



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:44 PM GMT

PDB ID : 3RYT  
Title : The Plexin A1 intracellular region in complex with Rac1  
Authors : Zhang, X.; He, H.  
Deposited on : 2011-05-11  
Resolution : 3.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

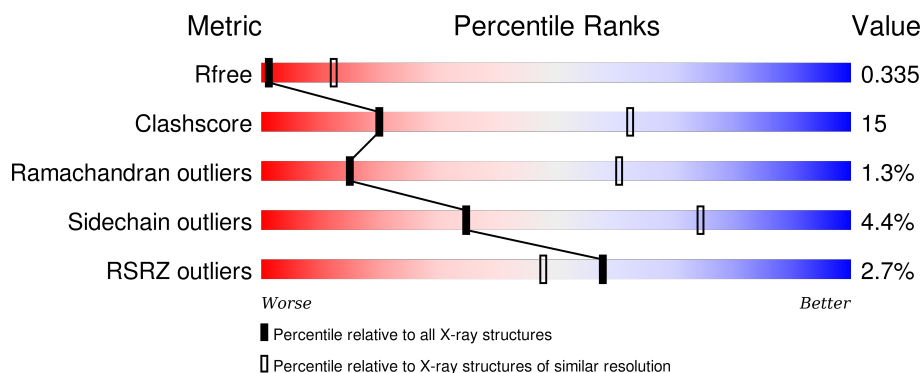
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.58 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	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

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	626	<div> <div>2%</div> <div>58%</div> <div>25%</div> <div>15%</div> </div>
1	B	626	<div> <div>2%</div> <div>64%</div> <div>19%</div> <div>15%</div> </div>
2	C	180	<div> <div>4%</div> <div>64%</div> <div>30%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9112 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 Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			3954	2533	663	737	21			
1	B	531	Total	C	N	O	S	0	0	0
			3852	2447	663	721	21			

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1273	820	208	239	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P63000
C	-1	PRO	-	EXPRESSION TAG	UNP P63000
C	0	HIS	-	EXPRESSION TAG	UNP P63000
C	61	LEU	GLN	ENGINEERED MUTATION	UNP P63000

