:O	2:D:477:ALA:CB	2.57	0.52
2:D:516:LEU:HD11	2:D:645:VAL:HG21	1.90	0.52
2:D:774:LYS:HE3	2:D:801:PHE:CE1	2.45	0.52
2:D:631:ASP:HB3	2:D:633:SER:H	1.76	0.51
2:D:975:VAL:O	2:D:976:PHE:HB2	2.10	0.50
2:D:569:HIS:HD2	2:D:625:SER:OG	1.95	0.50
2:D:398:ARG:HD3	2:D:400:TRP:CE2	2.47	0.50
2:D:401:ARG:NH2	2:D:487:GLU:OE1	2.45	0.50
2:D:309:ARG:HG2	2:D:456:TRP:CE2	2.46	0.50
2:D:564:TRP:HZ2	5:D:1502:1PE:C24	2.26	0.49
2:D:321:LEU:HD12	2:D:389:THR:HG23	1.94	0.49
1:B:-2:A:O2'	2:D:544:PRO:HD3	2.13	0.49
2:D:284:ASN:ND2	2:D:286:LEU:H	2.10	0.49
2:D:284:ASN:HD22	2:D:284:ASN:C	2.17	0.48
2:D:564:TRP:CH2	5:D:1502:1PE:H122	2.48	0.48
2:D:920:LYS:HB3	2:D:927:VAL:HB	1.96	0.48
2:D:570[A]:ILE:HD11	2:D:843:THR:HG22	1.96	0.47
2:D:570[A]:ILE:HD13	2:D:842:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:543:ASP:O	2:D:653:SER:HA	2.14	0.47
2:D:566:VAL:HG11	2:D:730:PHE:CE2	2.49	0.47
2:D:557:LYS:HD2	6:D:2091:HOH:O	2.16	0.46
2:D:532:LYS:HE2	6:D:2117:HOH:O	2.14	0.46
2:D:615:LEU:HD22	2:D:646[B]:ILE:HD11	1.97	0.46
2:D:778:ILE:CG2	2:D:786:LEU:HD13	2.46	0.46
2:D:337:GLU:HG3	2:D:425:ILE:HD13	1.98	0.46
2:D:434:VAL:HG22	2:D:463:PRO:HG2	1.99	0.45
2:D:655:GLU:O	2:D:659:LEU:HD13	2.17	0.45
2:D:804:LEU:HD22	2:D:808:MSE:SE	2.67	0.45
2:D:641:PHE:HB2	2:D:862:ILE:HG21	1.97	0.45
2:D:416:SER:O	6:D:2057:HOH:O	2.21	0.45
2:D:825:SER:OG	2:D:827:PRO:HD2	2.16	0.45
2:D:558:LYS:HZ3	5:D:1502:1PE:H132	1.81	0.44
2:D:842:PHE:O	2:D:855:HIS:HE1	2.00	0.44
2:D:764:GLU:O	2:D:768:GLU:HG3	2.17	0.44
2:D:326:TRP:CD1	2:D:389:THR:HG22	2.51	0.44
2:D:573:VAL:HB	2:D:845:PRO:HB2	2.00	0.44
2:D:283:TYR:HB2	6:D:2018:HOH:O	2.18	0.44
2:D:402:GLN:NE2	2:D:468:VAL:HG11	2.32	0.44
2:D:677:LEU:HB3	2:D:726:LEU:HD13	2.00	0.44
2:D:294:ARG:O	2:D:295:PHE:O	2.35	0.43
2:D:749:THR:O	2:D:877:MSE:HE2	2.18	0.43
2:D:772:THR:HG23	2:D:773[A]:ARG:HG2	1.99	0.43
2:D:419:THR:HG22	2:D:439:ARG:CB	2.48	0.43
2:D:554:LEU:HD23	2:D:568:VAL:HG22	2.00	0.43
2:D:721:LEU:H	2:D:724:ASN:ND2	2.15	0.43
2:D:476:SER:O	2:D:477:ALA:HB3	2.18	0.43
2:D:539:ILE:HG23	2:D:553:ALA:HB1	2.00	0.43
2:D:564:TRP:HZ3	5:D:1502:1PE:H122	1.81	0.43
2:D:264:VAL:HG21	2:D:394:TYR:CG	2.55	0.42
1:B:-8:A:C8	2:D:291:SER:HB3	2.55	0.42
2:D:471:LEU:HG	2:D:482:GLU:HG2	2.01	0.42
2:D:845:PRO:HA	2:D:851:ASP:HB2	2.00	0.42
2:D:280:ILE:CD1	2:D:285:PHE:HA	2.43	0.41
2:D:549:ASP:N	2:D:549:ASP:OD1	2.52	0.41
2:D:727:VAL:O	2:D:731:MSE:HG2	2.21	0.41
2:D:265:MSE:HG2	2:D:265:MSE:H	1.67	0.41
2:D:404:VAL:HG11	2:D:483:ALA:HB1	2.03	0.41
2:D:710:SER:HB2	6:D:2270:HOH:O	2.20	0.41
2:D:795:ASP:HA	2:D:796:PRO:HD2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:559:LEU:HD12	2:D:629:GLU:HG3	2.03	0.41
2:D:610:THR:HG23	6:D:2210:HOH:O	2.20	0.41
2:D:923:ASN:HA	2:D:953:PHE:HB2	2.02	0.41
2:D:725:SER:O	2:D:729:GLU:HG2	2.22	0.40
2:D:970:PRO:HB2	6:D:2424:HOH:O	2.20	0.40
2:D:548:VAL:CB	6:D:2207:HOH:O	2.70	0.40
2:D:539:ILE:CG2	2:D:553:ALA:HB1	2.51	0.40
2:D:617:PRO:HA	2:D:648:SER:HB3	2.03	0.40
2:D:440:ARG:HG2	2:D:444:LEU:HG	2.04	0.40
2:D:539:ILE:CD1	2:D:646[A]:ILE:HD12	2.51	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
2	D	695/760 (91%)	669 (96%)	19 (3%)	7 (1%)	15 17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	295	PHE
2	D	477	ALA
2	D	489	ASP
2	D	293	PRO
2	D	476	SER
2	D	631	ASP
2	D	546	GLY

