



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:31 AM GMT

PDB ID : 2XCS
Title : THE 2.1A CRYSTAL STRUCTURE OF S. AUREUS GYRASE COMPLEX WITH GSK299423 AND DNA
Authors : Bax, B.D.; Chan, P.F.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.W.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.F.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.
Deposited on : 2010-04-25
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

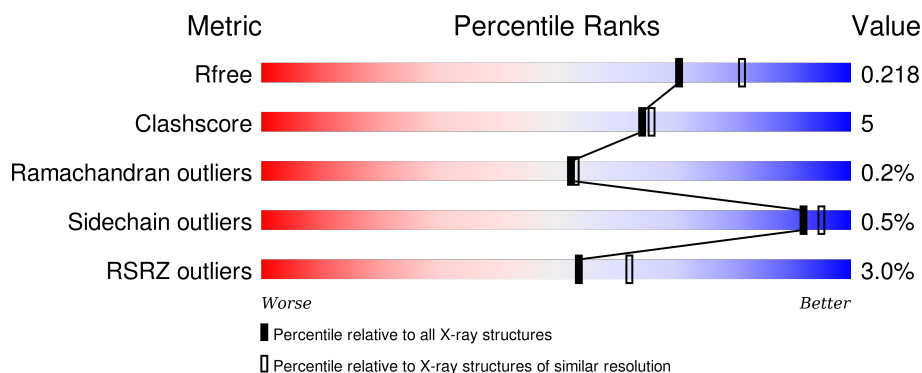
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	692	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>• •</div> </div>
1	D	692	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
2	E	20	<div> <div>60%</div> <div>40%</div> </div>
2	F	20	<div> <div>40%</div> <div>50%</div> <div>5%</div> <div>5%</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	RXV	F	1021[A]	-	-	-	X
4	RXV	F	1021[B]	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12713 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 DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	672	Total	C	N	O	S	0	26	0
			5543	3438	1009	1069	27			
1	D	670	Total	C	N	O	S	0	20	0
			5470	3394	995	1055	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	EXPRESSION TAG	UNP P66937
B	544	THR	-	INSERTION	UNP P66937
B	545	GLY	-	INSERTION	UNP P66937
B	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
D	409	MET	-	EXPRESSION TAG	UNP P66937
D	544	THR	-	INSERTION	UNP P66937
D	545	GLY	-	INSERTION	UNP P66937
D	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5

- Molecule 2 is a DNA chain called 5'-5UA*D(GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*C P *CP*TP*AP*CP*GP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	0	0
			410	194	77	120	19			
2	F	19	Total	C	N	O	P	0	0	0
			390	184	75	113	18			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

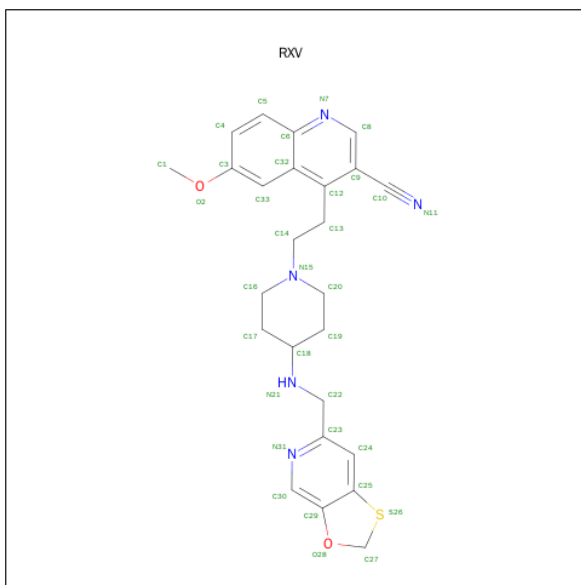
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 6-METHOXY-4-(2-{4-[(1,3]OXATHIOLO[5,4-C]PYRIDIN-6-YLMETHYL) AMINO]PIPERIDIN-1-YL}ETHYL)QUINOLINE-3-CARBONITRILE (three-letter code: RXV) (formula: C₂₅H₂₇N₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	S	0	1
			66	50	10	4	2		

