Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:53 am BST

PDB ID	:	2OQV
Title	:	Human Dipeptidyl Peptidase IV (DPP4) with piperidine-constrained phenethylamine
Authors	:	Pei, Z.; Li, X.; von Geldern, T.W.; Longenecker, K.L.; Pireh, D.; Stewart, K.D.
Deposited on	:	2007-02-01
Resolution	:	2.80 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:

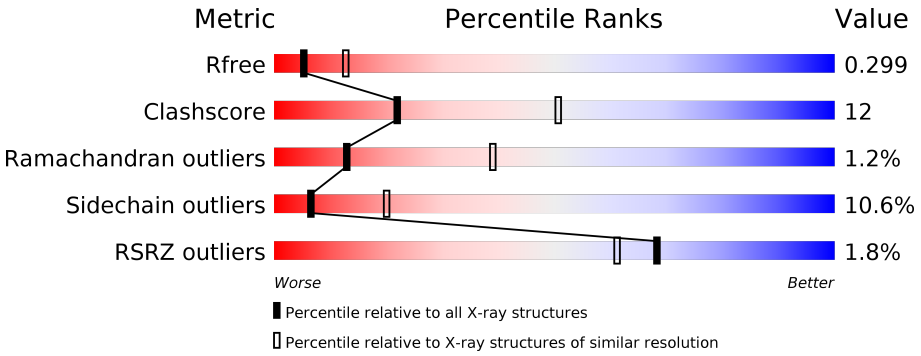
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	726	2% 71% 24% 5%
1	B	726	2% 73% 22%

2 Entry composition

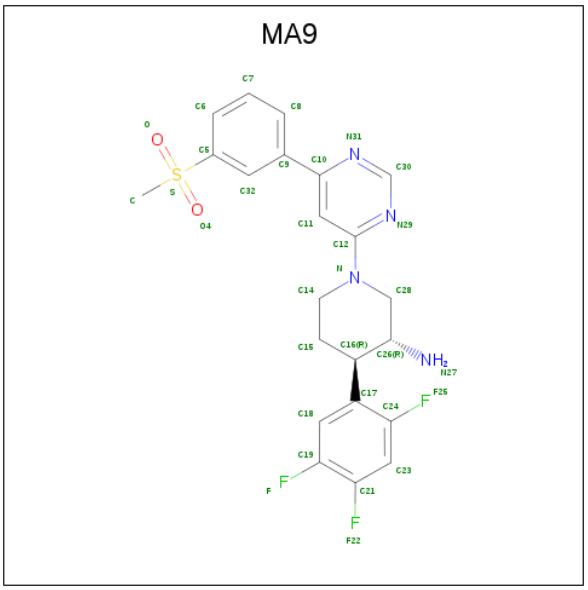
There are 2 unique types of molecules in this entry. The entry contains 11930 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	B	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			

- Molecule 2 is (3R,4R)-1-{6-[3-(METHYLSULFONYL)PHENYL]PYRIMIDIN-4-YL}-4-(2,4,5-TRIFLUOROPHENYL)PIPERIDIN-3-AMINE (three-letter code: MA9) (formula: $C_{22}H_{21}F_3N_4O_2S$).



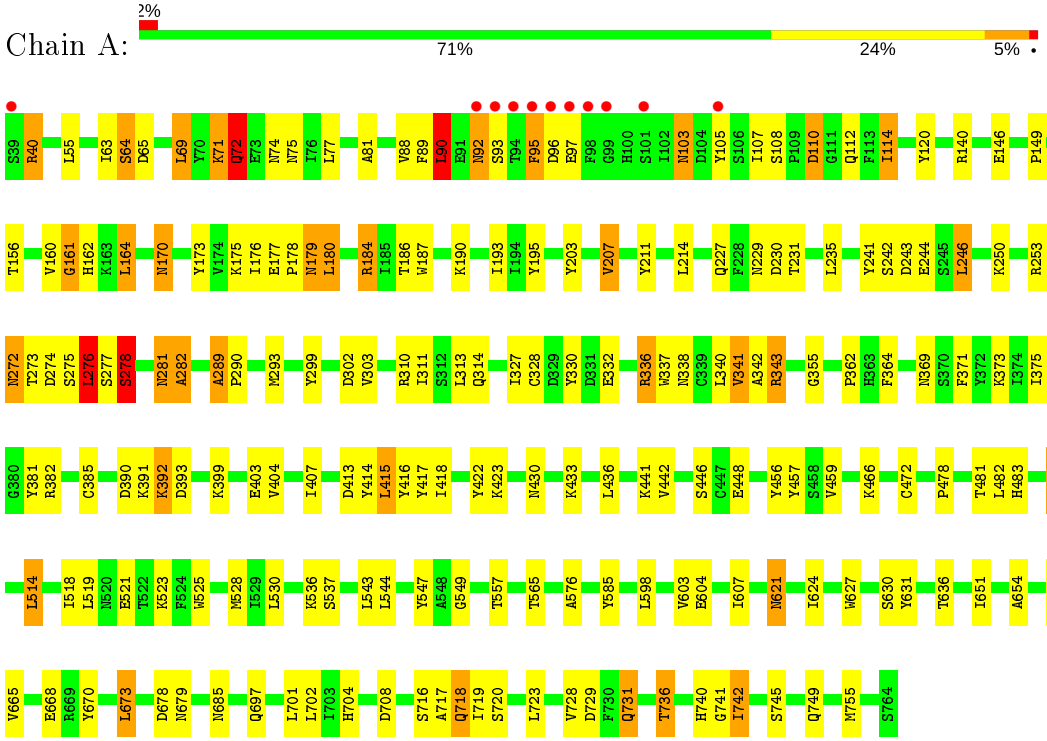
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			32	22	3	4	2	1		

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.

