Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 06:32 AM EDT

PDB ID	:	5ES8
Title	:	Crystal structure of the initiation module of LgrA in the thiolation state
Authors	:	Reimer, J.M.; Aloise, M.N.; Schmeing, T.M.
Deposited on	:	2015-11-16
Resolution	:	2.55 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

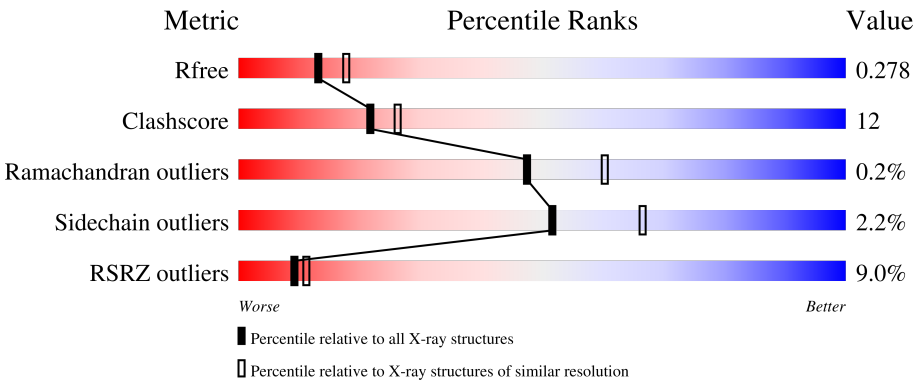
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	776	11% 71% 26% • •
1	B	776	7% 71% 27% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12255 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 Linear gramicidin synthetase subunit A.

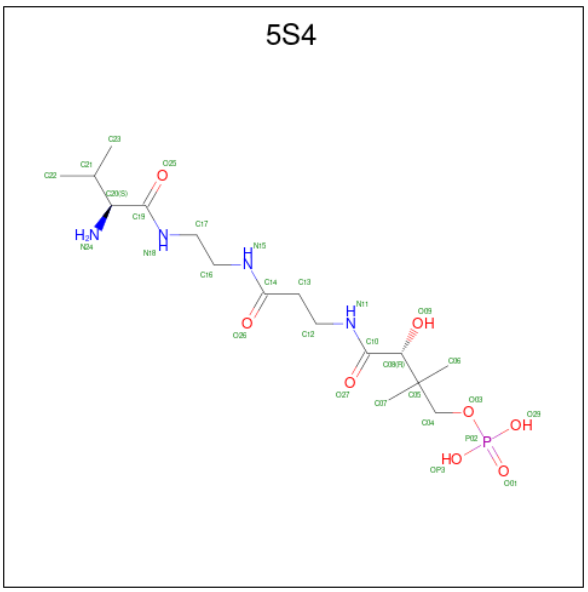
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	759	6054	3862	1041	1125	26	0	0	0
1	B	768	6126	3907	1051	1142	26	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	768	ALA	-	expression tag	UNP Q70LM7
A	769	ALA	-	expression tag	UNP Q70LM7
A	770	ALA	-	expression tag	UNP Q70LM7
A	771	GLU	-	expression tag	UNP Q70LM7
A	772	ASN	-	expression tag	UNP Q70LM7
A	773	LEU	-	expression tag	UNP Q70LM7
A	774	TYR	-	expression tag	UNP Q70LM7
A	775	PHE	-	expression tag	UNP Q70LM7
A	776	GLN	-	expression tag	UNP Q70LM7
B	1	MET	-	initiating methionine	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
B	768	ALA	-	expression tag	UNP Q70LM7
B	769	ALA	-	expression tag	UNP Q70LM7
B	770	ALA	-	expression tag	UNP Q70LM7
B	771	GLU	-	expression tag	UNP Q70LM7
B	772	ASN	-	expression tag	UNP Q70LM7
B	773	LEU	-	expression tag	UNP Q70LM7
B	774	TYR	-	expression tag	UNP Q70LM7
B	775	PHE	-	expression tag	UNP Q70LM7
B	776	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is [(3 {R})-4-[[3-[2-[[(2 {S})-2-azanyl-3-methyl-butanoyl]amino]ethylamino]-3 -oxidanylidene-propyl]amino]-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-butyl] dihydrogen

phosphate (three-letter code: 5S4) (formula: $C_{16}H_{33}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	28	16	4	7	1	0	0
			Total	C	N	O	P		
2	B	1	28	16	4	7	1	0	0

- Molecule 3 is water.

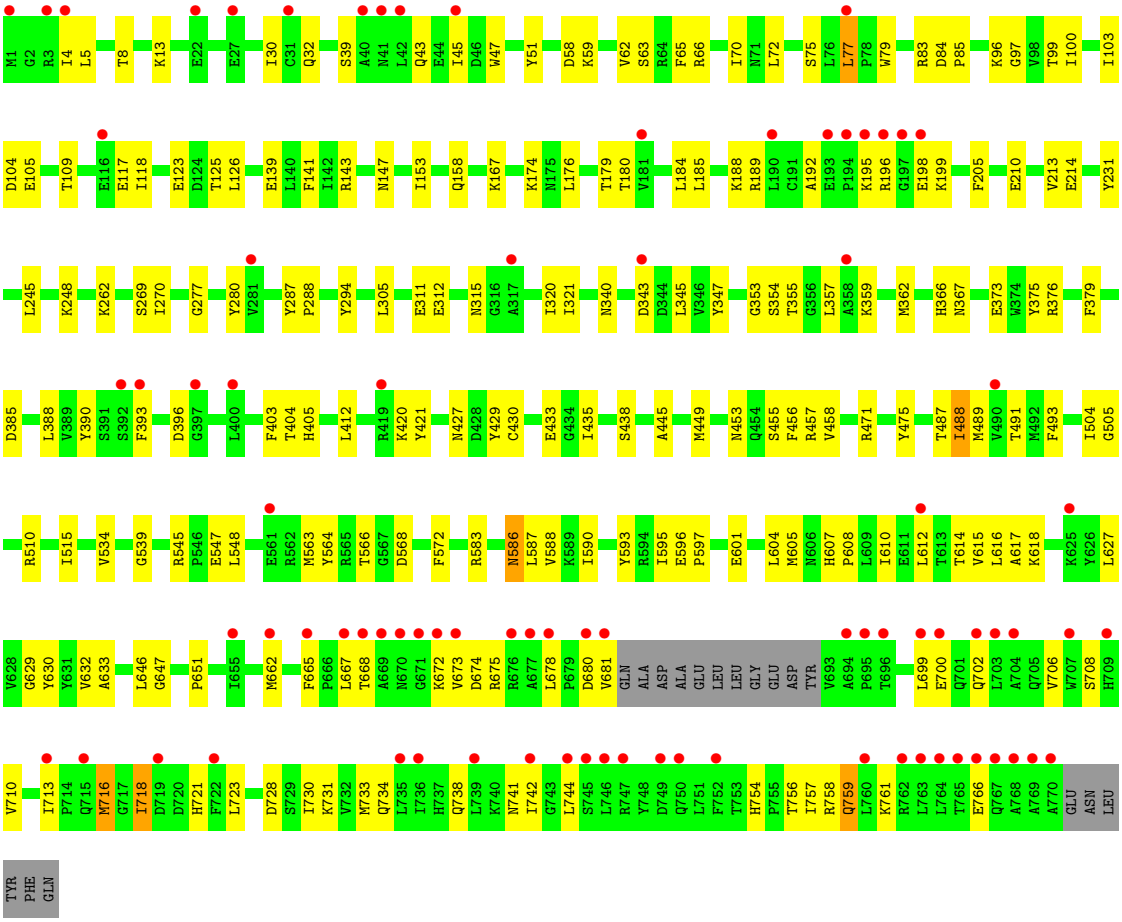
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	8	8	8	0	0
			Total	O		
3	B	11	11	11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