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
2	D	581/655 (89%)	537 (92%)	44 (8%)	13 16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	280	ILE
2	D	284	ASN
2	D	325	GLU
2	D	398	ARG
2	D	401	ARG
2	D	426	LEU
2	D	440	ARG
2	D	445	LEU
2	D	453[A]	ILE
2	D	453[B]	ILE
2	D	458	THR
2	D	471	LEU
2	D	493	ARG
2	D	516	LEU
2	D	547	CYS
2	D	558	LYS
2	D	596	LEU
2	D	599	LYS
2	D	604	LEU
2	D	618	TYR
2	D	624	PHE
2	D	630	LEU
2	D	645	VAL
2	D	669	GLU
2	D	670	LEU
2	D	684	LEU
2	D	686	GLN
2	D	698	SER
2	D	700	GLU
2	D	701	VAL

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Mol	Chain	Res	Type
2	D	726	LEU
2	D	732	LEU
2	D	738	VAL
2	D	744	ASP
2	D	773[A]	ARG
2	D	773[B]	ARG
2	D	786	LEU
2	D	804	LEU
2	D	807	ILE
2	D	817	GLN
2	D	830	ARG
2	D	837	ASP
2	D	851	ASP
2	D	981	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	275	GLN
2	D	284	ASN
2	D	315	GLN
2	D	569	HIS
2	D	704	HIS
2	D	724	ASN
2	D	748	GLN
2	D	755	HIS
2	D	771	ASN
2	D	855	HIS
2	D	875	ASN
2	D	910	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	8/10 (80%)	4 (50%)	2 (25%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	-8	A

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Mol	Chain	Res	Type
1	B	-7	A
1	B	-6	A
1	B	-5	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	-8	A
1	B	-5	A

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	1PE	D	1502	-	15,15,15	0.55	0	14,14,14	0.44	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
5	1PE	D	1502	-	-	12/13/13/13	-

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
5	D	1502	1PE	OH5-C14-C24-OH4
5	D	1502	1PE	OH4-C13-C23-OH3
5	D	1502	1PE	OH6-C15-C25-OH5
5	D	1502	1PE	OH2-C12-C22-OH3
5	D	1502	1PE	C12-C22-OH3-C23
5	D	1502	1PE	C16-C26-OH6-C15
5	D	1502	1PE	C15-C25-OH5-C14
5	D	1502	1PE	C13-C23-OH3-C22
5	D	1502	1PE	C14-C24-OH4-C13
5	D	1502	1PE	OH7-C16-C26-OH6
5	D	1502	1PE	C23-C13-OH4-C24
5	D	1502	1PE	C25-C15-OH6-C26

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1502	1PE	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	322:PRO	C	323:GLN	N	1.18

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	B	10/10 (100%)	1.46	4 (40%) 0 0	13, 19, 49, 53	0
2	D	676/760 (88%)	0.32	34 (5%) 28 35	2, 16, 24, 35	0
All	All	686/770 (89%)	0.33	38 (5%) 25 31	2, 16, 24, 53	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	570[A]	ILE	5.6
2	D	842	PHE	3.9
2	D	843	THR	3.8
1	B	-10	A	3.8
1	B	-8	A	3.7
2	D	852	VAL	3.7
1	B	-9	A	3.5
2	D	846	ILE	3.4
2	D	417	SER	3.4
1	B	-7	A	3.2
2	D	845	PRO	3.1
2	D	965	THR	3.0
2	D	734	ALA	2.9
2	D	624	PHE	2.8
2	D	854	ALA	2.8
2	D	738	VAL	2.8
2	D	293	PRO	2.7
2	D	604	LEU	2.7
2	D	773[A]	ARG	2.7
2	D	573	VAL	2.7
2	D	323	GLN	2.6
2	D	571	ALA	2.5
2	D	568	VAL	2.5
2	D	626	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	386	ILE	2.5
2	D	554	LEU	2.4
2	D	400	TRP	2.4
2	D	268	LEU	2.4
2	D	310	ALA	2.3
2	D	841	HIS	2.3
2	D	848	ARG	2.3
2	D	699	PRO	2.3
2	D	732	LEU	2.2
2	D	295	PHE	2.2
2	D	742	ILE	2.2
2	D	851	ASP	2.1
2	D	474	ILE	2.1
2	D	912	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
5	1PE	D	1502	16/16	0.92	0.15	23,24,26,26	0
3	MG	D	1500	1/1	0.94	0.05	16,16,16,16	0
4	NA	D	1501	1/1	0.98	0.17	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.