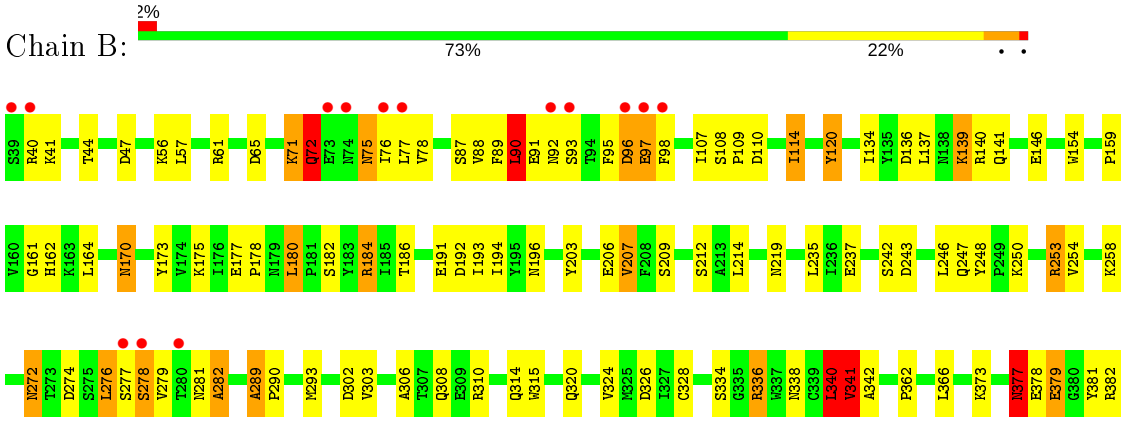
- Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV)

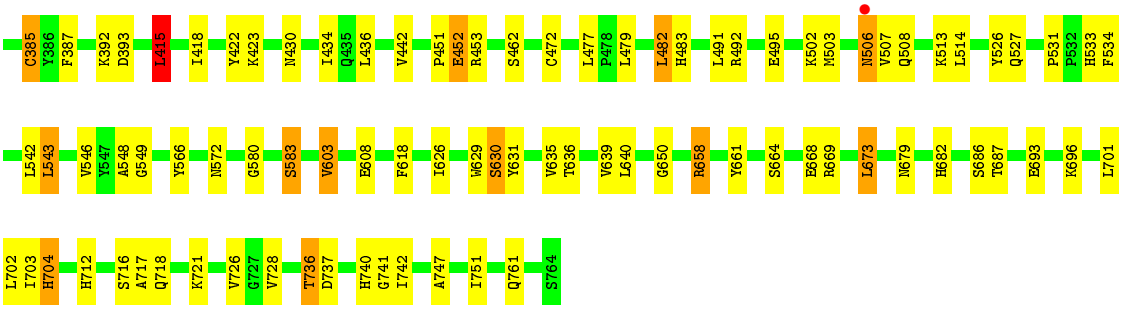
Chain A:



- Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV)

Chain B:




C385 Y386 F387 K392 D393 L415 I418 Y422 K423 N430 I434 Q435 L436 V442 P451 E452 R453 S462 C472 L477 P478 L479 L492 H493 L491 R492 E495 K502 M503 N506 V507 Q508 K513 L514 Y526 Q527 P531 P532 H533 F534
L542 L543 V546 Y547 A548 G549 Y566 N572 G580 S583 V603 E608 F618 I626 W629 S630 Y631 V635 T636 V639 L640 G650 R658 Y661 S664 E668 R669 L673 N679 H682 S686 T687 E693 K696 L701
L702 I703 H704 H712 S716 A717 Q718 K721 V726 G727 V728 T736 D737 H740 G741 I742 A747 I751 Q761 S764

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.01Å 118.20Å 232.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.80 45.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.2 (119.52-2.80) 82.1 (45.90-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.243 , 0.309 0.235 , 0.299	Depositor DCC
R_{free} test set	1884 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 20.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	11930	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MA9

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	0.62	0/6120	0.72	2/8321 (0.0%)
1	B	0.62	0/6120	0.73	4/8321 (0.0%)
All	All	0.62	0/12240	0.73	6/16642 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	LEU	CA-CB-CG	6.07	129.27	115.30
1	B	114	ILE	CB-CA-C	-5.86	99.88	111.60
1	A	276	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	90	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	340	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	415	LEU	CA-CB-CG	5.38	127.68	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	GLN	Peptide

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	5949	0	5667	143	0
1	B	5949	0	5667	138	0
2	A	32	0	21	1	0
All	All	11930	0	11355	274	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 12.