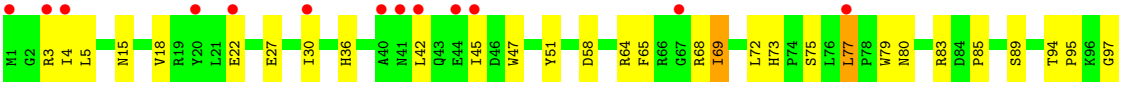
• Molecule 1: Linear gramicidin synthetase subunit A

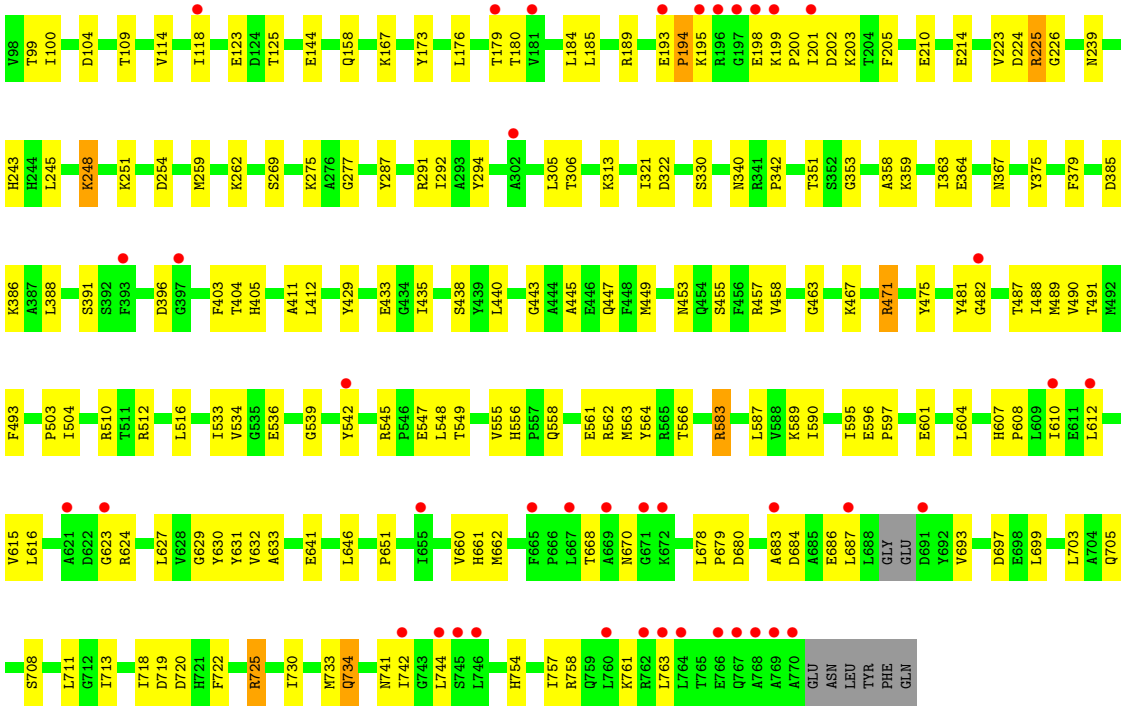
Chain A:



• Molecule 1: Linear gramicidin synthetase subunit A

Chain B:




V98 T99 I100 D104 T109 V114 I118 E123 D124 T125 E144 Q158 K167 Y173 L176 T179 T180 V181 L184 L185 R189 E193 P194 K195 R196 G197 E198 K199 P200 I201 D202 K203 T204 F205 E210 E214 V223 D224 R225 G226 N239
H243 H244 L245 K248 K251 D254 M259 K262 S269 K275 A276 G277 Y287 R291 I292 A293 Y294 A302 L305 T306 K313 I321 D322 S330 N340 R341 P342 T351 S352 G353 A358 K359 I363 E364 N367 Y375 F379 D385
K386 A387 L388 S391 S392 F393 D396 G397 F403 T404 H405 A411 L412 Y429 E433 G434 I435 S438 Y439 L440 G443 A444 A445 E446 Q447 F448 M449 N453 Q454 S455 F456 R457 V458 G463 K467 R471 Y475 Y481 G482 T487 I488 M489 V490 T491 M492
F493 P503 I504 R510 T511 R512 L516 I533 V534 G535 E536 G539 Y542 R545 P546 E547 L548 T549 V555 H556 P557 Q558 E561 R562 M563 Y564 R565 T566 R583 L587 V588 K589 I590 I595 E596 P597 E601 L604 H607 P608 L609 I610 E611 L612
V615 L616 A621 D622 G623 R624 L627 V628 G629 Y630 Y631 V632 A633 E641 L646 P651 I655 V660 H661 M662 F665 P666 L667 T668 A669 N670 G671 K672 L678 P679 D680 A683 D684 A685 E686 L687 L688 GLY GLU D691 Y692 V693 D697 E698 L699 L703 A704 Q705
S708 L711 G712 I713 I718 D719 D720 H721 F722 R725 I730 M733 Q734 N741 I742 G743 L744 S745 L746 H754 I757 R758 Q759 L760 K761 R762 L763 L764 T765 E766 Q767 A768 A769 A770 GLU ASN LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.55Å 101.05Å 138.74Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	47.47 – 2.55 47.47 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.0 (47.47-2.55) 85.2 (47.47-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.05 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.274 0.234 , 0.278	Depositor DCC
R_{free} test set	3292 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12255	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.03% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5S4

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	0.35	0/6194	0.57	1/8407 (0.0%)
1	B	0.35	0/6267	0.57	0/8507
All	All	0.35	0/12461	0.57	1/16914 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	744	LEU	CA-CB-CG	-5.72	102.14	115.30