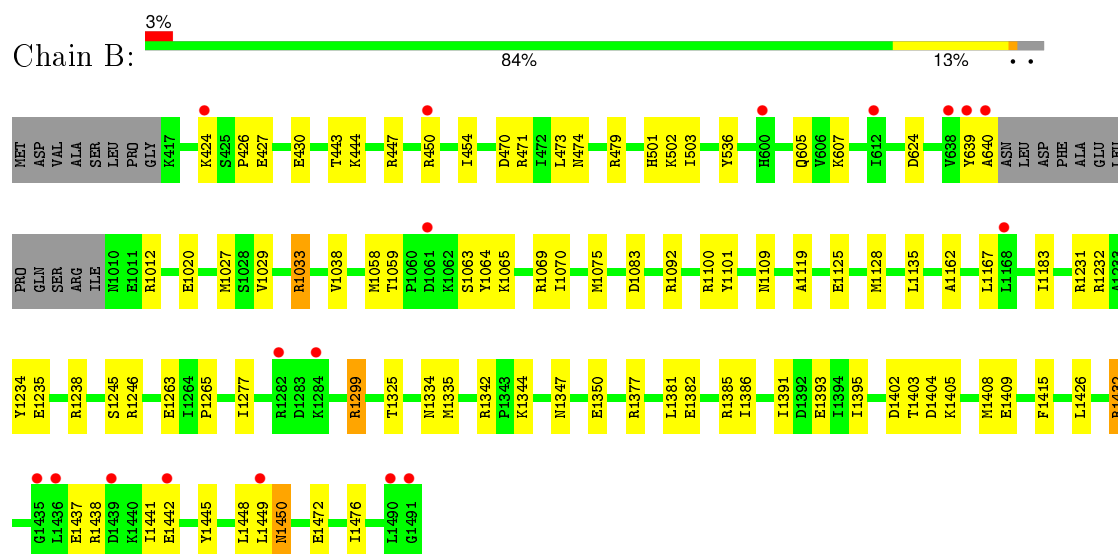
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	386	Total	O	0	2
			388	388		
5	D	365	Total	O	0	1
			366	366		
5	E	40	Total	O	0	0
			40	40		
5	F	35	Total	O	0	1
			36	36		

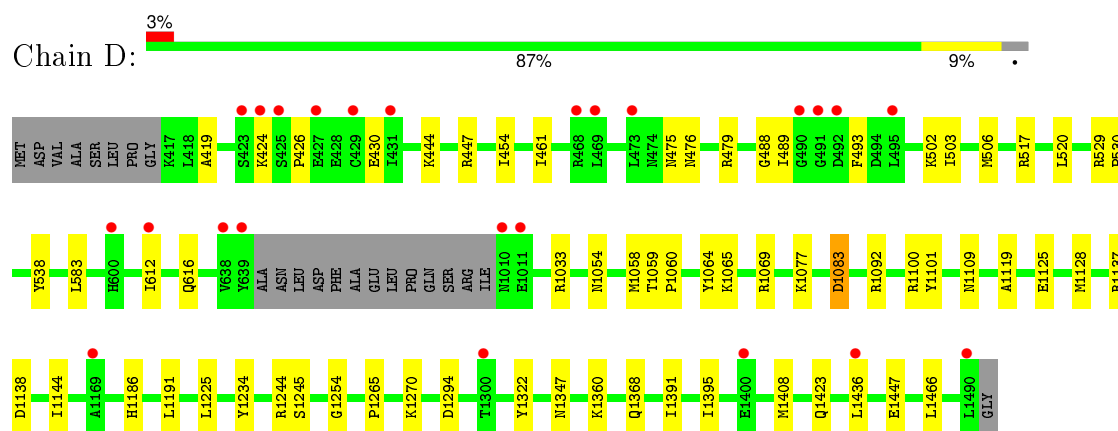
3 Residue-property plots

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: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

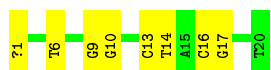


- Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A



- Molecule 2: 5'-5UA*D(GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3'





● Molecule 2: 5'-5UA*D(GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP *CP*TP*AP*CP*GP*GP*CP*T)-3'