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

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

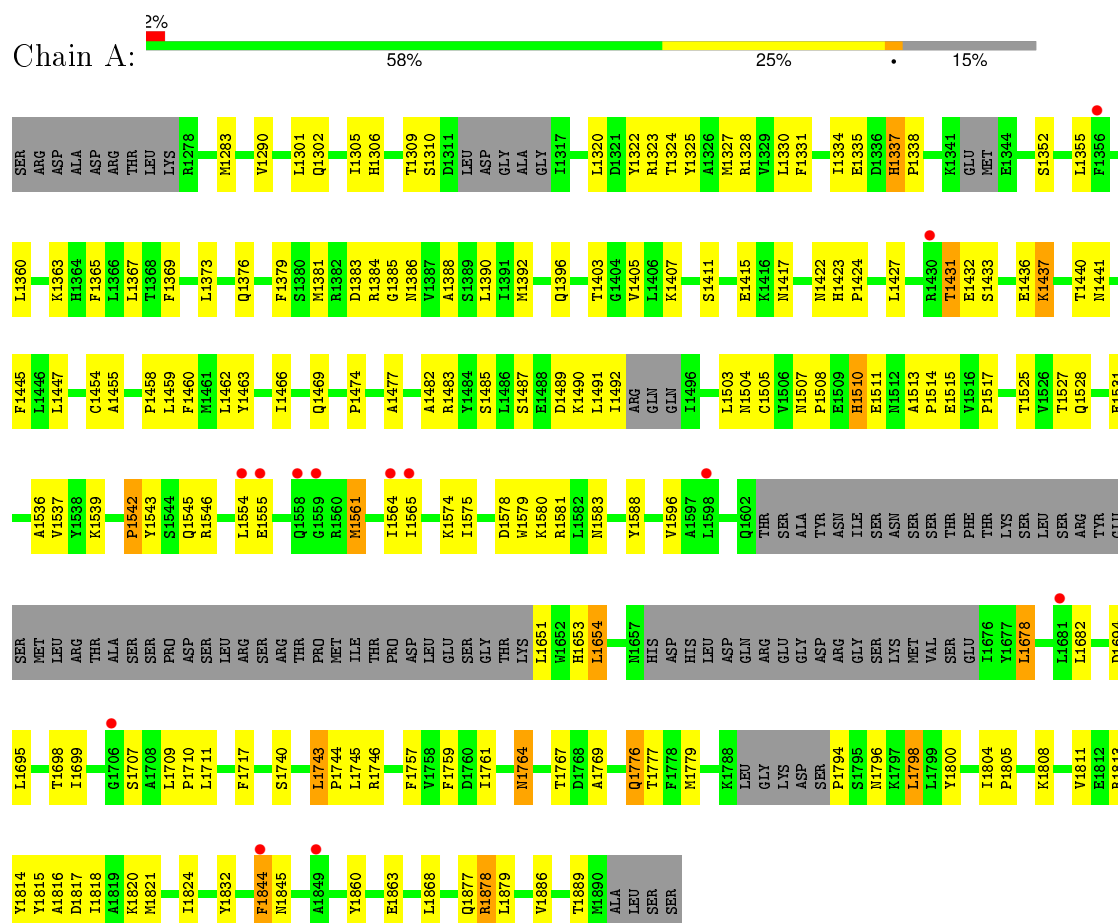


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

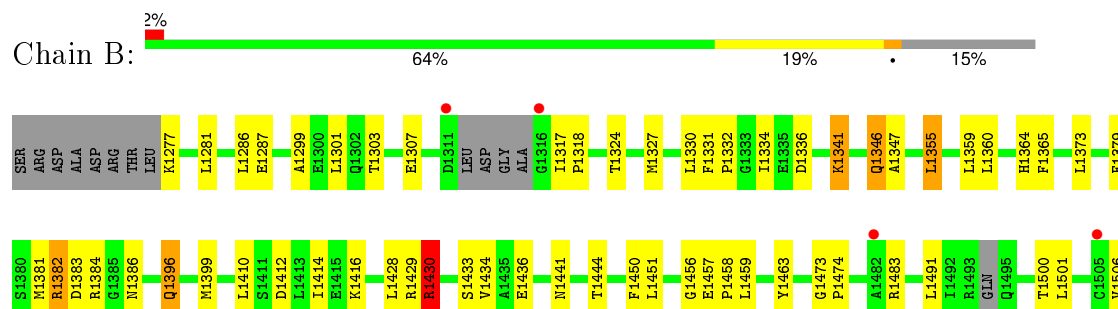
### 3 Residue-property plots

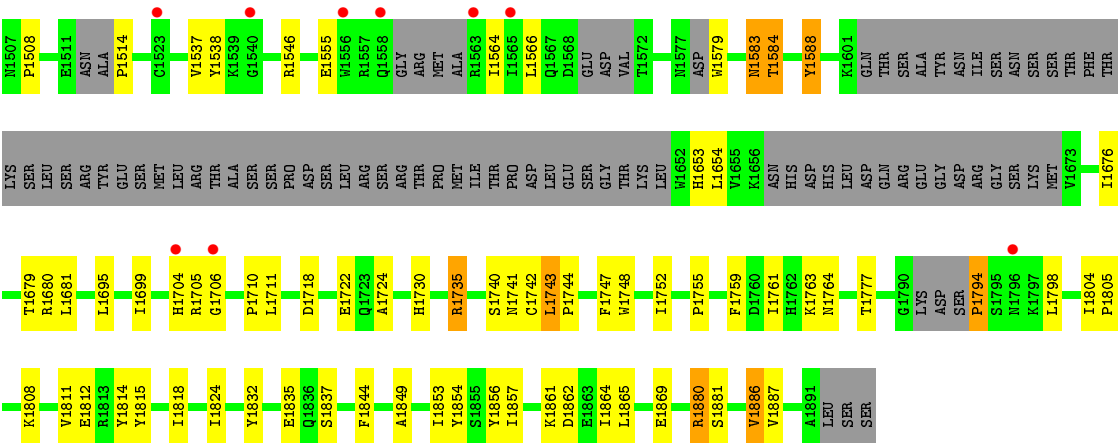
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Plexin-A1

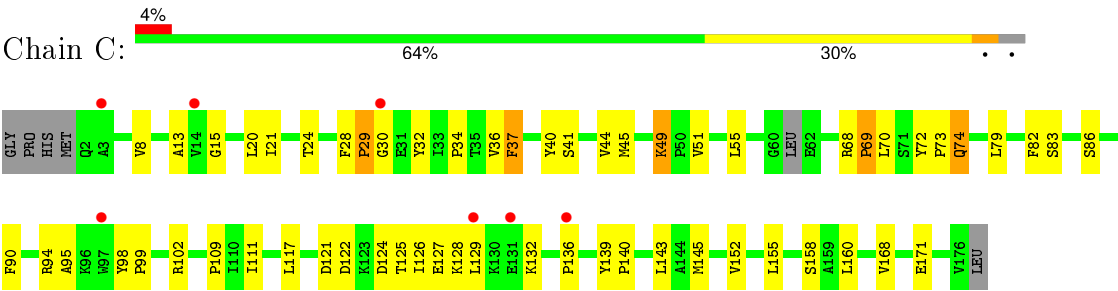


#### • Molecule 1: Plexin-A1





● Molecule 2: Ras-related C3 botulinum toxin substrate 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.78 Å 110.78 Å 265.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 3.58 49.54 – 3.58	Depositor EDS
% Data completeness (in resolution range)	91.4 (49.54-3.58) 91.4 (49.54-3.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 3.57 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.270 , 0.340 0.255 , 0.335	Depositor DCC
$R_{free}$ test set	901 reflections (4.77%)	DCC
Wilson B-factor (Å <sup>2</sup> )	126.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 183.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 20028 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.26	0/4029	0.37	1/5490 (0.0%)
1	B	0.29	0/3923	0.38	2/5351 (0.0%)
2	C	0.25	0/1302	0.38	0/1787
All	All	0.27	0/9254	0.38	3/12628 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1794	PRO	N-CA-CB	6.01	110.52	103.30
1	B	1514	PRO	N-CA-CB	5.93	110.42	103.30
1	B	1794	PRO	N-CA-CB	5.88	110.35	103.30

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	A	3954	0	3660	125	0
1	B	3852	0	3398	95	0
2	C	1273	0	1198	45	0
3	C	1	0	0	0	0
4	C	32	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9112	0	8269	258	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 15.