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	6054	0	5990	140	0
1	B	6126	0	6053	156	0
2	A	28	0	31	2	0
2	B	28	0	31	2	0
3	A	8	0	0	2	0
3	B	11	0	0	4	0
All	All	12255	0	12105	290	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 (290) 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:367:ASN:HB3	1:B:487:THR:HG21	1.39	1.05
1:A:199:LYS:O	1:A:510:ARG:NH1	2.05	0.90
1:A:668:THR:HG23	1:A:674:ASP:HB3	1.56	0.88
1:B:699:LEU:HD23	1:B:761:LYS:HE2	1.56	0.86
1:B:224:ASP:OD2	3:B:902:HOH:O	1.97	0.83
1:B:262:LYS:NZ	1:B:391:SER:O	2.12	0.82
1:B:199:LYS:O	1:B:510:ARG:NH1	2.15	0.80
1:A:605:MET:O	1:B:167:LYS:NZ	2.16	0.79
1:B:471:ARG:NH1	1:B:475:TYR:O	2.16	0.78
1:B:64:ARG:O	1:B:68:ARG:NH2	2.16	0.78
1:A:615:VAL:HG12	1:A:629:GLY:HA2	1.67	0.76
1:B:396:ASP:OD1	2:B:801:5S4:N24	2.18	0.76
1:B:539:GLY:O	1:B:562:ARG:NH2	2.19	0.76
1:B:512:ARG:NH2	1:B:561:GLU:OE1	2.19	0.76
1:B:687:LEU:HD11	1:B:725:ARG:HG3	1.68	0.75
1:A:270:ILE:HD11	1:A:393:PHE:HE1	1.49	0.74
1:A:718:ILE:HG12	1:A:757:ILE:HB	1.69	0.74
1:B:353:GLY:HA3	1:B:359:LYS:HD3	1.70	0.74
1:B:587:LEU:HD13	1:B:596:GLU:HG2	1.71	0.73
1:B:615:VAL:HG12	1:B:629:GLY:HA2	1.71	0.72
1:A:610:ILE:HG22	1:A:633:ALA:HB2	1.70	0.72
1:A:396:ASP:OD1	2:A:801:5S4:N24	2.22	0.72
1:B:610:ILE:HG22	1:B:633:ALA:HB2	1.72	0.70
1:A:457:ARG:HD2	1:A:458:VAL:HG23	1.73	0.69
1:B:616:LEU:HD11	1:B:678:LEU:HD12	1.73	0.68
1:A:245:LEU:HD21	1:A:305:LEU:HD11	1.76	0.68
1:A:104:ASP:OD2	1:A:109:THR:OG1	2.09	0.68
1:B:195:LYS:HA	1:B:198:GLU:HG2	1.74	0.68
1:A:277:GLY:O	1:A:340:ASN:ND2	2.25	0.68
1:B:730:ILE:HD13	1:B:733:MET:HE1	1.75	0.68
1:B:693:VAL:HB	1:B:718:ILE:HG22	1.75	0.67
1:A:355:THR:O	1:A:359:LYS:NZ	2.24	0.67
1:A:587:LEU:HD13	1:A:596:GLU:HG2	1.76	0.67
1:B:542:TYR:H	1:B:549:THR:HG22	1.58	0.67
1:A:83:ARG:NH2	1:B:608:PRO:O	2.26	0.67
1:A:388:LEU:HG	1:A:435:ILE:HG21	1.77	0.67
1:B:453:ASN:HD21	1:B:455:SER:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:VAL:HB	1:B:718:ILE:CG2	2.25	0.66
1:B:3:ARG:HD2	1:B:27:GLU:HB3	1.79	0.65
1:B:534:VAL:HG22	1:B:563:MET:HG2	1.77	0.65
1:B:443:GLY:HA2	1:B:624:ARG:HH12	1.63	0.64
1:B:457:ARG:HD2	1:B:458:VAL:HG23	1.80	0.64
1:A:534:VAL:HG22	1:A:563:MET:HG2	1.80	0.63
1:A:5:LEU:N	1:A:45:ILE:HD11	2.14	0.63
1:B:245:LEU:HD21	1:B:305:LEU:HD11	1.79	0.63
1:B:104:ASP:OD2	1:B:109:THR:OG1	2.09	0.62
1:B:668:THR:HG22	1:B:670:ASN:H	1.64	0.62
1:A:754:HIS:HB3	1:A:759:GLN:HB2	1.81	0.62
1:A:608:PRO:O	1:B:83:ARG:NH2	2.33	0.62
1:B:195:LYS:HG2	1:B:198:GLU:HG3	1.80	0.62
1:B:491:THR:HG22	1:B:504:ILE:O	1.98	0.62
1:A:367:ASN:HD21	1:A:539:GLY:HA2	1.63	0.62
1:A:84:ASP:OD2	3:A:901:HOH:O	2.16	0.62
1:B:719:ASP:OD1	1:B:758:ARG:HB2	1.99	0.62
1:B:562:ARG:NE	3:B:901:HOH:O	1.85	0.62
1:B:225:ARG:CD	1:B:226:GLY:H	2.13	0.61
1:A:125:THR:HA	1:A:180:THR:HA	1.83	0.61
1:A:420:LYS:NZ	3:A:902:HOH:O	2.32	0.61
1:A:590:ILE:HB	1:A:595:ILE:HD12	1.81	0.61
1:A:77:LEU:HB2	1:A:99:THR:HG21	1.82	0.61
1:B:385:ASP:OD1	1:B:457:ARG:NH2	2.34	0.61
1:A:718:ILE:HD11	1:A:758:ARG:HB2	1.82	0.61
1:B:77:LEU:HB2	1:B:99:THR:HG21	1.83	0.61
1:A:491:THR:HG22	1:A:504:ILE:O	2.01	0.60
1:B:741:ASN:OD1	1:B:742:ILE:N	2.35	0.60
1:A:72:LEU:HD22	1:A:100:ILE:HG12	1.85	0.59
1:A:4:ILE:HG12	1:A:47:TRP:HB2	1.85	0.59
1:A:595:ILE:HG21	1:A:627:LEU:HD11	1.85	0.58
1:A:45:ILE:HG23	1:A:65:PHE:HE2	1.69	0.58
1:B:595:ILE:HG21	1:B:627:LEU:HD11	1.86	0.57
1:B:259:MET:HE1	1:B:313:LYS:HB3	1.87	0.57
1:B:405:HIS:HB2	1:B:412:LEU:HD21	1.85	0.57
1:B:123:GLU:OE1	1:B:123:GLU:N	2.38	0.57
1:B:18:VAL:HG11	1:B:30:ILE:HD11	1.87	0.57
1:B:556:HIS:HE1	1:B:558:GLN:HB2	1.70	0.57
1:A:311:GLU:HG3	1:A:320:ILE:HD13	1.87	0.57
1:B:367:ASN:ND2	1:B:536:GLU:O	2.38	0.56
1:B:15:ASN:OD1	1:B:15:ASN:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:HIS:CE1	1:B:558:GLN:HB2	2.40	0.56
1:A:616:LEU:HD11	1:A:678:LEU:HD12	1.87	0.56
1:B:75:SER:OG	1:B:79:TRP:O	2.23	0.56
1:A:612:LEU:H	1:A:632:VAL:HG12	1.71	0.56
1:B:607:HIS:HB3	1:B:610:ILE:HG12	1.87	0.56
1:A:75:SER:OG	1:A:79:TRP:O	2.24	0.55
1:B:443:GLY:HA2	1:B:624:ARG:NH1	2.21	0.55
1:B:683:ALA:HB1	1:B:713:ILE:HG12	1.87	0.55
1:A:262:LYS:NZ	1:A:390:TYR:O	2.40	0.55
1:A:604:LEU:O	1:A:610:ILE:HD11	2.06	0.55
1:A:269:SER:HB2	1:A:305:LEU:HD23	1.89	0.55
1:A:75:SER:HB2	1:A:85:PRO:HB2	1.89	0.55
1:B:590:ILE:HB	1:B:595:ILE:HD12	1.89	0.55
1:A:59:LYS:HA	1:A:62:VAL:HG12	1.88	0.54
1:A:680:ASP:O	1:A:681:VAL:HB	2.08	0.54
1:A:607:HIS:O	1:B:167:LYS:NZ	2.41	0.54
1:B:89:SER:HA	1:B:94:THR:HG22	1.88	0.54
1:A:58:ASP:OD1	1:A:58:ASP:N	2.41	0.54
1:A:167:LYS:NZ	1:B:607:HIS:O	2.39	0.54
1:A:373:GLU:OE1	1:A:376:ARG:NH1	2.41	0.54
1:A:421:TYR:CD1	1:A:733:MET:HE3	2.43	0.54
1:B:287:TYR:CE1	1:B:651:PRO:HB3	2.43	0.53
1:A:590:ILE:HG13	1:A:627:LEU:HG	1.91	0.53
1:B:720:ASP:OD2	1:B:725:ARG:NH1	2.41	0.53
1:B:277:GLY:O	1:B:340:ASN:ND2	2.41	0.53
1:B:58:ASP:N	1:B:58:ASP:OD1	2.33	0.53
1:B:248:LYS:HD2	1:B:321:ILE:HD11	1.90	0.53
1:A:630:TYR:CD1	1:A:662:MET:HE2	2.43	0.53
1:A:353:GLY:O	1:A:596:GLU:HG3	2.09	0.53
1:A:355:THR:H	1:A:359:LYS:HZ3	1.57	0.53
1:A:665:PHE:HD2	1:A:673:VAL:HG11	1.73	0.53
1:B:545:ARG:O	1:B:549:THR:HG23	2.08	0.52
1:A:287:TYR:CE1	1:A:651:PRO:HB3	2.45	0.52
1:B:353:GLY:O	1:B:596:GLU:HG3	2.10	0.52
1:A:45:ILE:HG23	1:A:65:PHE:CE2	2.44	0.52
1:A:453:ASN:HD21	1:A:455:SER:HB3	1.74	0.51
1:B:612:LEU:HB3	1:B:632:VAL:HG12	1.91	0.51
1:A:77:LEU:HD12	1:A:158:GLN:NE2	2.25	0.51
1:B:719:ASP:OD2	1:B:758:ARG:NE	2.43	0.51
1:A:63:SER:O	1:A:66:ARG:HG3	2.11	0.51
1:A:70:ILE:HD11	1:A:141:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:TYR:HD1	1:A:662:MET:HE2	1.74	0.51
1:B:447:GLN:NE2	1:B:734:GLN:HG2	2.25	0.51
1:B:251:LYS:O	1:B:254:ASP:HB2	2.11	0.51
1:A:270:ILE:HD11	1:A:393:PHE:CE1	2.39	0.50
1:A:456:PHE:O	1:A:475:TYR:HB3	2.11	0.50
1:A:741:ASN:OD1	1:A:742:ILE:N	2.44	0.50
1:B:601:GLU:HG3	1:B:615:VAL:HG22	1.93	0.50
1:A:728:ASP:OD1	1:A:731:LYS:HG2	2.11	0.50
1:A:39:SER:O	1:A:43:GLN:NE2	2.44	0.50
1:A:179:THR:HG21	1:A:184:LEU:HD13	1.94	0.50
1:A:311:GLU:HG3	1:A:320:ILE:CD1	2.41	0.50
1:A:488:ILE:HG22	1:A:489:MET:H	1.76	0.50
1:B:467:LYS:HD3	1:B:623:GLY:HA3	1.93	0.50
1:B:4:ILE:C	1:B:45:ILE:HD11	2.33	0.49
1:B:65:PHE:O	1:B:69:ILE:HG13	2.12	0.49
1:B:202:ASP:HA	1:B:342:PRO:HG2	1.95	0.49
1:B:201:ILE:HG22	1:B:203:LYS:H	1.78	0.49
1:B:386:LYS:HB2	1:B:435:ILE:HA	1.94	0.49
1:A:379:PHE:O	1:A:457:ARG:NH1	2.44	0.49
1:A:210:GLU:O	1:A:214:GLU:HG2	2.13	0.49
1:B:379:PHE:O	1:B:457:ARG:NH1	2.46	0.49
1:A:13:LYS:HG2	1:A:30:ILE:HG21	1.95	0.49
1:A:367:ASN:ND2	1:A:539:GLY:HA2	2.25	0.49
1:A:564:TYR:CE2	1:A:566:THR:HA	2.48	0.49
1:A:608:PRO:HA	1:B:167:LYS:HD3	1.95	0.49
1:A:721:HIS:HE1	1:A:723:LEU:HG	1.78	0.49
