



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:55 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

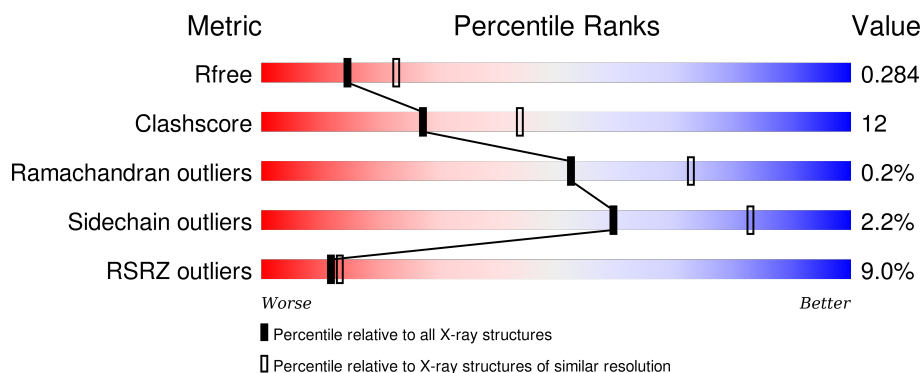
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	776	<div> <div>11%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	B	776	<div> <div>7%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5S4	B	801	-	-	-	X

2 Entry composition

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.

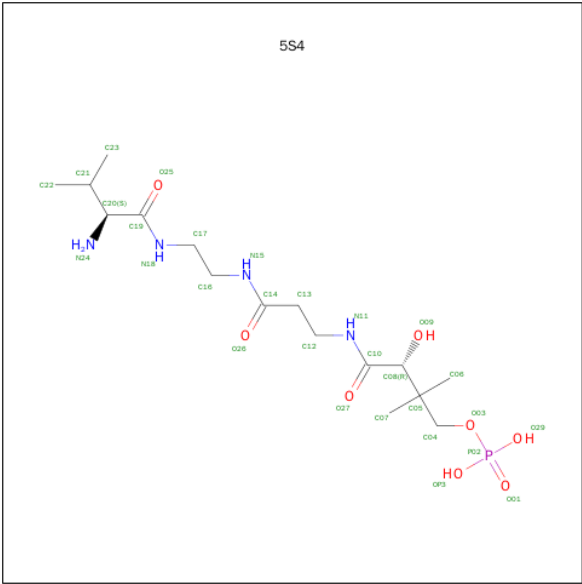
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			6054	3862	1041	1125	26			
1	B	768	Total	C	N	O	S	0	0	0
			6126	3907	1051	1142	26			

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

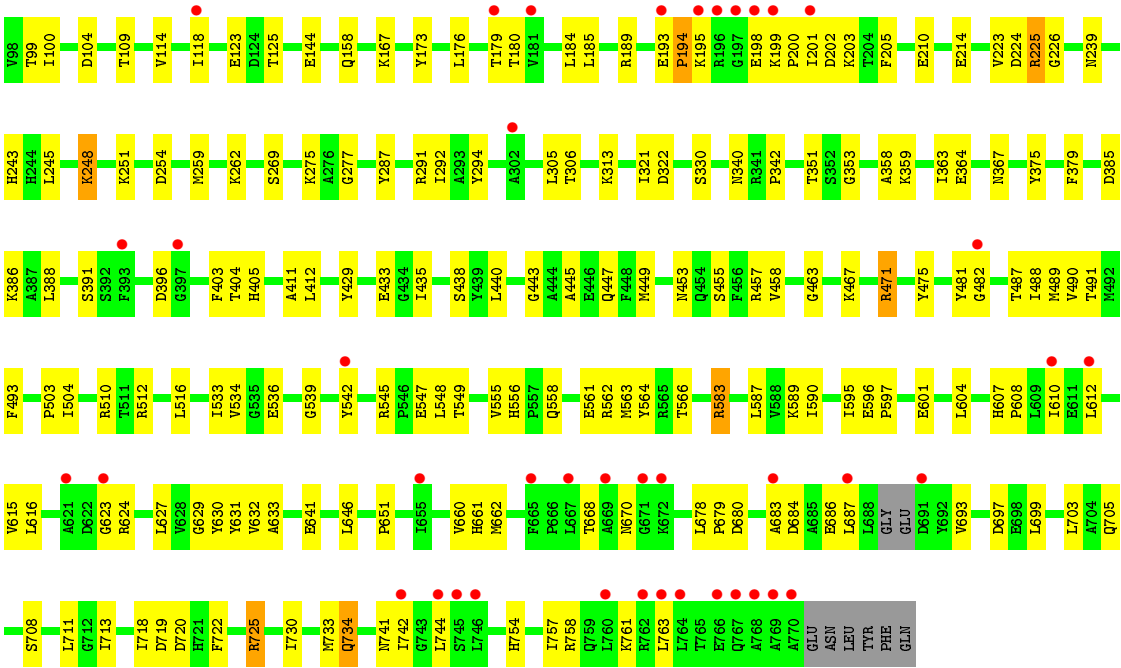
phosphate (three-letter code: 5S4) (formula: C₁₆H₃₃N₄O₈P).



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

- Molecule 3 is water.