All (258) 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:1337:HIS:HB3	1:A:1338:PRO:HA	1.26	1.09
1:A:1743:LEU:HB3	1:A:1744:PRO:HD3	1.51	0.92
1:B:1373:LEU:HB3	1:B:1379:PHE:HZ	1.35	0.90
1:A:1580:LYS:HB3	1:A:1651:LEU:HG	1.54	0.89
1:A:1381:MET:HA	1:A:1384:ARG:HD3	1.58	0.85
1:A:1365:PHE:HB2	1:A:1879:LEU:HD11	1.59	0.84
1:A:1510:HIS:CD2	1:A:1513:ALA:HB3	2.12	0.84
1:B:1331:PHE:HB3	1:B:1334:ILE:HD12	1.59	0.82
1:A:1508:PRO:HD2	1:A:1537:VAL:HG11	1.63	0.81
1:A:1337:HIS:HB3	1:A:1338:PRO:CA	2.11	0.79
1:B:1373:LEU:HB3	1:B:1379:PHE:CZ	2.20	0.76
1:B:1711:LEU:HD22	1:B:1824:ILE:HD13	1.68	0.76
1:A:1474:PRO:HD2	1:A:1483:ARG:HB2	1.69	0.75
1:A:1477:ALA:HB2	1:A:1528:GLN:HE21	1.52	0.74
1:B:1341:LYS:H	1:B:1341:LYS:HD2	1.51	0.74
1:B:1346:GLN:HA	1:B:1346:GLN:HE21	1.54	0.72
2:C:8:VAL:HG21	2:C:20:LEU:HD21	1.72	0.72
2:C:45:MET:HG2	2:C:49:LYS:H	1.55	0.71
1:B:1743:LEU:HB3	1:B:1744:PRO:HD3	1.71	0.70
1:A:1440:THR:OG1	1:A:1746:ARG:HD3	1.91	0.70
1:A:1695:LEU:O	1:A:1699:ILE:HG13	1.92	0.69
1:B:1459:LEU:HD22	1:B:1759:PHE:HE2	1.57	0.69
1:A:1379:PHE:HB2	1:A:1383:ASP:HB2	1.75	0.69
1:A:1507:ASN:HB3	1:A:1510:HIS:CE1	2.28	0.68
1:A:1561:MET:CE	2:C:41:SER:HB2	2.25	0.67
1:A:1816:ALA:O	1:A:1820:LYS:HG2	1.96	0.66
1:B:1412:ASP:HB3	1:B:1416:LYS:HE3	1.76	0.66
1:B:1396:GLN:HE21	1:B:1396:GLN:HA	1.60	0.66
2:C:36:VAL:O	2:C:37:PHE:HB3	1.96	0.65
1:A:1513:ALA:HB1	1:A:1514:PRO:HD2	1.78	0.64
2:C:83:SER:HB3	2:C:86:SER:HB3	1.78	0.64
1:A:1365:PHE:HD1	1:A:1879:LEU:HD21	1.62	0.64
1:B:1382:ARG:HD3	1:B:1382:ARG:C	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1423:HIS:H	1:B:1303:THR:HG21	1.63	0.63
1:B:1755:PRO:HD2	1:B:1763:LYS:HD3	1.80	0.63
1:A:1525:THR:HB	1:A:1528:GLN:HG3	1.81	0.62
1:A:1525:THR:HG22	1:A:1527:THR:H	1.64	0.62
1:A:1800:TYR:O	1:A:1804:ILE:HG12	1.98	0.62
1:B:1832:TYR:O	1:B:1835:GLU:HG2	2.00	0.62
1:A:1808:LYS:O	1:A:1811:VAL:HG12	2.00	0.61
1:B:1491:LEU:HD12	1:B:1681:LEU:HD21	1.83	0.61
1:A:1776:GLN:HB3	1:A:1796:ASN:HD21	1.66	0.61
1:A:1423:HIS:H	1:B:1303:THR:CG2	2.14	0.60
1:A:1564:ILE:HG21	2:C:70:LEU:HB3	1.82	0.60
1:B:1724:ALA:HB1	1:B:1735:ARG:HD2	1.83	0.60
1:B:1428:LEU:O	1:B:1741:ASN:HB3	2.02	0.60
2:C:13:ALA:H	4:C:179:GNP:HNB3	1.49	0.59
1:A:1355:LEU:HD13	1:A:1886:VAL:HA	1.84	0.59
2:C:32:TYR:CE1	2:C:34:PRO:HD3	2.37	0.59
1:A:1337:HIS:CB	1:A:1338:PRO:HA	2.16	0.59
1:B:1346:GLN:HG3	1:B:1347:ALA:H	1.67	0.59
1:B:1330:LEU:HD22	1:B:1441:ASN:ND2	2.19	0.58
1:B:1814:TYR:O	1:B:1818:ILE:HG13	2.04	0.58
1:B:1584:THR:HG22	1:B:1653:HIS:CD2	2.39	0.58
1:B:1506:VAL:O	1:B:1508:PRO:HD3	2.03	0.58
1:A:1694:ASP:O	1:A:1698:THR:HG23	2.03	0.58
1:A:1555:GLU:HG2	1:A:1565:ILE:HG12	1.85	0.58
2:C:117:LEU:HB3	2:C:158:SER:HB2	1.85	0.58
1:B:1811:VAL:HG22	1:B:1815:TYR:CE2	2.38	0.58
1:B:1330:LEU:O	1:B:1332:PRO:HD3	2.03	0.58
1:A:1283:MET:SD	1:A:1798:LEU:HD22	2.45	0.57
1:A:1417:ASN:HB3	1:A:1427:LEU:HD22	1.86	0.57
1:B:1341:LYS:NZ	1:B:1341:LYS:HB3	2.20	0.57
1:A:1574:LYS:O	1:A:1581:ARG:HB3	2.05	0.56
1:B:1854:TYR:O	1:B:1857:ILE:HG22	2.04	0.56
1:B:1864:ILE:HG13	1:B:1865:LEU:N	2.20	0.56