1:B:388:LEU:HG	1:B:435:ILE:HG21	1.93	0.49
1:A:721:HIS:CE1	1:A:723:LEU:HG	2.48	0.48
1:A:139:GLU:HG3	1:A:143:ARG:NH1	2.28	0.48
1:B:375:TYR:CD1	1:B:404:THR:HB	2.47	0.48
1:B:194:PRO:HG3	1:B:512:ARG:CD	2.43	0.48
1:B:73:HIS:HE1	1:B:80:ASN:O	1.97	0.48
1:B:705:GLN:N	1:B:705:GLN:OE1	2.47	0.48
1:A:123:GLU:OE1	1:A:123:GLU:N	2.47	0.48
1:A:515:ILE:HD13	1:A:572:PHE:CE2	2.47	0.48
1:A:176:LEU:O	1:A:179:THR:HG22	2.14	0.48
1:A:427:ASN:ND2	1:A:453:ASN:HD22	2.11	0.48
1:A:213:VAL:HG22	1:A:231:TYR:HB3	1.96	0.48
1:A:343:ASP:HA	1:A:366:HIS:HD2	1.78	0.47
1:B:388:LEU:HB2	1:B:438:SER:OG	2.14	0.47
1:B:75:SER:HB2	1:B:85:PRO:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:CG	1:B:226:GLY:H	2.26	0.47
1:B:179:THR:HG21	1:B:184:LEU:HD13	1.96	0.47
1:A:248:LYS:HD2	1:A:321:ILE:HD11	1.97	0.47
1:B:607:HIS:HB3	1:B:610:ILE:CG1	2.44	0.47
1:A:367:ASN:HB3	1:A:487:THR:OG1	2.14	0.47
1:B:195:LYS:HA	1:B:198:GLU:CG	2.43	0.47
1:B:607:HIS:HE1	1:B:641:GLU:OE2	1.98	0.47
1:A:601:GLU:HG3	1:A:615:VAL:HG22	1.97	0.47
1:A:728:ASP:OD1	1:A:730:ILE:HG13	2.15	0.46
1:B:239:ASN:OD1	1:B:275:LYS:HE3	2.15	0.46
1:B:259:MET:CE	1:B:292:ILE:HD13	2.45	0.46
1:B:481:TYR:CG	1:B:482:GLY:N	2.83	0.46
1:A:354:SER:HA	1:A:596:GLU:HG3	1.97	0.46
1:A:388:LEU:HB2	1:A:438:SER:OG	2.16	0.46
1:A:445:ALA:O	1:A:449:MET:HG3	2.15	0.46
1:B:225:ARG:HD2	1:B:226:GLY:H	1.79	0.46
1:A:597:PRO:HB3	1:A:615:VAL:HG23	1.97	0.46
1:A:716:MET:O	1:A:716:MET:HG3	2.14	0.46
1:B:632:VAL:HA	1:B:662:MET:O	2.15	0.46
1:A:699:LEU:O	1:A:702:GLN:HG2	2.16	0.46
1:B:4:ILE:HG12	1:B:47:TRP:HB2	1.98	0.46
1:B:388:LEU:H	1:B:438:SER:HG	1.64	0.46
1:A:435:ILE:O	1:A:455:SER:OG	2.31	0.46
1:B:223:VAL:N	1:B:412:LEU:O	2.40	0.46
1:B:547:GLU:CD	1:B:547:GLU:H	2.19	0.46
1:A:375:TYR:CD1	1:A:404:THR:HB	2.51	0.46
1:A:596:GLU:HA	1:A:597:PRO:HD2	1.80	0.46
1:B:590:ILE:HG12	1:B:627:LEU:HG	1.98	0.46
1:B:730:ILE:HD13	1:B:733:MET:CE	2.45	0.46
1:B:630:TYR:CD1	1:B:660:VAL:HB	2.50	0.45
1:A:59:LYS:HD3	1:A:105:GLU:HG3	1.97	0.45
1:A:205:PHE:CE1	1:A:403:PHE:HB3	2.51	0.45
1:A:294:TYR:OH	1:A:545:ARG:NH2	2.48	0.45
1:A:734:GLN:O	1:A:738:GLN:HG3	2.15	0.45
1:B:562:ARG:NH2	3:B:901:HOH:O	2.50	0.45
1:B:363:ILE:HD12	1:B:487:THR:HG22	1.99	0.45
1:B:453:ASN:ND2	1:B:455:SER:HB3	2.30	0.45
1:A:294:TYR:CE1	1:A:357:LEU:HD23	2.52	0.45
1:A:96:LYS:O	1:A:117:GLU:HG3	2.16	0.45
1:A:700:GLU:HG3	1:A:761:LYS:HD3	1.98	0.45
1:B:210:GLU:O	1:B:214:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:LEU:HD21	1:B:722:PHE:CZ	2.51	0.45
1:A:708:SER:HB2	1:A:713:ILE:O	2.16	0.45
1:B:306:THR:O	1:B:322:ASP:HA	2.16	0.45
1:B:259:MET:HE1	1:B:292:ILE:HD13	1.99	0.45
1:A:405:HIS:HB2	1:A:412:LEU:HD21	1.99	0.44
1:B:114:VAL:HG11	1:B:144:GLU:HG3	2.00	0.44
1:B:547:GLU:HG2	1:B:548:LEU:N	2.33	0.44
1:A:195:LYS:O	1:A:198:GLU:HG2	2.17	0.44
1:A:429:TYR:CZ	1:A:433:GLU:HG3	2.52	0.44
1:A:568:ASP:HA	1:A:583:ARG:HG2	2.00	0.44
1:B:80:ASN:OD1	1:B:94:THR:HG21	2.17	0.44
1:B:194:PRO:HG3	1:B:512:ARG:HD3	1.98	0.44
1:A:126:LEU:HD12	1:A:176:LEU:O	2.17	0.44
1:A:345:LEU:HD21	1:A:362:MET:HB3	2.00	0.44
1:B:445:ALA:O	1:B:449:MET:HG3	2.16	0.44
1:A:185:LEU:O	1:A:189:ARG:HG3	2.17	0.44
1:A:188:LYS:O	1:A:192:ALA:N	2.51	0.44
1:B:490:VAL:HG11	1:B:533:ILE:HD13	2.00	0.44
1:B:516:LEU:HD11	1:B:563:MET:HE1	2.00	0.44
1:B:596:GLU:HA	1:B:597:PRO:HD2	1.73	0.44
1:A:8:THR:O	1:A:32:GLN:HG3	2.17	0.44
1:A:421:TYR:HA	1:A:733:MET:CE	2.47	0.44
1:B:77:LEU:HD12	1:B:158:GLN:NE2	2.33	0.44
1:B:125:THR:HA	1:B:180:THR:HA	2.00	0.44
1:B:291:ARG:HH22	1:B:358:ALA:HB2	1.83	0.44
1:A:312:GLU:O	1:A:315:ASN:N	2.38	0.43
1:A:586:ASN:HD22	1:A:675:ARG:NH1	2.16	0.43
1:B:199:LYS:HG2	1:B:200:PRO:O	2.18	0.43
1:A:662:MET:HE1	1:A:678:LEU:HD22	1.99	0.43
1:B:564:TYR:CE2	1:B:566:THR:HA	2.53	0.43
1:B:583:ARG:HH11	1:B:587:LEU:HB3	1.84	0.43
1:B:693:VAL:HB	1:B:718:ILE:HG21	1.99	0.43
1:A:62:VAL:HG21	1:A:103:ILE:HG22	2.00	0.43
1:A:174:LYS:HD2	1:A:174:LYS:HA	1.59	0.43
1:A:593:TYR:CZ	2:A:801:5S4:H22	2.53	0.43
1:A:706:VAL:O	1:A:710:VAL:HG23	2.18	0.43
1:A:385:ASP:OD1	1:A:457:ARG:NH2	2.47	0.43
1:B:18:VAL:O	1:B:22:GLU:HG2	2.19	0.43
1:B:243:HIS:HB2	1:B:330:SER:OG	2.19	0.43
1:A:547:GLU:HG2	1:A:548:LEU:N	2.34	0.43
1:B:386:LYS:HD3	1:B:411:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLY:O	1:B:589:LYS:HD3	2.19	0.43
1:B:205:PHE:CE1	1:B:403:PHE:HB3	2.54	0.42
1:A:294:TYR:CD1	1:A:357:LEU:HD23	2.54	0.42
1:A:604:LEU:HD13	1:A:646:LEU:HD11	2.01	0.42
1:A:427:ASN:ND2	1:A:453:ASN:HB2	2.34	0.42
1:B:42:LEU:HD12	1:B:42:LEU:HA	1.75	0.42
1:A:147:ASN:HB3	1:A:153:ILE:HG13	2.02	0.42
1:B:5:LEU:N	1:B:45:ILE:HD11	2.35	0.42
1:B:94:THR:HG23	1:B:95:PRO:O	2.19	0.42
1:B:604:LEU:HD13	1:B:646:LEU:HD21	2.01	0.42
1:B:173:TYR:HB3	1:B:176:LEU:HD12	2.02	0.42
1:B:269:SER:HB2	1:B:305:LEU:HD23	2.01	0.42
1:B:467:LYS:O	3:B:903:HOH:O	2.22	0.42
1:B:754:HIS:CE1	1:B:763:LEU:HD13	2.55	0.42
1:A:4:ILE:C	1:A:45:ILE:HD11	2.39	0.42
1:A:288:PRO:HG3	1:A:647:GLY:O	2.20	0.42
1:B:435:ILE:O	1:B:455:SER:OG	2.32	0.42
1:A:196:ARG:HA	1:A:196:ARG:HD3	1.84	0.41
1:B:364:GLU:O	1:B:367:ASN:HB2	2.20	0.41
1:B:493:PHE:CZ	1:B:503:PRO:HG2	2.55	0.41
1:B:678:LEU:HA	1:B:679:PRO:HD2	1.88	0.41
1:A:280:TYR:CE2	1:A:347:TYR:HB3	2.55	0.41
1:B:72:LEU:HD22	1:B:100:ILE:HG12	2.01	0.41
1:B:510:ARG:HD2	1:B:536:GLU:HG3	2.01	0.41
1:B:719:ASP:OD2	1:B:758:ARG:CZ	2.68	0.41
1:B:185:LEU:O	1:B:189:ARG:HG3	2.19	0.41
1:B:630:TYR:OH	1:B:679:PRO:O	2.24	0.41
1:B:97:GLY:HA2	1:B:118:ILE:HG22	2.03	0.41
1:A:312:GLU:O	1:A:312:GLU:HG2	2.21	0.41
1:A:493:PHE:HB2	1:A:505:GLY:HA3	2.01	0.41
1:B:294:TYR:OH	1:B:545:ARG:NH2	2.54	0.41
1:B:429:TYR:CZ	1:B:433:GLU:HG3	2.55	0.41
1:B:718:ILE:O	1:B:757:ILE:HB	2.21	0.41
1:A:430:CYS:HA	1:A:435:ILE:HG12	2.03	0.41
1:B:703:LEU:HD23	1:B:703:LEU:HA	1.88	0.41
1:A:96:LYS:HB2	1:A:118:ILE:O	2.21	0.40
1:A:614:THR:O	1:A:630:TYR:HB2	2.21	0.40
1:A:667:LEU:HB3	1:A:672:LYS:O	2.21	0.40
1:B:440:LEU:HB2	1:B:445:ALA:HB2	2.02	0.40
1:B:489:MET:HE2	2:B:801:5S4:H7	2.03	0.40
1:B:612:LEU:HB3	1:B:632:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASN:HD21	1:A:453:ASN:HB2	1.86	0.40
1:B:631:TYR:CZ	1:B:661:HIS:HB2	2.56	0.40
1:A:97:GLY:HA2	1:A:118:ILE:HG22	2.03	0.40
1:A:612:LEU:N	1:A:632:VAL:HG12	2.36	0.40
1:A:617:ALA:O	1:A:618:LYS:HD2	2.22	0.40
1:B:5:LEU:HB2	1:B:45:ILE:HG12	2.03	0.40
1:B:194:PRO:HD3	1:B:512:ARG:HD3	2.03	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	755/776 (97%)	742 (98%)	12 (2%)	1 (0%)	51	65
1	B	764/776 (98%)	746 (98%)	16 (2%)	2 (0%)	41	51
All	All	1519/1552 (98%)	1488 (98%)	28 (2%)	3 (0%)	47	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	GLU
1	A	488	ILE
1	B	488	ILE