All (274) 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:289:ALA:HB1	1:B:290:PRO:HA	1.36	1.07
1:B:136:ASP:OD2	1:B:139:LYS:HG2	1.63	0.97
1:A:731:GLN:HE21	1:A:731:GLN:HA	1.32	0.95
1:A:272:ASN:ND2	1:A:274:ASP:H	1.65	0.93
1:B:630:SER:HG	1:B:740:HIS:HE2	0.92	0.90
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.01	0.89
1:B:289:ALA:CB	1:B:290:PRO:HA	2.05	0.86
1:A:107:ILE:HG13	1:A:114:ILE:HG23	1.59	0.85
1:A:407:ILE:HG23	1:A:415:LEU:HD11	1.59	0.84
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.44	0.83
1:A:272:ASN:HD22	1:A:274:ASP:H	1.25	0.81
1:A:630:SER:OG	1:A:740:HIS:NE2	2.13	0.81
1:A:93:SER:HA	1:A:96:ASP:OD2	1.83	0.79
1:A:40:ARG:HE	1:A:508:GLN:HG2	1.49	0.77
1:B:237:GLU:HG2	1:B:253:ARG:HB2	1.67	0.76
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.16	0.76
1:A:281:ASN:O	1:A:282:ALA:HB3	1.86	0.75
1:B:272:ASN:HD22	1:B:274:ASP:H	1.34	0.75
1:A:55:LEU:HD21	1:A:478:PRO:HG2	1.69	0.75
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.67	0.75
1:A:281:ASN:O	1:A:282:ALA:CB	2.34	0.74
1:B:184:ARG:HD3	1:B:186:THR:O	1.87	0.73
1:A:110:ASP:HB3	1:A:112:GLN:HG3	1.70	0.73
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLN:HE21	1:A:731:GLN:CA	2.01	0.71
1:B:508:GLN:OE1	1:B:533:HIS:CE1	2.44	0.71
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.73	0.71
1:A:277:SER:O	1:A:278:SER:HB3	1.90	0.71
1:A:184:ARG:HD3	1:A:186:THR:O	1.91	0.70
1:A:731:GLN:NE2	1:A:731:GLN:HA	2.07	0.69
1:B:237:GLU:HG2	1:B:253:ARG:CB	2.22	0.69
1:A:71:LYS:O	1:A:72:GLN:HG3	1.92	0.69
1:B:718:GLN:NE2	1:B:718:GLN:HA	2.08	0.68
1:A:103:ASN:OD1	1:A:120:TYR:HB2	1.94	0.68
1:A:377:ASN:HB3	1:A:379:GLU:H	1.60	0.67
1:B:503:MET:O	1:B:506:ASN:ND2	2.27	0.67
1:B:77:LEU:HD23	1:B:88:VAL:HA	1.75	0.67
1:A:704:HIS:HD2	1:A:716:SER:OG	1.79	0.66
1:B:415:LEU:HB3	1:B:434:ILE:HG23	1.78	0.65
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.31	0.65
1:A:272:ASN:C	1:A:272:ASN:HD22	2.00	0.65
1:A:723:LEU:HD22	1:A:728:VAL:HG11	1.78	0.65
1:A:448:GLU:OE2	1:A:448:GLU:HA	1.96	0.65
1:A:40:ARG:NE	1:A:508:GLN:HG2	2.12	0.65
1:B:704:HIS:HD2	1:B:716:SER:HB2	1.62	0.64
1:B:747:ALA:O	1:B:751:ILE:HG22	1.98	0.64
1:B:219:ASN:HB3	1:B:308:GLN:NE2	2.13	0.63
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.96	0.62
1:B:97:GLU:O	1:B:97:GLU:HG3	1.99	0.62
1:A:377:ASN:HB2	1:A:381:TYR:H	1.63	0.62
1:A:92:ASN:N	1:A:92:ASN:HD22	1.98	0.61
1:B:114:ILE:CG1	1:B:137:LEU:HD21	2.31	0.61
1:B:508:GLN:OE1	1:B:533:HIS:HE1	1.83	0.61
1:B:139:LYS:HD3	1:B:141:GLN:HE21	1.66	0.60
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.36	0.60
1:B:175:LYS:HE3	1:B:180:LEU:O	2.01	0.60
1:B:206:GLU:OE1	1:B:206:GLU:HA	2.01	0.60
1:B:664:SER:O	1:B:668:GLU:HB2	2.01	0.60
1:B:580:GLY:O	1:B:583:SER:HB3	2.02	0.60
1:B:451:PRO:HG2	1:B:452:GLU:OE2	2.02	0.59
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.84	0.59
1:A:242:SER:OG	1:A:243:ASP:N	2.35	0.58
1:A:63:ILE:HG21	1:A:69:LEU:HD11	1.85	0.58
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.02	0.58
1:A:179:ASN:ND2	1:A:180:LEU:HD13	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:SER:HA	1:B:96:ASP:OD1	2.03	0.58
1:B:341:VAL:O	1:B:342:ALA:HB3	2.03	0.58
1:A:258:LYS:HD2	1:B:247:GLN:HG2	1.86	0.57
1:A:289:ALA:CB	1:A:290:PRO:CA	2.82	0.57
1:A:289:ALA:CB	1:A:290:PRO:HA	2.33	0.57
1:B:293:MET:HE2	1:B:324:VAL:HG23	1.86	0.57
1:A:621:ASN:HB3	1:A:624:ILE:HD11	1.87	0.57
1:A:407:ILE:HG23	1:A:415:LEU:CD1	2.31	0.57
1:B:290:PRO:HD2	1:B:315:TRP:CD1	2.39	0.57
1:B:718:GLN:CA	1:B:718:GLN:HE21	2.15	0.57
1:B:293:MET:CE	1:B:324:VAL:HG23	2.35	0.57
1:A:708:ASP:OD2	1:A:740:HIS:HA	2.04	0.57
1:B:281:ASN:O	1:B:282:ALA:HB3	2.05	0.56
1:B:146:GLU:O	1:B:175:LYS:HE2	2.04	0.56
1:A:720:SER:OG	1:B:736:THR:CG2	2.54	0.56
1:A:340:LEU:O	1:A:343:ARG:HB2	2.05	0.56
1:A:377:ASN:HB2	1:A:381:TYR:N	2.20	0.56
1:A:310:ARG:NH2	1:A:369:ASN:ND2	2.54	0.56
1:A:456:TYR:HB2	1:A:557:THR:OG1	2.05	0.56
1:A:657:SER:HB3	1:A:719:ILE:HD11	1.88	0.56
1:B:56:LYS:HD2	1:B:495:GLU:OE2	2.05	0.56
1:A:164:LEU:HB2	1:A:175:LYS:HB3	1.88	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.87	0.56
1:B:491:LEU:HB3	1:B:492:ARG:NH1	2.20	0.55
1:A:518:ILE:O	1:A:519:LEU:HD23	2.06	0.55
1:B:703:ILE:HG21	1:B:751:ILE:HD12	1.89	0.55
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.88	0.55