Chain F: 40% 50% 5% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.32Å 93.32Å 412.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10 24.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 98.6 (24.97-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.183 , 0.214 0.186 , 0.218	Depositor DCC
R_{free} test set	2907 reflections (2.57%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.1	EDS
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 116140 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12713	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.375 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: MN, 5UA, RXV

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	0.39	0/5615	0.58	0/7556
1	D	0.37	0/5542	0.57	0/7466
2	E	0.76	0/435	1.47	10/669 (1.5%)
2	F	0.76	0/413	1.53	10/635 (1.6%)
All	All	0.42	0/12005	0.70	20/16326 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	17	DG	O4'-C1'-N9	-9.64	101.25	108.00
2	E	9	DG	O4'-C4'-C3'	-8.64	100.82	106.00
2	E	13	DC	C4'-C3'-C2'	-8.22	95.70	103.10
2	F	14	DT	C4'-C3'-C2'	-7.01	96.79	103.10
2	F	3	DC	P-O3'-C3'	-6.58	111.81	119.70
2	F	19	DC	O4'-C1'-N1	6.50	112.55	108.00
2	E	17	DG	O4'-C1'-N9	-6.44	103.49	108.00
2	E	6	DT	O4'-C1'-N1	6.11	112.28	108.00
2	F	9	DG	O4'-C1'-N9	5.87	112.11	108.00
2	E	13	DC	O4'-C4'-C3'	-5.81	102.18	104.50
2	F	16	DC	C1'-O4'-C4'	-5.80	104.30	110.10
2	F	13	DC	O4'-C1'-N1	5.69	111.98	108.00
2	F	6	DT	O4'-C1'-N1	5.61	111.93	108.00
2	E	10	DG	P-O3'-C3'	-5.57	113.01	119.70
2	F	14	DT	O4'-C1'-N1	5.45	111.82	108.00
2	E	14	DT	C4'-C3'-C2'	-5.40	98.24	103.10
2	E	9	DG	C4'-C3'-C2'	-5.25	98.37	103.10
2	F	9	DG	C4'-C3'-C2'	-5.12	98.49	103.10
2	E	16	DC	C1'-O4'-C4'	-5.09	105.01	110.10
2	E	14	DT	O4'-C4'-C3'	-5.07	102.47	104.50

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	B	5543	0	5540	73	0
1	D	5470	0	5453	45	0
2	E	410	0	224	1	0
2	F	390	0	212	4	0
3	B	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	F	66	0	54	2	0
5	B	388	0	0	3	0
5	D	366	0	0	4	0
5	E	40	0	0	1	0
5	F	36	0	0	0	0
All	All	12713	0	11483	120	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 5.