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/666 (98%)	641 (98%)	10 (2%)	65	77
1	B	658/666 (99%)	639 (97%)	19 (3%)	42	57
All	All	1309/1332 (98%)	1280 (98%)	29 (2%)	52	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	77	LEU
1	A	471	ARG
1	A	586	ASN
1	A	588	VAL
1	A	716	MET
1	A	718	ILE
1	A	756	THR
1	A	759	GLN
1	A	766	GLU
1	B	36	HIS
1	B	51	TYR
1	B	69	ILE
1	B	77	LEU
1	B	194	PRO
1	B	225	ARG
1	B	248	LYS
1	B	351	THR
1	B	471	ARG
1	B	555	VAL
1	B	583	ARG
1	B	680	ASP
1	B	684	ASP
1	B	686	GLU
1	B	697	ASP
1	B	708	SER
1	B	725	ARG
1	B	734	GLN
1	B	744	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	432	GLN
1	B	607	HIS
1	B	715	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5S4	B	801	1	20,27,28	2.22	4 (20%)	27,36,39	1.52	4 (14%)
2	5S4	A	801	1	20,27,28	2.25	5 (25%)	27,36,39	1.80	8 (29%)

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	5S4	B	801	1	-	11/35/37/38	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5S4	A	801	1	-	15/35/37/38	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	5S4	C10-N11	6.08	1.46	1.33
2	B	801	5S4	C10-N11	6.08	1.46	1.33
2	A	801	5S4	C14-N15	4.97	1.44	1.33
2	B	801	5S4	C14-N15	4.96	1.44	1.33
2	A	801	5S4	C19-N18	4.37	1.43	1.33
2	B	801	5S4	C19-N18	4.11	1.42	1.33
2	B	801	5S4	C13-C14	2.76	1.56	1.51
2	A	801	5S4	C13-C14	2.61	1.56	1.51
2	A	801	5S4	C20-N24	-2.13	1.41	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	5S4	C12-C13-C14	4.89	120.50	112.36
2	B	801	5S4	C12-C13-C14	4.61	120.04	112.36
2	A	801	5S4	C07-C05-C04	3.38	113.75	108.23
2	A	801	5S4	C13-C14-N15	2.94	121.38	116.42
2	A	801	5S4	C19-C20-N24	-2.58	106.34	110.28
2	B	801	5S4	C07-C05-C08	2.38	112.95	108.82
2	B	801	5S4	C12-N11-C10	2.36	126.80	122.59
2	B	801	5S4	C13-C14-N15	2.32	120.33	116.42
2	A	801	5S4	O09-C08-C05	-2.26	104.92	110.25
2	A	801	5S4	C16-N15-C14	-2.23	118.71	122.84
2	A	801	5S4	O26-C14-C13	-2.19	118.01	122.02
2	A	801	5S4	C12-N11-C10	2.02	126.20	122.59