1:B:415:LEU:HB3	1:B:434:ILE:CG2	2.37	0.55
1:B:281:ASN:O	1:B:282:ALA:CB	2.55	0.55
1:A:175:LYS:HE3	1:A:178:PRO:O	2.07	0.54
1:A:544:LEU:HD12	1:A:576:ALA:O	2.07	0.54
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.72	0.54
1:A:289:ALA:HB1	1:A:290:PRO:C	2.28	0.54
1:A:731:GLN:NE2	1:A:731:GLN:CA	2.70	0.53
1:A:341:VAL:O	1:A:342:ALA:HB3	2.09	0.53
1:B:661:TYR:OH	1:B:718:GLN:HG3	2.09	0.53
1:A:377:ASN:HB3	1:A:379:GLU:N	2.23	0.53
1:B:191:GLU:O	1:B:192:ASP:HB2	2.08	0.53
1:B:219:ASN:HB3	1:B:308:GLN:HE22	1.74	0.52
1:A:179:ASN:HD21	1:A:180:LEU:HD13	1.73	0.52
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PRO:HD2	1:B:161:GLY:O	2.09	0.52
1:B:668:GLU:HG2	1:B:673:LEU:HD12	1.92	0.52
1:A:390:ASP:O	1:A:391:LYS:HG3	2.10	0.52
1:B:71:LYS:O	1:B:72:GLN:HG2	2.10	0.52
1:B:136:ASP:OD2	1:B:139:LYS:CG	2.48	0.52
1:A:281:ASN:N	1:A:281:ASN:OD1	2.39	0.52
1:A:177:GLU:HB2	1:A:180:LEU:HB2	1.92	0.52
1:A:736:THR:HG21	1:B:717:ALA:O	2.10	0.52
1:B:453:ARG:HH21	1:B:477:LEU:HB2	1.75	0.52
1:A:328:CYS:HA	1:A:338:ASN:O	2.09	0.51
1:A:418:ILE:HA	1:A:430:ASN:O	2.10	0.51
1:B:704:HIS:HD2	1:B:716:SER:CB	2.23	0.51
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.93	0.51
1:B:630:SER:HG	1:B:740:HIS:CE1	2.27	0.51
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.45	0.51
1:B:91:GLU:HA	1:B:91:GLU:OE1	2.11	0.51
1:A:514:LEU:HD22	1:A:525:TRP:CE3	2.46	0.51
1:A:547:TYR:OH	2:A:901:MA9:H152	2.11	0.51
1:B:704:HIS:CD2	1:B:716:SER:HB2	2.44	0.51
1:B:682:HIS:CE1	1:B:686:SER:HB3	2.46	0.51
1:A:190:LYS:HE3	1:A:193:ILE:HG21	1.93	0.50
1:B:258:LYS:NZ	1:B:712:HIS:ND1	2.59	0.50
1:A:149:PRO:O	1:A:152:THR:OG1	2.29	0.50
1:A:77:LEU:HA	1:A:89:PHE:H	1.76	0.50
1:A:90:LEU:HD21	1:A:95:PHE:CE1	2.47	0.50
1:B:377:ASN:HB2	1:B:381:TYR:H	1.76	0.50
1:B:482:LEU:HD23	1:B:483:HIS:N	2.26	0.50
1:B:549:GLY:HA2	1:B:631:TYR:CE1	2.46	0.50
1:B:120:TYR:C	1:B:120:TYR:CD2	2.85	0.50
1:A:549:GLY:HA2	1:A:631:TYR:CE1	2.47	0.50
1:A:92:ASN:HD22	1:A:93:SER:H	1.59	0.50
1:B:693:GLU:OE1	1:B:696:LYS:HE3	2.12	0.50
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.94	0.49
1:A:92:ASN:ND2	1:A:92:ASN:N	2.60	0.49
1:B:334:SER:OG	1:B:336:ARG:HG3	2.11	0.49
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.93	0.49
1:B:630:SER:OG	1:B:740:HIS:NE2	2.16	0.49
1:B:289:ALA:HB1	1:B:290:PRO:C	2.32	0.49
1:A:63:ILE:CG2	1:A:69:LEU:HD11	2.42	0.49
1:B:377:ASN:HB3	1:B:379:GLU:H	1.77	0.49
1:A:636:THR:HG21	1:A:651:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:PRO:HA	1:A:373:LYS:HB3	1.95	0.49
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.48	0.48
1:A:418:ILE:HD11	1:A:459:VAL:HG12	1.94	0.48
1:A:720:SER:OG	1:B:736:THR:HG21	2.14	0.48
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.13	0.48
1:A:720:SER:OG	1:B:736:THR:HG22	2.13	0.48
1:A:90:LEU:HD21	1:A:95:PHE:HE1	1.78	0.48
1:B:139:LYS:HG3	1:B:141:GLN:HB3	1.95	0.48
1:B:173:TYR:CZ	1:B:184:ARG:HG3	2.48	0.48
1:B:76:ILE:HG22	1:B:89:PHE:HB3	1.95	0.48
1:A:314:GLN:HE22	1:A:373:LYS:NZ	2.11	0.48
1:A:40:ARG:H	1:A:40:ARG:HG3	1.36	0.48
1:B:603:VAL:HB	1:B:635:VAL:HG13	1.96	0.47
1:A:146:GLU:O	1:A:175:LYS:NZ	2.42	0.47
1:A:745:SER:O	1:A:749:GLN:HG3	2.15	0.47
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.79	0.47
1:B:482:LEU:HD23	1:B:483:HIS:H	1.79	0.47
1:A:514:LEU:HD22	1:A:525:TRP:HE3	1.79	0.47
1:B:526:TYR:C	1:B:526:TYR:CD1	2.88	0.47
1:A:241:TYR:O	1:A:242:SER:HB3	2.14	0.47
1:A:40:ARG:HE	1:A:508:GLN:CG	2.22	0.47
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.97	0.47
1:B:306:ALA:HB3	1:B:310:ARG:HB3	1.97	0.47
1:A:258:LYS:HG3	1:B:248:TYR:CZ	2.50	0.47
1:A:604:GLU:HA	1:A:607:ILE:HD12	1.96	0.47
1:A:717:ALA:O	1:B:736:THR:HG21	2.16	0.46
1:B:742:ILE:HG22	1:B:742:ILE:O	2.15	0.46
1:A:179:ASN:ND2	1:A:180:LEU:CD1	2.78	0.46
1:A:75:ASN:HB3	1:A:92:ASN:N	2.31	0.46
1:A:107:ILE:HG22	1:A:108:SER:O	2.15	0.46
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.23	0.46
1:A:355:GLY:HA2	1:A:382:ARG:HH12	1.79	0.46
1:B:114:ILE:HD11	1:B:137:LEU:HD21	1.97	0.46
1:B:362:PRO:HA	1:B:373:LYS:HB3	1.96	0.46
1:A:446:SER:HB2	1:A:457:TYR:CD1	2.50	0.46
1:B:328:CYS:HA	1:B:338:ASN:O	2.15	0.46
1:B:542:LEU:HD23	1:B:543:LEU:C	2.36	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.50	0.46
1:A:330:TYR:HB2	1:A:337:TRP:CH2	2.51	0.46