1:A:1392:MET:HB3	1:A:1445:PHE:HE2	1.71	0.56
1:A:1561:MET:HE2	2:C:41:SER:HB2	1.88	0.56
2:C:21:ILE:HG21	2:C:29:PRO:HG3	1.87	0.56
1:A:1431:THR:HG23	1:A:1436:GLU:OE2	2.06	0.55
1:B:1653:HIS:ND1	1:B:1654:LEU:HG	2.21	0.55
1:A:1301:LEU:O	1:A:1305:ILE:HG22	2.06	0.55
1:A:1454:CYS:SG	1:A:1707:SER:HB2	2.46	0.55
2:C:95:ALA:O	2:C:99:PRO:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1777:THR:HG23	1:A:1804:ILE:HD11	1.89	0.55
1:A:1323:ARG:O	1:A:1327:MET:HG2	2.06	0.54
1:A:1328:ARG:NH2	1:A:1335:GLU:HG2	2.22	0.54
1:B:1711:LEU:HD12	1:B:1832:TYR:CB	2.38	0.54
1:B:1286:LEU:HD22	1:B:1679:THR:HB	1.89	0.54
2:C:155:LEU:HD13	2:C:168:VAL:HA	1.88	0.54
1:B:1379:PHE:HB2	1:B:1383:ASP:CB	2.38	0.54
1:A:1388:ALA:O	1:A:1392:MET:HG2	2.08	0.54
2:C:72:TYR:N	2:C:73:PRO:CD	2.71	0.53
1:A:1403:THR:O	1:A:1407:LYS:HG3	2.08	0.53
1:A:1460:PHE:HB2	1:A:1759:PHE:CZ	2.44	0.52
1:A:1583:ASN:HB3	1:A:1588:TYR:CE2	2.45	0.52
1:A:1814:TYR:O	1:A:1818:ILE:HG13	2.10	0.52
1:A:1543:TYR:C	1:A:1545:GLN:H	2.13	0.52
2:C:125:THR:O	2:C:129:LEU:HG	2.09	0.51
1:A:1561:MET:HE1	2:C:41:SER:HB2	1.92	0.51
1:A:1322:TYR:CE2	1:A:1844:PHE:HZ	2.29	0.51
2:C:139:TYR:HB3	2:C:140:PRO:HD3	1.93	0.51
1:B:1384:ARG:HH21	1:B:1433:SER:HB2	1.74	0.51
1:A:1542:PRO:O	1:A:1546:ARG:HG3	2.11	0.51
1:B:1444:THR:HA	1:B:1747:PHE:CE1	2.45	0.51
1:B:1555:GLU:HA	1:B:1564:ILE:O	2.11	0.51
1:A:1504:ASN:HB3	1:A:1515:GLU:HG3	1.92	0.51
2:C:20:LEU:HD22	2:C:55:LEU:HD13	1.93	0.51
2:C:109:PRO:HB3	2:C:152:VAL:HG21	1.93	0.51
1:B:1410:LEU:O	1:B:1414:ILE:HG13	2.11	0.51
1:B:1748:TRP:O	1:B:1752:ILE:HG13	2.12	0.50
1:B:1508:PRO:HD2	1:B:1537:VAL:HG11	1.93	0.50
1:B:1869:GLU:OE1	1:B:1880:ARG:HG2	2.11	0.50
1:A:1474:PRO:HD2	1:A:1483:ARG:CB	2.41	0.50
1:B:1459:LEU:HD22	1:B:1759:PHE:CE2	2.43	0.50
1:A:1320:LEU:HD22	1:A:1324:THR:HG21	1.92	0.50
1:B:1744:PRO:HA	1:B:1748:TRP:HB2	1.94	0.50
1:A:1510:HIS:CG	1:A:1511:GLU:N	2.80	0.50
1:A:1376:GLN:HE22	1:A:1860:TYR:HB3	1.77	0.49
1:B:1861:LYS:HG3	1:B:1862:ASP:N	2.28	0.49
1:A:1379:PHE:HB2	1:A:1383:ASP:CB	2.42	0.49
1:A:1305:ILE:O	1:A:1309:THR:HG22	2.13	0.49
1:A:1352:SER:HB3	1:A:1889:THR:HG22	1.94	0.49
1:B:1336:ASP:HA	1:B:1341:LYS:HE2	1.93	0.49
2:C:28:PHE:CD2	2:C:160:LEU:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1450:PHE:CD2	1:B:1710:PRO:HG3	2.48	0.49
1:A:1711:LEU:HD12	1:A:1832:TYR:CG	2.48	0.49
1:A:1330:LEU:HD11	1:A:1445:PHE:CZ	2.48	0.49
1:A:1536:ALA:O	1:A:1539:LYS:HG3	2.12	0.49
1:A:1360:LEU:HD23	1:A:1360:LEU:O	2.12	0.49
2:C:72:TYR:N	2:C:73:PRO:HD2	2.27	0.49
2:C:20:LEU:HD22	2:C:55:LEU:HB3	1.94	0.48
1:B:1740:SER:O	1:B:1744:PRO:HD2	2.13	0.48
2:C:32:TYR:CD2	4:C:179:GNP:H5'1	2.47	0.48
1:A:1776:GLN:HB3	1:A:1796:ASN:ND2	2.27	0.48
1:A:1459:LEU:HD22	1:A:1759:PHE:HE2	1.78	0.48
1:B:1444:THR:HA	1:B:1747:PHE:HE1	1.78	0.48
1:A:1331:PHE:HB3	1:A:1334:ILE:HG13	1.94	0.48
1:A:1437:LYS:O	1:A:1437:LYS:HE2	2.14	0.48
1:B:1360:LEU:HD23	1:B:1360:LEU:O	2.13	0.48
2:C:15:GLY:HA2	4:C:179:GNP:H8	1.96	0.48
1:A:1322:TYR:HE2	1:A:1844:PHE:HZ	1.59	0.48
1:B:1473:GLY:HA3	1:B:1483:ARG:HB3	1.95	0.48