All (120) 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:424:LYS:O	1:B:426:PRO:HD3	1.57	1.05
1:D:424:LYS:O	1:D:426:PRO:HD3	1.63	0.98
1:B:1438:ARG:HH12	1:B:1442[B]:GLU:HG3	1.31	0.93
1:B:450[A]:ARG:HH11	1:B:450[A]:ARG:HG2	1.35	0.89
1:B:1432:ARG:HG3	1:B:1432:ARG:HH11	1.36	0.89
1:B:1438:ARG:NH1	1:B:1442[B]:GLU:HG3	1.92	0.83
1:B:1075:MET:HE1	4:F:1021[A]:RXV:H30	1.64	0.79
2:E:1:5UA:OP3	5:E:2038:HOH:O	2.04	0.76
1:D:475:ASN:O	1:D:479:ARG:HG3	1.87	0.74
1:B:450[A]:ARG:NH1	1:B:450[A]:ARG:HG2	2.00	0.73
1:B:470:ASP:O	1:B:474[A]:ASN:ND2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1432:ARG:O	1:B:1437:GLU:HG3	1.94	0.68
1:D:1092[A]:ARG:NH1	2:F:5:DG:OP1	2.30	0.65
1:D:503:ILE:N	1:D:503:ILE:HD12	2.12	0.64
1:D:1360:LYS:HE2	1:D:1466:LEU:HD13	1.80	0.64
1:D:461:ILE:HD13	1:D:520:LEU:HD23	1.78	0.64
1:B:1432:ARG:HG3	1:B:1432:ARG:NH1	2.08	0.63
1:B:1069[B]:ARG:HG3	1:B:1070:ILE:N	2.13	0.62
1:B:1058:MET:HG2	1:B:1065:LYS:HG3	1.84	0.60
1:D:1137[B]:ARG:O	1:D:1138[B]:ASP:OD2	2.19	0.60
1:B:473:LEU:O	1:B:479:ARG:HD2	2.01	0.60
1:B:1063:SER:O	1:B:1065:LYS:HE3	2.01	0.60
1:B:1238[B]:ARG:HE	1:B:1334:ASN:ND2	1.99	0.60
1:B:1450[A]:ASN:N	1:B:1450[A]:ASN:HD22	2.00	0.59
1:D:1408:MET:CE	1:D:1423:GLN:HG2	2.33	0.59
1:D:1058:MET:HG2	1:D:1065:LYS:HG3	1.85	0.58
1:B:1381:LEU:HD22	1:B:1441:ILE:HG23	1.85	0.58
1:D:488:GLY:O	1:D:489:ILE:CG2	2.51	0.58
1:B:1083[B]:ASP:OD2	5:B:2110[B]:HOH:O	2.17	0.57
1:D:488:GLY:O	1:D:489:ILE:HG23	2.04	0.56
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.40	0.56
1:D:488:GLY:C	1:D:489:ILE:HG23	2.25	0.56
1:D:1447:GLU:HG3	5:D:2331:HOH:O	2.05	0.56
1:B:1445:TYR:CE1	1:B:1449:LEU:HD11	2.41	0.56
1:D:1109:ASN:HB3	1:D:1119:ALA:HB2	1.88	0.56
1:B:1393[B]:GLU:HA	1:B:1393[B]:GLU:OE1	2.06	0.56
1:D:1100:ARG:HG3	1:D:1101:TYR:CE2	2.41	0.56
1:B:1405[B]:LYS:O	1:B:1409[B]:GLU:HG3	2.06	0.56
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.36	0.55
1:B:1109:ASN:HB3	1:B:1119:ALA:HB2	1.88	0.55
1:D:1391:ILE:O	1:D:1395:ILE:HG12	2.06	0.55
1:D:430:GLU:HB3	1:D:502:LYS:HB2	1.89	0.54
1:D:1368:GLN:NE2	5:D:2283:HOH:O	2.40	0.54
1:B:1069[A]:ARG:HG3	5:D:2080:HOH:O	2.07	0.53
1:D:419:ALA:HB2	1:D:444:LYS:HE2	1.89	0.53
2:F:1:5UA:H2'2	2:F:2:DG:C8	2.44	0.53
1:D:447:ARG:HD3	1:D:454:ILE:HD11	1.91	0.52
1:B:1092[A]:ARG:NH2	5:B:2118:HOH:O	2.41	0.52
1:B:1391:ILE:O	1:B:1395:ILE:HG12	2.10	0.52
1:B:1234:TYR:O	1:B:1347:ASN:HB2	2.09	0.52
1:B:1402[A]:ASP:OD1	1:B:1403:THR:N	2.44	0.51
1:B:605:GLN:NE2	1:B:607:LYS:HE2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1054:ASN:HA	1:D:1128:MET:CE	2.41	0.51
1:D:447:ARG:HD3	1:D:454:ILE:CD1	2.42	0.50
1:B:503:ILE:HD12	1:B:503:ILE:N	2.27	0.50
1:B:1012:ARG:HH22	1:B:1020:GLU:CD	2.14	0.50
1:B:1472:GLU:O	1:B:1476:ILE:HG12	2.12	0.49
1:B:1059:THR:HA	1:B:1128:MET:HE3	1.93	0.49
1:B:1438:ARG:HH12	1:B:1442[B]:GLU:CG	2.14	0.49
1:D:1225:LEU:HD21	1:D:1244:ARG:HD2	1.94	0.49
1:D:1234:TYR:O	1:D:1347:ASN:HB2	2.13	0.48
1:B:1382:GLU:O	1:B:1385[A]:ARG:HG2	2.13	0.48
1:B:1299:ARG:N	1:B:1299:ARG:HD3	2.28	0.48
1:B:1393[B]:GLU:HG3	1:B:1415:PHE:HZ	1.79	0.48
1:B:1100:ARG:HG3	1:B:1101:TYR:CE2	2.49	0.48
1:B:1403:THR:HG22	1:D:1436:LEU:HD22	1.96	0.47
1:D:1083[A]:ASP:OD2	5:D:2089[A]:HOH:O	2.20	0.47
1:B:427:GLU:HA	1:B:501:HIS:CG	2.50	0.47
1:B:1377:ARG:HG3	1:B:1448:LEU:HD11	1.97	0.46
1:B:471:ARG:HH21	2:F:14:DT:P	2.39	0.46