1:B:531:PRO:HB3	1:B:572:ASN:HD22	1.81	0.46
1:B:377:ASN:HB3	1:B:379:GLU:N	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:PHE:HD1	1:B:90:LEU:HD12	1.81	0.45
1:B:71:LYS:O	1:B:72:GLN:CG	2.64	0.45
1:A:414:TYR:CE2	1:A:433:LYS:HE3	2.52	0.45
1:A:627:TRP:CE3	1:A:755:MET:HE3	2.51	0.45
1:A:336:ARG:CZ	1:A:338:ASN:HD21	2.30	0.45
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.98	0.45
1:A:299:TYR:CE1	1:A:665:VAL:HG22	2.52	0.45
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.65	0.45
1:A:81:ALA:O	1:A:492:ARG:NH2	2.50	0.45
1:B:139:LYS:O	1:B:141:GLN:HB2	2.17	0.45
1:B:377:ASN:HD22	1:B:379:GLU:CB	2.30	0.45
1:B:630:SER:HB3	1:B:631:TYR:H	1.39	0.45
1:A:373:LYS:HD3	1:A:375:ILE:CG2	2.47	0.44
1:B:629:TRP:CZ2	1:B:742:ILE:HD12	2.53	0.44
1:B:95:PHE:HD1	1:B:98:PHE:HB2	1.82	0.44
1:B:242:SER:OG	1:B:243:ASP:N	2.48	0.44
1:A:310:ARG:NH2	1:A:369:ASN:HD21	2.15	0.44
1:B:75:ASN:N	1:B:75:ASN:OD1	2.50	0.44
1:A:327:ILE:HB	1:A:343:ARG:HB3	2.00	0.44
1:B:340:LEU:C	1:B:341:VAL:O	2.56	0.44
1:A:364:PHE:CD2	1:A:371:PHE:HB3	2.53	0.44
1:A:657:SER:CB	1:A:719:ILE:HD11	2.47	0.44
1:B:77:LEU:HA	1:B:89:PHE:H	1.82	0.44
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.99	0.44
1:B:272:ASN:ND2	1:B:274:ASP:H	2.11	0.44
1:B:626:ILE:HG12	1:B:636:THR:HG23	2.00	0.44
1:B:107:ILE:HG22	1:B:108:SER:O	2.18	0.43
1:B:44:THR:O	1:B:47:ASP:HB2	2.18	0.43
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.53	0.43
1:A:64:SER:OG	1:A:65:ASP:N	2.49	0.43
1:B:726:VAL:HG13	1:B:728:VAL:HG23	2.00	0.43
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.43
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.54	0.43
1:A:179:ASN:HD21	1:A:180:LEU:CD1	2.31	0.43
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.53	0.43
1:B:377:ASN:HB2	1:B:381:TYR:N	2.33	0.43
1:B:65:ASP:HA	1:B:462:SER:HB2	2.01	0.43
1:A:242:SER:HB3	1:A:246:LEU:HD12	2.01	0.43
1:A:415:LEU:HD12	1:A:416:TYR:N	2.33	0.43
1:B:235:LEU:HD13	1:B:253:ARG:HG3	2.00	0.43
1:B:377:ASN:HD22	1:B:379:GLU:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:HB3	1:A:193:ILE:HB	2.00	0.42
1:A:77:LEU:HD23	1:A:88:VAL:HG13	1.99	0.42
1:B:603:VAL:HG23	1:B:639:VAL:CG2	2.49	0.42
1:A:704:HIS:CD2	1:A:716:SER:OG	2.66	0.42
1:B:170:ASN:O	1:B:196:ASN:HB2	2.20	0.42
1:B:340:LEU:O	1:B:341:VAL:C	2.58	0.42
1:B:548:ALA:HB3	1:B:635:VAL:HG21	2.01	0.42
1:A:311:ILE:HG12	1:A:313:LEU:CD1	2.49	0.42
1:A:170:ASN:N	1:A:170:ASN:HD22	2.18	0.42
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.19	0.42
1:A:404:VAL:HG13	1:A:417:TYR:CD1	2.55	0.42
1:B:718:GLN:HE22	1:B:721:LYS:CE	2.32	0.42
1:B:237:GLU:HG2	1:B:253:ARG:HB3	1.99	0.42
1:B:418:ILE:HA	1:B:430:ASN:O	2.19	0.42
1:A:272:ASN:ND2	1:A:272:ASN:C	2.71	0.42
1:B:177:GLU:HB2	1:B:180:LEU:HB2	2.01	0.42
1:B:453:ARG:NH1	1:B:479:LEU:HD22	2.35	0.42
1:B:170:ASN:HD22	1:B:170:ASN:N	2.17	0.42
1:A:92:ASN:HD22	1:A:93:SER:N	2.18	0.41
1:A:422:TYR:CE2	1:A:423:LYS:HD2	2.55	0.41
1:B:658:ARG:HB3	1:B:687:THR:HG22	2.02	0.41
1:B:718:GLN:HE22	1:B:721:LYS:HE2	1.84	0.41
1:A:195:TYR:O	1:A:227:GLN:HA	2.20	0.41
1:A:310:ARG:HG3	1:A:310:ARG:HH11	1.86	0.41
1:B:78:VAL:HG12	1:B:87:SER:O	2.20	0.41
1:A:598:LEU:HD11	1:A:670:TYR:HB2	2.03	0.41
1:A:290:PRO:HG2	1:A:293:MET:HG2	2.02	0.41
1:A:741:GLY:O	1:A:742:ILE:C	2.59	0.41
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.56	0.41
1:A:272:ASN:HD22	1:A:274:ASP:N	2.04	0.41
1:A:272:ASN:HD22	1:A:273:THR:N	2.18	0.41
1:B:276:LEU:CD2	1:B:276:LEU:H	2.34	0.41
1:A:160:VAL:HG23	1:A:161:GLY:H	1.86	0.41
1:A:392:LYS:HG3	1:A:392:LYS:H	1.61	0.41
1:B:277:SER:O	1:B:278:SER:OG	2.35	0.41
1:A:664:SER:O	1:A:668:GLU:HB2	2.20	0.40
1:B:513:LYS:O	1:B:527:GLN:HA	2.21	0.40
1:A:673:LEU:O	1:A:678:ASP:HB3	2.21	0.40
1:B:219:ASN:C	1:B:219:ASN:OD1	2.59	0.40
1:B:340:LEU:O	1:B:341:VAL:O	2.39	0.40
1:B:377:ASN:HB2	1:B:381:TYR:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:PHE:HZ	1:B:618:PHE:CD1	2.39	0.40
1:B:736:THR:O	1:B:737:ASP:HB2	2.21	0.40
1:A:229:ASN:OD1	1:A:231:THR:OG1	2.28	0.40
1:A:310:ARG:HG3	1:A:310:ARG:NH1	2.36	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	724/726 (100%)	663 (92%)	51 (7%)	10 (1%)	11	34
1	B	724/726 (100%)	661 (91%)	55 (8%)	8 (1%)	14	41
All	All	1448/1452 (100%)	1324 (91%)	106 (7%)	18 (1%)	13	39