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	5S4	O03-C04-C05-C08
2	B	801	5S4	N11-C12-C13-C14
2	A	801	5S4	N15-C16-C17-N18
2	A	801	5S4	C13-C12-N11-C10
2	B	801	5S4	C13-C12-N11-C10
2	A	801	5S4	O25-C19-N18-C17

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Mol	Chain	Res	Type	Atoms
2	B	801	5S4	O25-C19-N18-C17
2	B	801	5S4	N15-C16-C17-N18
2	A	801	5S4	C20-C19-N18-C17
2	B	801	5S4	C20-C19-N18-C17
2	A	801	5S4	C12-C13-C14-O26
2	A	801	5S4	C12-C13-C14-N15
2	A	801	5S4	O25-C19-C20-N24
2	B	801	5S4	O25-C19-C20-N24
2	A	801	5S4	N18-C19-C20-N24
2	B	801	5S4	N18-C19-C20-N24
2	A	801	5S4	O03-C04-C05-C06
2	A	801	5S4	O03-C04-C05-C07
2	B	801	5S4	C05-C08-C10-O27
2	A	801	5S4	O09-C08-C10-N11
2	B	801	5S4	O09-C08-C10-N11
2	A	801	5S4	N11-C12-C13-C14
2	A	801	5S4	O25-C19-C20-C21
2	B	801	5S4	C05-C08-C10-N11
2	B	801	5S4	C12-C13-C14-N15
2	A	801	5S4	N18-C19-C20-C21