1:D:1245:SER:OG	1:D:1265:PRO:HD3	2.15	0.46
1:D:612:ILE:O	1:D:616:GLN:HG3	2.15	0.46
1:B:1183:ILE:HG12	1:B:1335:MET:HG2	1.98	0.46
1:D:1408:MET:HE1	1:D:1423:GLN:HG2	1.96	0.46
1:D:1244:ARG:HG2	1:D:1322:TYR:CE1	2.51	0.46
1:D:503:ILE:CD1	1:D:503:ILE:N	2.79	0.46
5:B:2103:HOH:O	1:D:1069:ARG:HG3	2.15	0.46
1:B:1238[B]:ARG:HH21	1:B:1334:ASN:HD21	1.64	0.45
1:D:502:LYS:HG2	1:D:538:TYR:CE1	2.51	0.45
1:D:1064:TYR:HB3	1:D:1125:GLU:HB3	1.97	0.45
1:B:624[B]:ASP:N	1:B:624[B]:ASP:OD2	2.49	0.45
1:D:506:MET:HG2	1:D:583:LEU:HD11	1.98	0.45
1:D:529:ARG:N	1:D:530:PRO:CD	2.80	0.45
1:B:1038:VAL:HA	1:B:1167:LEU:HD22	1.98	0.45
1:B:639:TYR:O	1:B:640:ALA:HB2	2.16	0.45
1:B:1246:ARG:HB3	1:B:1263:GLU:HB2	1.99	0.44
1:B:1135:LEU:HA	1:B:1162:ALA:HA	1.99	0.44
1:B:450[A]:ARG:HH11	1:B:450[A]:ARG:CG	2.15	0.44
1:B:1409[A]:GLU:HA	1:B:1409[A]:GLU:OE1	2.18	0.44
1:B:1408:MET:HG2	1:B:1426:LEU:CD1	2.48	0.44
1:B:605:GLN:NE2	1:B:607:LYS:CE	2.81	0.44
1:B:1245:SER:OG	1:B:1265:PRO:HD3	2.18	0.44
1:B:474[A]:ASN:N	1:B:474[A]:ASN:HD22	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069[A]:ARG:NH1	1:D:1077:LYS:HE3	2.34	0.43
1:B:639:TYR:CG	1:B:1342:ARG:HG2	2.54	0.43
2:F:1:5UA:N3	2:F:1:5UA:H2'1	2.34	0.43
1:B:1382:GLU:O	1:B:1385[A]:ARG:CG	2.67	0.43
1:B:1277:ILE:HG12	1:B:1325:THR:HG21	2.00	0.43
1:B:1385[A]:ARG:HG3	1:B:1386:ILE:N	2.33	0.43
1:D:1186:HIS:HB2	1:D:1191:LEU:HD11	2.01	0.43
1:D:1137[A]:ARG:O	1:D:1138[A]:ASP:HB2	2.18	0.42
1:B:1450[A]:ASN:ND2	1:B:1450[A]:ASN:N	2.68	0.42
1:B:1382:GLU:HA	1:B:1385[A]:ARG:HG2	2.00	0.42
1:D:1270:LYS:NZ	1:D:1294:ASP:OD2	2.46	0.42
1:B:1232[B]:ARG:HG2	1:B:1238[B]:ARG:O	2.19	0.41
1:B:444:LYS:O	1:B:447:ARG:HG2	2.19	0.41
1:B:1344:LYS:HZ2	1:B:1350[B]:GLU:CD	2.24	0.41
1:D:1144:ILE:HD12	1:D:1144:ILE:C	2.41	0.41
1:B:444:LYS:HA	1:B:454:ILE:CD1	2.51	0.41
1:D:488:GLY:C	1:D:489:ILE:CG2	2.88	0.41
1:B:430:GLU:HB3	1:B:502:LYS:HB2	2.02	0.41
1:D:476:ASN:HA	1:D:479:ARG:HD3	2.03	0.41
1:D:1059:THR:HB	1:D:1060:PRO:HD2	2.03	0.41
1:B:1064:TYR:HB3	1:B:1125:GLU:HB3	2.03	0.41
1:B:1231:ARG:O	1:B:1235[A]:GLU:HG3	2.21	0.41
1:B:1408:MET:SD	1:B:1426:LEU:HD12	2.61	0.40
4:F:1021[B]:RXV:H132	4:F:1021[B]:RXV:H201	1.82	0.40
1:B:501:HIS:CE1	1:B:536:TYR:OH	2.74	0.40
1:B:1029:VAL:HA	1:B:1033:ARG:HB3	2.03	0.40
1:B:1027[A]:MET:HE2	1:B:1027[A]:MET:HB3	1.93	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	B	694/692 (100%)	677 (98%)	16 (2%)	1 (0%)	56	58
1	D	686/692 (99%)	667 (97%)	17 (2%)	2 (0%)	46	45
All	All	1380/1384 (100%)	1344 (97%)	33 (2%)	3 (0%)	52	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1033	ARG
1	B	1033	ARG
1	D	1254	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	
1	B	597/591 (101%)	592 (99%)	5 (1%)	86	91
1	D	587/591 (99%)	584 (100%)	3 (0%)	92	95
All	All	1184/1182 (100%)	1176 (99%)	8 (1%)	92	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1299	ARG
1	B	1404	ASP
1	B	1432	ARG
1	B	1450[A]	ASN
1	B	1450[B]	ASN
1	D	517	ARG
1	D	1083[A]	ASP
1	D	1083[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	480	GLN
1	B	501	HIS
1	B	605	GLN
1	B	1324	GLN
1	B	1334	ASN
1	B	1368	GLN
1	B	1423	GLN
1	D	476	ASN
1	D	1334	ASN
1	D	1368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	5UA	E	1	3,2	16,23,23	2.60	2 (12%)	17,33,33	4.90	5 (29%)
2	5UA	F	1	2	16,23,23	2.67	2 (12%)	17,33,33	4.67	4 (23%)