1:B:1695:LEU:O	1:B:1699:ILE:HG13	2.13	0.48
2:C:44:VAL:O	2:C:51:VAL:HG22	2.13	0.47
1:B:1864:ILE:HG13	1:B:1865:LEU:H	1.79	0.47
1:B:1676:ILE:O	1:B:1680:ARG:HG2	2.13	0.47
1:B:1277:LYS:O	1:B:1281:LEU:HG	2.13	0.47
1:A:1764:ASN:ND2	1:A:1767:THR:H	2.12	0.47
1:A:1505:CYS:HA	1:A:1596:VAL:O	2.15	0.47
1:A:1743:LEU:HB3	1:A:1744:PRO:CD	2.34	0.47
1:A:1365:PHE:CD1	1:A:1879:LEU:HD21	2.47	0.47
1:B:1704:HIS:CG	1:B:1705:ARG:H	2.33	0.47
1:A:1503:LEU:O	1:A:1517:PRO:HA	2.15	0.47
1:A:1507:ASN:HB3	1:A:1510:HIS:ND1	2.30	0.46
1:B:1396:GLN:CA	1:B:1396:GLN:HE21	2.26	0.46
1:A:1385:GLY:HA2	1:A:1437:LYS:HD3	1.97	0.46
1:B:1711:LEU:HD12	1:B:1832:TYR:CG	2.50	0.46
1:A:1373:LEU:HB3	1:A:1379:PHE:CE2	2.51	0.46
2:C:139:TYR:HE1	2:C:143:LEU:HD22	1.80	0.46
1:A:1302:GLN:HA	1:A:1305:ILE:HG22	1.96	0.46
1:A:1490:LYS:HD2	1:A:1769:ALA:CB	2.45	0.46
1:B:1463:TYR:CZ	1:B:1761:ILE:HD12	2.51	0.46
1:A:1510:HIS:NE2	1:A:1513:ALA:HB3	2.31	0.46
1:B:1355:LEU:CB	1:B:1886:VAL:HG13	2.46	0.46
1:B:1299:ALA:O	1:B:1303:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1566:LEU:HD22	1:B:1588:TYR:CZ	2.51	0.46
1:B:1324:THR:HG22	1:B:1324:THR:O	2.16	0.46
1:A:1717:PHE:HE2	1:A:1815:TYR:CD1	2.34	0.46
1:B:1500:THR:C	1:B:1501:LEU:HD12	2.36	0.46
1:B:1849:ALA:O	1:B:1853:ILE:HG13	2.16	0.46
2:C:24:THR:HG21	2:C:40:TYR:HB3	1.98	0.46
1:A:1463:TYR:CZ	1:A:1761:ILE:HD12	2.50	0.46
2:C:44:VAL:HG12	2:C:45:MET:N	2.31	0.46
1:A:1528:GLN:HE22	1:A:1653:HIS:CE1	2.33	0.46
1:A:1653:HIS:ND1	1:A:1654:LEU:HD22	2.32	0.45
2:C:124:ASP:O	2:C:127:GLU:HB3	2.15	0.45
1:A:1369:PHE:O	1:A:1373:LEU:HG	2.16	0.45
1:A:1392:MET:HB3	1:A:1445:PHE:CE2	2.52	0.45
1:A:1485:SER:HB3	1:A:1491:LEU:HA	1.98	0.45
1:A:1320:LEU:HD12	1:A:1757:PHE:O	2.17	0.45
1:A:1363:LYS:O	1:A:1367:LEU:HG	2.16	0.45
1:B:1428:LEU:HD13	1:B:1742:CYS:SG	2.57	0.45
2:C:20:LEU:CD2	2:C:55:LEU:HD13	2.47	0.45
1:A:1441:ASN:N	1:A:1441:ASN:HD22	2.14	0.45
1:B:1886:VAL:HG12	1:B:1887:VAL:N	2.32	0.45
1:B:1451:LEU:O	1:B:1456:GLY:HA3	2.17	0.45
1:B:1808:LYS:O	1:B:1811:VAL:HG12	2.17	0.45
1:B:1880:ARG:HG3	1:B:1881:SER:N	2.32	0.45
1:A:1360:LEU:HA	1:A:1365:PHE:CD2	2.52	0.45
1:A:1554:LEU:HD11	1:A:1596:VAL:HG11	1.98	0.45
2:C:68:ARG:HB3	2:C:69:PRO:HD3	1.99	0.44
1:B:1704:HIS:CG	1:B:1705:ARG:N	2.85	0.44
1:A:1709:LEU:HD12	1:A:1710:PRO:HD2	1.99	0.44
2:C:155:LEU:HD11	2:C:171:GLU:HB2	1.99	0.44
1:A:1462:LEU:O	1:A:1466:ILE:HG12	2.17	0.44
1:A:1320:LEU:HD13	1:A:1324:THR:HG22	1.99	0.44
1:B:1705:ARG:HA	1:B:1706:GLY:HA2	1.53	0.44
2:C:82:PHE:CE2	2:C:90:PHE:HD1	2.36	0.44
2:C:37:PHE:CG	2:C:37:PHE:O	2.71	0.44
1:A:1386:ASN:O	1:A:1390:LEU:HG	2.17	0.44
1:A:1432:GLU:OE2	1:A:1432:GLU:HA	2.17	0.44
1:B:1359:LEU:O	1:B:1365:PHE:CD1	2.71	0.44
1:A:1423:HIS:HB2	1:B:1303:THR:HB	1.99	0.44
1:A:1868:LEU:HD22	1:A:1879:LEU:HD22	2.00	0.43
2:C:44:VAL:HG12	2:C:45:MET:H	1.84	0.43
1:B:1301:LEU:HD23	1:B:1301:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1538:TYR:HB2	1:B:1546:ARG:HD3	2.00	0.43
1:B:1869:GLU:HG3	1:B:1869:GLU:O	2.18	0.43
1:A:1817:ASP:O	1:A:1821:MET:HG3	2.19	0.43
1:B:1584:THR:HG22	1:B:1653:HIS:NE2	2.34	0.43