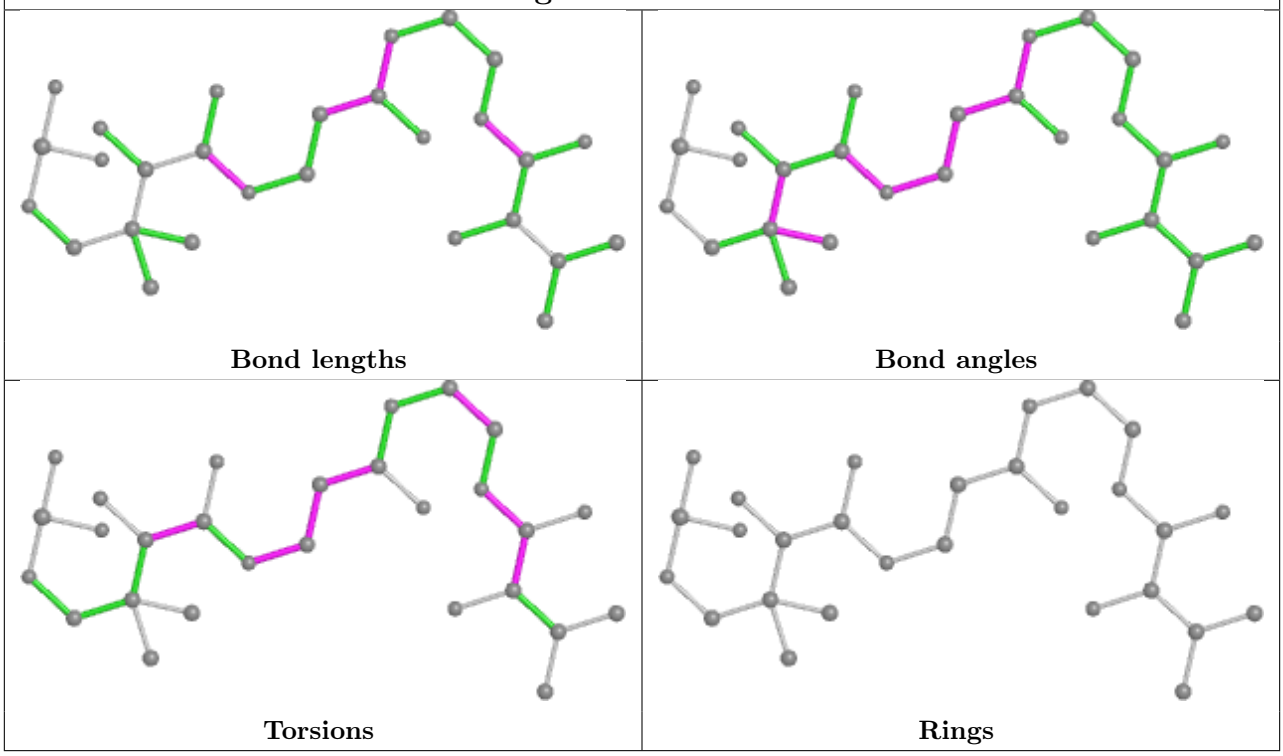
There are no ring outliers.

2 monomers are involved in 4 short contacts:

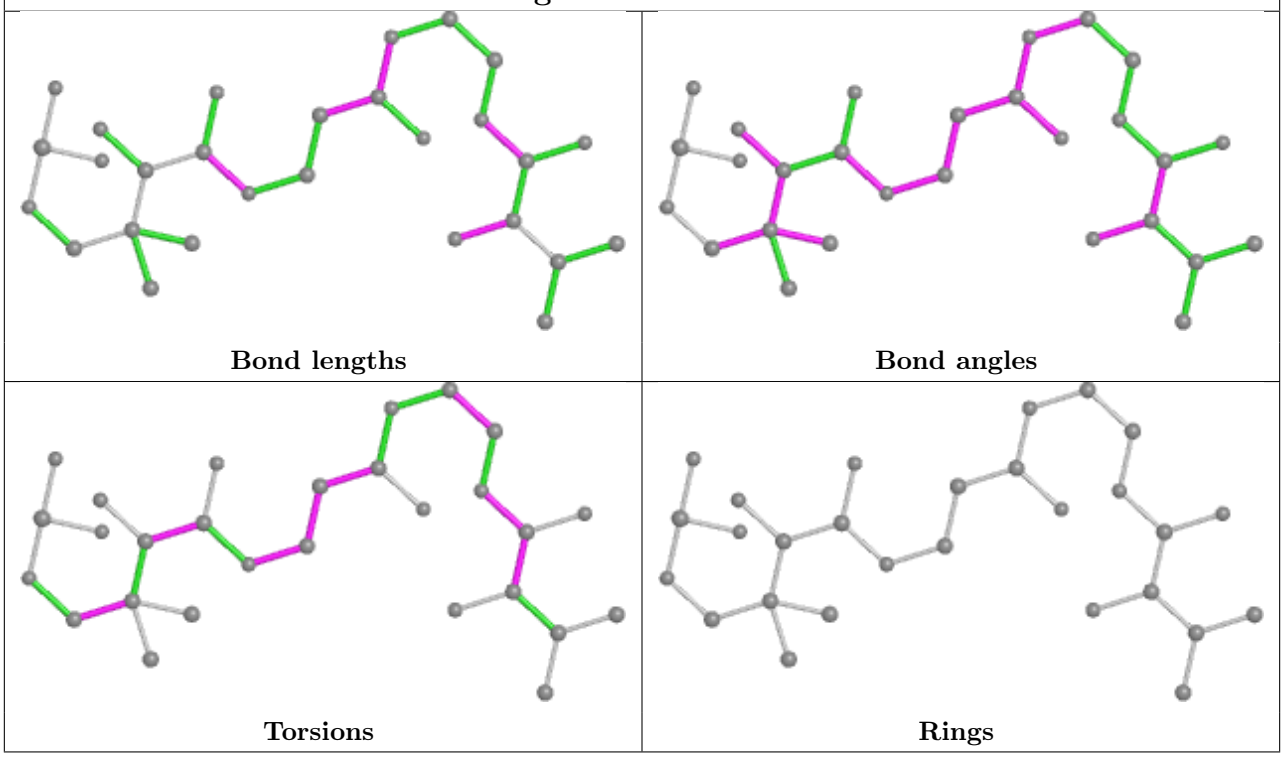
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	5S4	2	0
2	A	801	5S4	2	0