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	5UA	E	1	3,2	-	0/3/21/21	0/3/3/3
2	5UA	F	1	2	-	0/3/21/21	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	5UA	C2-N1	6.42	1.46	1.33
2	F	1	5UA	C2-N1	6.52	1.46	1.33
2	E	1	5UA	C2-N3	7.50	1.45	1.32
2	F	1	5UA	C2-N3	7.92	1.46	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	5UA	N3-C2-N1	-18.24	114.93	128.89
2	F	1	5UA	N3-C2-N1	-18.06	115.07	128.89
2	F	1	5UA	C4-C5-N7	-4.17	105.64	109.48
2	E	1	5UA	C4-C5-N7	-4.15	105.66	109.48
2	E	1	5UA	O4'-C1'-N9	2.09	111.34	107.72
2	F	1	5UA	C2-N1-C6	2.91	123.97	118.77
2	F	1	5UA	O5'-C5'-C4'	2.97	114.47	109.08
2	E	1	5UA	C2-N1-C6	3.09	124.29	118.77
2	E	1	5UA	O5'-C5'-C4'	6.46	120.78	109.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	5UA	1	0
2	F	1	5UA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
4	RXV	F	1021[A]	-	35,37,37	2.00	2 (5%)	40,51,51	1.38	8 (20%)
4	RXV	F	1021[B]	-	35,37,37	2.00	2 (5%)	40,51,51	1.32	6 (15%)