1:B:1396:GLN:O	1:B:1837:SER:HB2	2.18	0.43
1:A:1455:ALA:O	1:A:1458:PRO:HD2	2.19	0.43
1:A:1651:LEU:HD12	1:A:1651:LEU:N	2.33	0.43
1:A:1740:SER:O	1:A:1744:PRO:HD2	2.19	0.42
1:A:1580:LYS:O	1:A:1651:LEU:HA	2.19	0.42
1:B:1399:MET:HB2	1:B:1837:SER:HB3	2.00	0.42
2:C:129:LEU:HD13	2:C:136:PRO:HG3	2.01	0.42
1:B:1869:GLU:HA	1:B:1869:GLU:OE1	2.19	0.42
1:A:1678:LEU:HD12	1:A:1682:LEU:CD1	2.49	0.42
1:A:1411:SER:O	1:A:1415:GLU:HG2	2.19	0.42
1:B:1428:LEU:HD23	1:B:1436:GLU:OE2	2.19	0.42
1:A:1330:LEU:HD22	1:A:1441:ASN:CG	2.40	0.42
2:C:68:ARG:N	2:C:69:PRO:CD	2.82	0.42
1:A:1305:ILE:HG23	1:A:1306:HIS:N	2.34	0.42
1:A:1306:HIS:O	1:A:1310:SER:N	2.45	0.42
1:B:1566:LEU:HD22	1:B:1588:TYR:CE1	2.53	0.42
1:A:1373:LEU:HD22	1:A:1860:TYR:HD2	1.85	0.42
2:C:98:TYR:HE1	2:C:102:ARG:HH11	1.68	0.42
1:A:1745:LEU:HD21	1:A:1779:MET:HA	2.01	0.42
1:A:1528:GLN:O	1:A:1531:GLU:HB2	2.19	0.42
1:A:1804:ILE:N	1:A:1805:PRO:CD	2.82	0.42
1:A:1290:VAL:O	1:A:1290:VAL:HG12	2.19	0.42
1:A:1877:GLN:O	1:A:1878:ARG:C	2.58	0.42
1:A:1490:LYS:HD2	1:A:1769:ALA:HB2	2.01	0.42
1:A:1487:SER:C	1:A:1489:ASP:H	2.24	0.42
1:B:1777:THR:HG23	1:B:1804:ILE:HD11	2.01	0.42
1:A:1653:HIS:C	1:A:1654:LEU:HD13	2.41	0.41
1:B:1384:ARG:HB3	1:B:1434:VAL:HG22	2.01	0.41
1:A:1367:LEU:CD2	1:A:1405:VAL:HG13	2.50	0.41
2:C:94:ARG:HE	2:C:145:MET:HE1	1.85	0.41
2:C:74:GLN:HE21	2:C:74:GLN:HB2	1.72	0.41
1:A:1463:TYR:CE1	1:A:1761:ILE:HD12	2.54	0.41
2:C:79:LEU:CD2	2:C:111:ILE:HB	2.50	0.41
1:B:1794:PRO:O	1:B:1798:LEU:HB2	2.20	0.41
1:A:1711:LEU:HD22	1:A:1824:ILE:HD11	2.03	0.41
1:B:1724:ALA:HB3	1:B:1735:ARG:HH11	1.85	0.41
2:C:68:ARG:O	2:C:70:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:PRO:O	1:A:1427:LEU:HG	2.21	0.41
2:C:139:TYR:N	2:C:140:PRO:CD	2.84	0.41
1:B:1317:ILE:HA	1:B:1318:PRO:HD3	1.84	0.41
2:C:128:LYS:O	2:C:132:LYS:HG3	2.21	0.41
1:A:1417:ASN:O	1:A:1422:ASN:HB2	2.20	0.41
1:B:1457:GLU:N	1:B:1458:PRO:HD2	2.35	0.41
1:A:1482:ALA:N	1:A:1492:ILE:HG13	2.35	0.41
2:C:122:ASP:O	2:C:126:ILE:HG12	2.20	0.41
1:A:1376:GLN:NE2	1:A:1863:GLU:HB2	2.36	0.41
1:B:1441:ASN:N	1:B:1441:ASN:HD22	2.19	0.41
1:A:1469:GLN:NE2	1:A:1469:GLN:HA	2.36	0.41
1:B:1808:LYS:O	1:B:1812:GLU:HG3	2.21	0.40
1:B:1474:PRO:HD2	1:B:1483:ARG:HB2	2.01	0.40
1:B:1583:ASN:HB3	1:B:1588:TYR:HE2	1.85	0.40
1:B:1382:ARG:HD3	1:B:1383:ASP:N	2.36	0.40
1:A:1447:LEU:HD11	1:A:1743:LEU:HD11	2.04	0.40
1:B:1718:ASP:O	1:B:1722:GLU:HG3	2.22	0.40
1:B:1384:ARG:HH21	1:B:1433:SER:CB	2.33	0.40
1:B:1804:ILE:N	1:B:1805:PRO:CD	2.85	0.40
1:B:1429:ARG:O	1:B:1430:ARG:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/626 (83%)	455 (88%)	56 (11%)	7 (1%)	14	59
1	B	511/626 (82%)	460 (90%)	46 (9%)	5 (1%)	19	66
2	C	170/180 (94%)	149 (88%)	17 (10%)	4 (2%)	7	49
All	All	1199/1432 (84%)	1064 (89%)	119 (10%)	16 (1%)	15	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	29	PRO
1	A	1575	ILE
1	B	1430	ARG
1	B	1583	ASN
2	C	37	PHE
1	A	1578	ASP
1	B	1584	THR
1	A	1433	SER
1	A	1845	ASN
1	B	1355	LEU
1	B	1743	LEU
1	A	1337	HIS
1	A	1542	PRO
2	C	30	GLY
1	A	1743	LEU
2	C	69	PRO