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ALA
1	A	341	VAL
1	B	282	ALA
1	B	341	VAL
1	B	377	ASN
1	A	71	LYS
1	A	72	GLN
1	A	278	SER
1	A	289	ALA
1	A	377	ASN
1	B	278	SER
1	B	289	ALA
1	A	74	ASN
1	B	71	LYS

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Mol	Chain	Res	Type
1	B	340	LEU
1	B	72	GLN
1	A	161	GLY
1	A	742	ILE

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	651/651 (100%)	579 (89%)	72 (11%)	6 19
1	B	651/651 (100%)	585 (90%)	66 (10%)	7 22
All	All	1302/1302 (100%)	1164 (89%)	138 (11%)	6 20

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	SER
1	A	69	LEU
1	A	90	LEU
1	A	92	ASN
1	A	95	PHE
1	A	97	GLU
1	A	103	ASN
1	A	105	TYR
1	A	110	ASP
1	A	114	ILE
1	A	140	ARG
1	A	156	THR
1	A	164	LEU
1	A	170	ASN
1	A	179	ASN
1	A	180	LEU
1	A	184	ARG
1	A	207	VAL

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Mol	Chain	Res	Type
1	A	211	TYR
1	A	214	LEU
1	A	230	ASP
1	A	235	LEU
1	A	244	GLU
1	A	246	LEU
1	A	250	LYS
1	A	253	ARG
1	A	254	VAL
1	A	272	ASN
1	A	275	SER
1	A	276	LEU
1	A	278	SER
1	A	281	ASN
1	A	303	VAL
1	A	332	GLU
1	A	336	ARG
1	A	343	ARG
1	A	376	SER
1	A	378	GLU
1	A	385	CYS
1	A	392	LYS
1	A	393	ASP
1	A	399	LYS
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	441	LYS
1	A	442	VAL
1	A	472	CYS
1	A	482	LEU
1	A	492	ARG
1	A	507	VAL
1	A	514	LEU
1	A	521	GLU
1	A	523	LYS
1	A	536	LYS
1	A	537	SER
1	A	543	LEU
1	A	565	THR
1	A	603	VAL
1	A	621	ASN