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 5S4 B 801



Ligand 5S4 A 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	759/776 (97%)	0.77	83 (10%)	5	7	59, 78, 135, 177	0
1	B	768/776 (98%)	0.62	54 (7%)	16	19	59, 78, 109, 154	0
All	All	1527/1552 (98%)	0.69	137 (8%)	9	11	59, 78, 121, 177	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	763	LEU	9.7
1	A	768	ALA	8.1
1	A	760	LEU	7.5
1	B	197	GLY	7.1
1	B	763	LEU	6.4
1	A	197	GLY	6.4
1	A	41	ASN	6.2
1	A	670	ASN	6.1
1	A	746	LEU	6.1
1	A	42	LEU	5.9
1	A	767	GLN	5.9
1	B	744	LEU	5.6
1	A	196	ARG	5.2
1	B	672	LYS	5.2
1	A	193	GLU	5.0
1	A	45	ILE	4.9
1	A	770	ALA	4.9
1	A	696	THR	4.9
1	A	703	LEU	4.8
1	A	702	GLN	4.6
1	A	694	ALA	4.5
1	A	769	ALA	4.5
1	B	687	LEU	4.5
1	A	695	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	77	LEU	4.3
1	B	671	GLY	4.1
1	B	198	GLU	4.1
1	B	769	ALA	4.1
1	B	4	ILE	4.1
1	A	752	PHE	4.0
1	A	673	VAL	4.0
1	A	765	THR	3.8
1	A	766	GLU	3.8
1	B	196	ARG	3.8
1	A	735	LEU	3.7
1	B	691	ASP	3.7
1	A	719	ASP	3.7
1	A	198	GLU	3.7
1	A	744	LEU	3.7
1	A	677	ALA	3.7
1	B	770	ALA	3.7
1	A	678	LEU	3.6
1	B	623	GLY	3.6
1	A	40	ALA	3.6
1	A	700	GLU	3.6
1	B	764	LEU	3.5
1	B	768	ALA	3.5
1	A	195	LYS	3.5
1	A	736	ILE	3.4
1	A	707	TRP	3.4
1	B	612	LEU	3.3
1	A	680	ASP	3.3
1	A	762	ARG	3.3
1	A	612	LEU	3.3
1	B	44	GLU	3.2
1	A	669	ALA	3.2
1	A	699	LEU	3.1
1	B	621	ALA	3.1
1	A	764	LEU	3.1
1	A	392	SER	3.0
1	A	709	HIS	3.0
1	B	195	LYS	3.0
1	A	393	PHE	3.0
1	A	676	ARG	3.0
1	A	194	PRO	3.0
1	A	704	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	749	ASP	2.9
1	A	715	GLN	2.9
1	B	22	GLU	2.9
1	B	199	LYS	2.9
1	A	739	LEU	2.9
1	A	672	LYS	2.8
1	B	762	ARG	2.8
1	B	118	ILE	2.7
1	B	302	ALA	2.6
1	A	722	PHE	2.6
1	B	30	ILE	2.6
1	B	41	ASN	2.6
1	B	67	GLY	2.6
1	A	662	MET	2.6
1	A	4	ILE	2.6
1	B	746	LEU	2.6
1	A	3	ARG	2.6
1	A	713	ILE	2.5
1	A	419	ARG	2.5
1	B	193	GLU	2.5
1	B	669	ALA	2.5
1	A	747	ARG	2.5
1	B	1	MET	2.5
1	A	27	GLU	2.5
1	B	42	LEU	2.5
1	A	77	LEU	2.5
1	B	45	ILE	2.5
1	A	1	MET	2.5
1	B	397	GLY	2.5
1	B	766	GLU	2.4
1	B	767	GLN	2.4
1	B	742	ILE	2.4
1	A	116	GLU	2.4
1	A	400	LEU	2.4
1	B	201	ILE	2.4
1	A	317	ALA	2.4
1	B	3	ARG	2.3
1	B	482	GLY	2.3
1	B	181	VAL	2.3
1	B	610	ILE	2.3
1	A	625	LYS	2.3
1	B	40	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	667	LEU	2.3
1	B	655	ILE	2.3
1	A	668	THR	2.3
1	A	745	SER	2.3
1	A	31	CYS	2.3
1	A	671	GLY	2.2
1	B	542	TYR	2.2
1	A	490	VAL	2.2
1	A	22	GLU	2.2
1	A	358	ALA	2.2
1	B	665	PHE	2.2
1	B	179	THR	2.2
1	B	393	PHE	2.2
1	A	561	GLU	2.2
1	A	281	VAL	2.2
1	A	750	GLN	2.2
1	B	667	LEU	2.2
1	B	760	LEU	2.2
1	A	665	PHE	2.1
1	B	683	ALA	2.1
1	A	190	LEU	2.1
1	A	397	GLY	2.1
1	B	745	SER	2.1
1	A	655	ILE	2.1
1	A	181	VAL	2.1
1	A	343	ASP	2.1
1	A	742	ILE	2.0
1	B	20	TYR	2.0
1	A	681	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

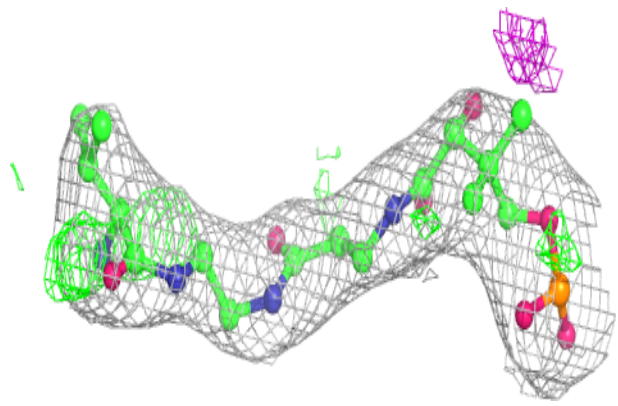
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

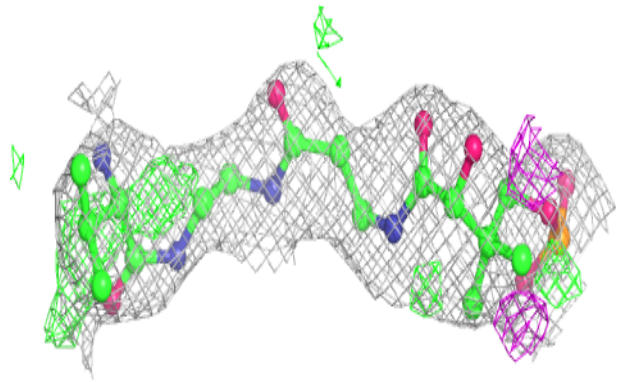
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5S4	A	801	28/29	0.93	0.31	69,81,95,119	0
2	5S4	B	801	28/29	0.93	0.32	65,78,99,126	0

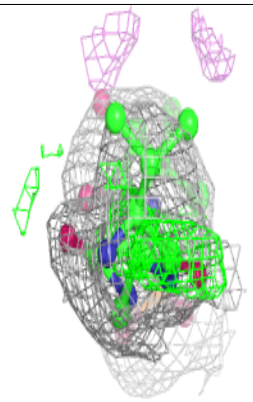
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5S4 A 801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

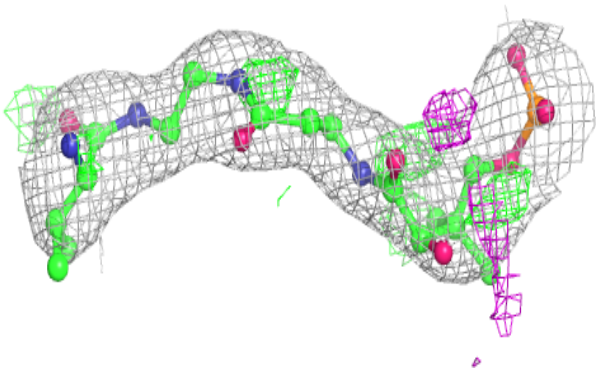


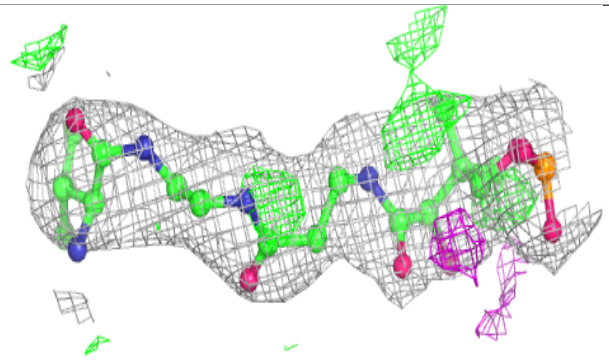


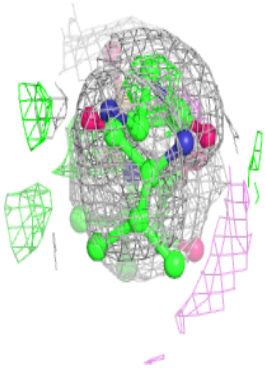


Electron density around 5S4 B 801:

$2mF_o$-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.