### 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	383/563 (68%)	368 (96%)	15 (4%)	39	76
1	B	350/563 (62%)	330 (94%)	20 (6%)	25	67
2	C	127/155 (82%)	124 (98%)	3 (2%)	57	85
All	All	860/1281 (67%)	822 (96%)	38 (4%)	35	74

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1325	TYR
1	A	1396	GLN
1	A	1431	THR
1	A	1437	LYS
1	A	1510	HIS

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Mol	Chain	Res	Type
1	A	1561	MET
1	A	1579	TRP
1	A	1654	LEU
1	A	1678	LEU
1	A	1764	ASN
1	A	1776	GLN
1	A	1798	LEU
1	A	1813	ARG
1	A	1844	PHE
1	A	1878	ARG
1	B	1287	GLU
1	B	1307	GLU
1	B	1327	MET
1	B	1341	LYS
1	B	1346	GLN
1	B	1364	HIS
1	B	1381	MET
1	B	1382	ARG
1	B	1386	ASN
1	B	1396	GLN
1	B	1430	ARG
1	B	1579	TRP
1	B	1588	TYR
1	B	1730	HIS
1	B	1735	ARG
1	B	1764	ASN
1	B	1844	PHE
1	B	1856	TYR
1	B	1880	ARG
1	B	1886	VAL
2	C	49	LYS
2	C	74	GLN
2	C	121	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1358	GLN
1	A	1376	GLN
1	A	1441	ASN
1	A	1468	GLN
1	A	1469	GLN