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Mol	Chain	Res	Type
1	A	658	ARG
1	A	673	LEU
1	A	679	ASN
1	A	685	ASN
1	A	697	GLN
1	A	701	LEU
1	A	702	LEU
1	A	718	GLN
1	A	729	ASP
1	A	731	GLN
1	A	736	THR
1	B	40	ARG
1	B	41	LYS
1	B	57	LEU
1	B	61	ARG
1	B	72	GLN
1	B	75	ASN
1	B	90	LEU
1	B	92	ASN
1	B	96	ASP
1	B	97	GLU
1	B	120	TYR
1	B	139	LYS
1	B	140	ARG
1	B	159	PRO
1	B	164	LEU
1	B	170	ASN
1	B	180	LEU
1	B	182	SER
1	B	184	ARG
1	B	207	VAL
1	B	209	SER
1	B	214	LEU
1	B	246	LEU
1	B	250	LYS
1	B	253	ARG
1	B	254	VAL
1	B	272	ASN
1	B	276	LEU
1	B	279	VAL
1	B	303	VAL
1	B	326	ASP

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Mol	Chain	Res	Type
1	B	336	ARG
1	B	341	VAL
1	B	366	LEU
1	B	377	ASN
1	B	378	GLU
1	B	379	GLU
1	B	382	ARG
1	B	385	CYS
1	B	392	LYS
1	B	393	ASP
1	B	415	LEU
1	B	436	LEU
1	B	442	VAL
1	B	452	GLU
1	B	472	CYS
1	B	482	LEU
1	B	502	LYS
1	B	506	ASN
1	B	507	VAL
1	B	514	LEU
1	B	543	LEU
1	B	546	VAL
1	B	566	TYR
1	B	583	SER
1	B	603	VAL
1	B	608	GLU
1	B	630	SER
1	B	658	ARG
1	B	673	LEU
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	704	HIS
1	B	736	THR
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	75	ASN
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	100	HIS
1	A	138	ASN
1	A	170	ASN
1	A	179	ASN
1	A	272	ASN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	483	HIS
1	A	505	GLN
1	A	533	HIS
1	A	572	ASN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	731	GLN
1	B	72	GLN
1	B	141	GLN
1	B	169	ASN
1	B	170	ASN
1	B	272	ASN
1	B	338	ASN
1	B	377	ASN
1	B	506	ASN
1	B	533	HIS
1	B	572	ASN
1	B	606	GLN
1	B	612	GLN
1	B	679	ASN
1	B	704	HIS
1	B	718	GLN
1	B	754	HIS
1	B	761	GLN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	MA9	A	901	-	35,35,35	2.66	2 (5%)	48,52,52	2.70	16 (33%)

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	MA9	A	901	-	-	4/18/31/31	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	MA9	C5-S	-14.78	1.61	1.77
2	A	901	MA9	C17-C16	-2.13	1.48	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	MA9	C30-N29-C12	7.62	121.60	114.94
2	A	901	MA9	N31-C30-N29	-6.11	119.05	128.60
2	A	901	MA9	C6-C5-S	5.56	124.74	119.58
2	A	901	MA9	C14-C15-C16	-5.38	106.47	111.58
2	A	901	MA9	C18-C17-C24	5.27	120.86	116.48
2	A	901	MA9	C32-C9-C10	-5.00	113.35	120.59
2	A	901	MA9	C14-N-C28	4.36	125.25	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	MA9	C30-N31-C10	4.07	121.25	115.74
2	A	901	MA9	O4-S-O	-4.06	110.93	117.92
2	A	901	MA9	C23-C24-C17	-3.67	119.44	123.83
2	A	901	MA9	C32-C5-S	-3.32	116.43	119.06
2	A	901	MA9	C-S-C5	3.12	108.27	104.58
2	A	901	MA9	C14-N-C12	-2.58	114.39	120.39
2	A	901	MA9	C8-C9-C10	2.57	125.34	121.28
2	A	901	MA9	C15-C14-N	-2.42	106.11	111.10
2	A	901	MA9	C8-C9-C32	2.20	121.27	118.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

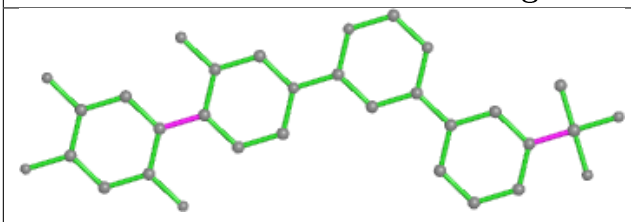
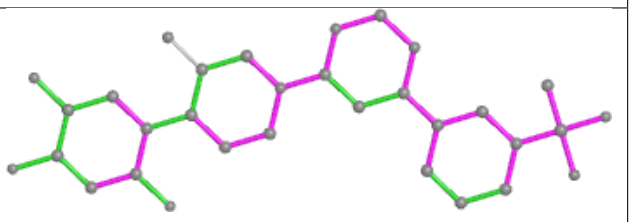
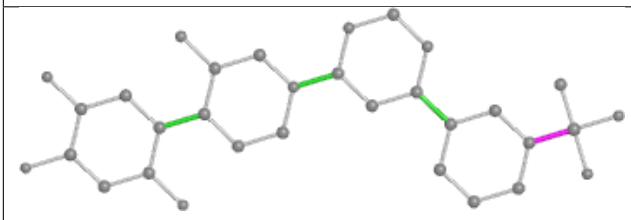
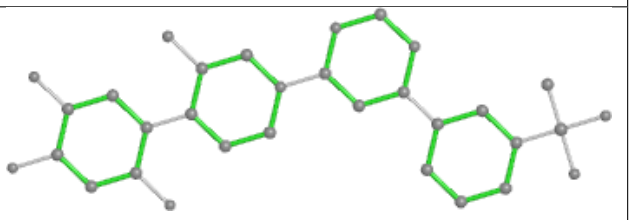
Mol	Chain	Res	Type	Atoms
2	A	901	MA9	C32-C5-S-O
2	A	901	MA9	C6-C5-S-O
2	A	901	MA9	C32-C5-S-C
2	A	901	MA9	C6-C5-S-C