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	RXV	F	1021[A]	-	-	0/14/30/30	0/4/5/5
4	RXV	F	1021[B]	-	-	0/14/30/30	0/4/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1021[A]	RXV	C9-C10	-10.44	1.28	1.44
4	F	1021[B]	RXV	C9-C10	-10.42	1.28	1.44
4	F	1021[B]	RXV	C12-C32	-2.13	1.39	1.43
4	F	1021[A]	RXV	C12-C32	-2.05	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1021[A]	RXV	C9-C10-N11	-2.90	172.79	177.82
4	F	1021[B]	RXV	C9-C8-N7	-2.44	120.64	124.30
4	F	1021[A]	RXV	C32-C6-N7	-2.26	120.47	122.88
4	F	1021[A]	RXV	C9-C8-N7	-2.25	120.93	124.30
4	F	1021[B]	RXV	C29-C30-N31	-2.24	118.87	122.72
4	F	1021[A]	RXV	C29-C30-N31	-2.22	118.90	122.72
4	F	1021[A]	RXV	C19-C18-C17	-2.21	107.05	110.82
4	F	1021[B]	RXV	C25-C24-C23	-2.18	117.77	121.42
4	F	1021[B]	RXV	C32-C6-N7	-2.15	120.59	122.88
4	F	1021[A]	RXV	C25-C24-C23	-2.00	118.06	121.42
4	F	1021[A]	RXV	O28-C29-C25	2.48	113.13	109.80
4	F	1021[B]	RXV	O28-C29-C25	2.56	113.24	109.80
4	F	1021[A]	RXV	C8-N7-C6	3.25	120.65	116.95
4	F	1021[B]	RXV	C8-N7-C6	3.38	120.80	116.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1021[A]	RXV	1	0
4	F	1021[B]	RXV	1	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, 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	672/692 (97%)	-0.02	18 (2%) 58 65	25, 37, 52, 67	0
1	D	670/692 (96%)	0.00	24 (3%) 46 55	25, 36, 58, 70	0
2	E	19/20 (95%)	-0.65	0 100 100	26, 34, 46, 48	0
2	F	18/20 (90%)	-0.31	0 100 100	28, 35, 49, 53	0
All	All	1379/1424 (96%)	-0.02	42 (3%) 54 62	25, 36, 55, 70	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	ALA	7.2
1	D	491	GLY	7.1
1	B	1490	LEU	5.9
1	B	1491	GLY	4.8
1	D	638	VAL	3.9
1	B	600	HIS	3.7
1	D	490	GLY	3.6
1	B	424	LYS	3.5
1	B	638	VAL	3.4
1	B	1435	GLY	3.2
1	B	1436	LEU	3.2
1	D	639	TYR	3.1
1	D	473	LEU	3.1
1	D	425	SER	3.0
1	B	1442[A]	GLU	2.9
1	D	468	ARG	2.8
1	D	423	SER	2.7
1	B	612	ILE	2.6
1	D	427	GLU	2.6
1	D	429	CYS	2.6
1	D	1400	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1011	GLU	2.4
1	B	1284	LYS	2.4
1	B	1061	ASP	2.3
1	D	1010	ASN	2.3
1	B	450[A]	ARG	2.3
1	D	1490	LEU	2.3
1	B	639	TYR	2.3
1	D	1169	ALA	2.2
1	D	600	HIS	2.2
1	D	1436	LEU	2.2
1	D	492	ASP	2.2
1	B	1282	ARG	2.1
1	D	431	ILE	2.1
1	D	424	LYS	2.1
1	B	1449	LEU	2.1
1	D	612	ILE	2.1
1	D	469	LEU	2.1
1	B	1168	LEU	2.1
1	D	1300	THR	2.0
1	B	1439	ASP	2.0
1	D	495	LEU	2.0

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

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	5UA	E	1	21/21	0.86	0.15	-	36,40,52,57	0
2	5UA	F	1	21/21	0.56	0.33	-	68,72,84,85	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	RXV	F	1021[B]	33/33	0.93	0.18	2.11	33,40,43,46	33
4	RXV	F	1021[A]	33/33	0.93	0.18	2.11	34,43,45,47	33
3	MN	B	2492	1/1	0.99	0.20	1.92	53,53,53,53	0
3	MN	D	2491	1/1	1.00	0.05	-1.56	32,32,32,32	0
3	MN	B	2493	1/1	1.00	0.04	-5.36	31,31,31,31	0
3	MN	E	1022	1/1	0.97	0.06	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.