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Mol	Chain	Res	Type
1	A	1528	GLN
1	A	1545	GLN
1	A	1583	ASN
1	A	1589	GLN
1	A	1602	GLN
1	A	1723	GLN
1	A	1727	HIS
1	A	1764	ASN
1	A	1776	GLN
1	A	1836	GLN
1	A	1845	ASN
1	B	1346	GLN
1	B	1376	GLN
1	B	1386	ASN
1	B	1396	GLN
1	B	1441	ASN
1	B	1468	GLN
1	B	1469	GLN
1	B	1545	GLN
1	B	1689	GLN
1	B	1723	GLN
1	B	1762	HIS
1	B	1764	ASN
1	B	1836	GLN
1	B	1845	ASN
2	C	74	GLN
2	C	104	HIS
2	C	107	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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$
4	GNP	C	179	3	28,34,34	1.87	6 (21%)	33,54,54	2.43	7 (21%)

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	GNP	C	179	3	-	0/12/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	179	GNP	PB-O3A	-5.22	1.52	1.59
4	C	179	GNP	PB-O2B	-2.98	1.48	1.56
4	C	179	GNP	C8-N7	-2.02	1.30	1.34
4	C	179	GNP	PB-O1B	2.02	1.48	1.46
4	C	179	GNP	C6-N1	3.51	1.39	1.33
4	C	179	GNP	PG-O1G	4.56	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	179	GNP	C5-C6-N1	-8.72	111.66	123.59
4	C	179	GNP	PA-O3A-PB	-3.71	120.23	132.67
4	C	179	GNP	O3G-PG-O1G	-3.43	104.38	113.49
4	C	179	GNP	N3-C2-N1	-2.22	124.06	127.44
4	C	179	GNP	O3G-PG-O2G	2.93	116.28	107.58
4	C	179	GNP	O2B-PB-O1B	3.99	118.33	110.00
4	C	179	GNP	C6-N1-C2	6.41	124.84	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	179	GNP	3	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	532/626 (84%)	-0.12	13 (2%)	62 52	88, 179, 275, 337	0
1	B	531/626 (84%)	-0.04	13 (2%)	62 52	126, 216, 304, 371	0
2	C	174/180 (96%)	0.14	7 (4%)	42 33	92, 183, 346, 410	7 (4%)
All	All	1237/1432 (86%)	-0.05	33 (2%)	58 48	88, 196, 302, 410	7 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	30	GLY	5.6
1	A	1555	GLU	4.4
1	B	1316	GLY	4.1
1	A	1564	ILE	4.1
1	A	1844	PHE	3.8
1	A	1849	ALA	3.8
1	B	1706	GLY	3.8
1	B	1796	ASN	3.4
1	A	1706	GLY	3.3
1	A	1565	ILE	3.2
1	B	1565	ILE	2.9
1	B	1558	GLN	2.9
1	A	1356	PHE	2.9
1	A	1598	LEU	2.9
1	A	1559	GLY	2.4
1	B	1523	CYS	2.4
1	B	1311	ASP	2.4
1	A	1681	LEU	2.4
1	B	1505	CYS	2.4
1	B	1563	ARG	2.3
2	C	14	VAL	2.3
1	B	1704	HIS	2.2
1	A	1430	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1556	TRP	2.2
1	A	1554	LEU	2.2
2	C	131	GLU	2.2
2	C	136	PRO	2.1
2	C	3	ALA	2.1
2	C	97	TRP	2.0
2	C	129	LEU	2.0
1	A	1558	GLN	2.0
1	B	1540	GLY	2.0
1	B	1482	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GNP	C	179	32/32	0.94	0.18	-0.89	126,165,181,392	0
3	MG	C	178	1/1	0.96	0.18	-1.77	148,148,148,148	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.