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	MA9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MA9 A 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	726/726 (100%)	-0.17	11 (1%)	73	68	18, 28, 41, 48	0
1	B	726/726 (100%)	-0.17	15 (2%)	63	54	18, 28, 41, 49	0
All	All	1452/1452 (100%)	-0.17	26 (1%)	68	61	18, 28, 41, 49	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	SER	4.9
1	A	39	SER	4.5
1	A	105	TYR	4.3
1	A	93	SER	4.2
1	A	97	GLU	4.0
1	B	73	GLU	3.8
1	B	277	SER	3.7
1	B	96	ASP	3.4
1	A	101	SER	3.4
1	A	94	THR	3.3
1	A	98	PHE	3.1
1	A	92	ASN	2.9
1	A	95	PHE	2.8
1	B	92	ASN	2.6
1	A	96	ASP	2.6
1	B	506	ASN	2.6
1	A	99	GLY	2.4
1	B	74	ASN	2.3
1	B	40	ARG	2.2
1	B	280	THR	2.1
1	B	97	GLU	2.1
1	B	278	SER	2.1
1	B	93	SER	2.1
1	B	76	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	77	LEU	2.0
1	B	98	PHE	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)

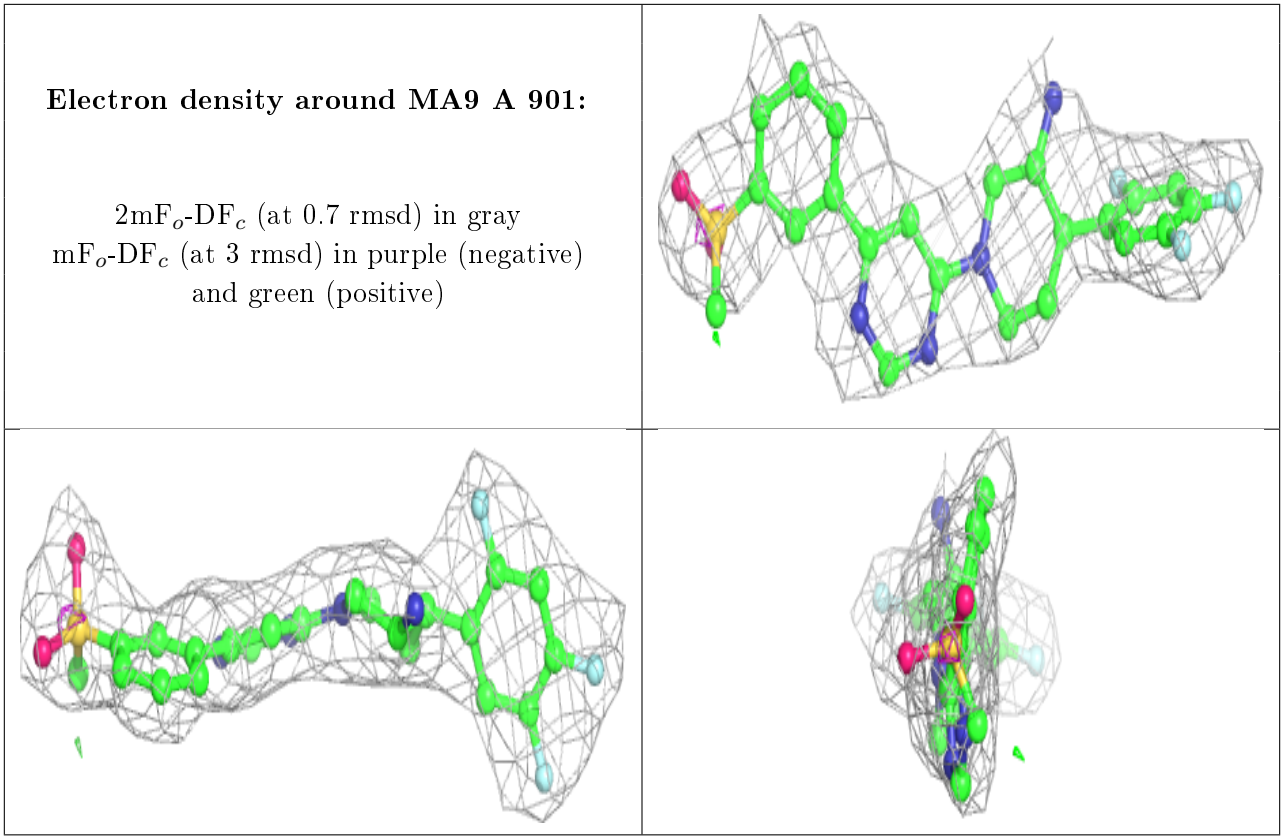
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MA9	A	901	32/32	0.92	0.20	28,38,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MA9 A 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.