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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.274 0.241 , 0.284	Depositor DCC
R_{free} test set	3292 reflections (5.87%)	DCC
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.8	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65675 reflections	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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(°)	Ideal(°)
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: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:355:THR:O	1:A:359:LYS:NZ	2.24	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:457:ARG:HD2	1:B:458:VAL:HG23	1.80	0.64
1:B:443:GLY:HA2	1:B:624:ARG:HH12	1.63	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:420:LYS:NZ	3:A:902:HOH:O	2.32	0.61
1:A:125:THR:HA	1:A:180:THR:HA	1.83	0.61
1:A:590:ILE:HB	1:A:595:ILE:HD12	1.81	0.61
1:B:385:ASP:OD1	1:B:457:ARG:NH2	2.34	0.61
1:A:77:LEU:HB2	1:A:99:THR:HG21	1.82	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:556:HIS:CE1	1:B:558:GLN:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASN:N	1:B:15:ASN:OD1	2.36	0.56
1:B:75:SER:OG	1:B:79:TRP:O	2.23	0.56
1:A:616:LEU:HD11	1:A:678:LEU:HD12	1.87	0.56
1:B:607:HIS:HB3	1:B:610:ILE:HG12	1.87	0.56
1:A:612:LEU:H	1:A:632:VAL:HG12	1.71	0.56
1:B:443:GLY:HA2	1:B:624:ARG:NH1	2.21	0.55
1:A:75:SER:OG	1:A:79:TRP:O	2.24	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:N	1:A:58:ASP:OD1	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:B:720:ASP:OD2	1:B:725:ARG:NH1	2.41	0.53
1:A:590:ILE:HG13	1:A:627:LEU:HG	1.91	0.53
1:B:277:GLY:O	1:B:340:ASN:ND2	2.41	0.53
1:B:58:ASP:OD1	1:B:58:ASP:N	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:B:719:ASP:OD2	1:B:758:ARG:NE	2.43	0.51
1:A:77:LEU:HD12	1:A:158:GLN:NE2	2.25	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:B:601:GLU:HG3	1:B:615:VAL:HG22	1.93	0.50
1:A:741:ASN:OD1	1:A:742:ILE:N	2.44	0.50
1:A:728:ASP:OD1	1:A:731:LYS:HG2	2.11	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:A:179:THR:HG21	1:A:184:LEU:HD13	1.94	0.50
1:A:39:SER:O	1:A:43:GLN:NE2	2.44	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:B:379:PHE:O	1:B:457:ARG:NH1	2.46	0.49
1:A:210:GLU:O	1:A:214:GLU:HG2	2.13	0.49
1:A:13:LYS:HG2	1:A:30:ILE:HG21	1.95	0.49
1:A:608:PRO:HA	1:B:167:LYS:HD3	1.95	0.49
1:B:388:LEU:HG	1:B:435:ILE:HG21	1.93	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:721:HIS:HE1	1:A:723:LEU:HG	1.78	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:OE1	1:B:705:GLN:N	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:B:388:LEU:HB2	1:B:438:SER:OG	2.14	0.47
1:A:343:ASP:HA	1:A:366:HIS:HD2	1.78	0.47
1:B:225:ARG:CG	1:B:226:GLY:H	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:SER:HB2	1:B:85:PRO:HB2	1.95	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:B:195:LYS:HA	1:B:198:GLU:CG	2.43	0.47
1:A:367:ASN:HB3	1:A:487:THR:OG1	2.14	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:B:259:MET:CE	1:B:292:ILE:HD13	2.45	0.46
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: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:B:225:ARG:HD2	1:B:226:GLY:H	1.79	0.46
1:A:445:ALA:O	1:A:449:MET:HG3	2.15	0.46
1:A:597:PRO:HB3	1:A:615:VAL:HG23	1.97	0.46
1:B:632:VAL:HA	1:B:662:MET:O	2.15	0.46
1:A:716:MET:O	1:A:716:MET:HG3	2.14	0.46
1:B:388:LEU:H	1:B:438:SER:HG	1.64	0.46
1:B:4:ILE:HG12	1:B:47:TRP:HB2	1.98	0.46
1:A:699:LEU:O	1:A:702:GLN:HG2	2.16	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:596:GLU:HA	1:A:597:PRO:HD2	1.80	0.46
1:B:730:ILE:HD13	1:B:733:MET:CE	2.45	0.46
1:B:590:ILE:HG12	1:B:627:LEU:HG	1.98	0.46
1:A:375:TYR:CD1	1:A:404:THR:HB	2.51	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:B:562:ARG:NH2	3:B:901:HOH:O	2.50	0.45
1:A:734:GLN:O	1:A:738:GLN:HG3	2.15	0.45
1:A:294:TYR:OH	1:A:545:ARG:NH2	2.48	0.45
1:A:205:PHE:CE1	1:A:403:PHE:HB3	2.51	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:B:306:THR:O	1:B:322:ASP:HA	2.16	0.45
1:A:708:SER:HB2	1:A:713:ILE:O	2.16	0.45
1:B:259:MET:HE1	1:B:292:ILE:HD13	1.99	0.45
1:B:114:VAL:HG11	1:B:144:GLU:HG3	2.00	0.44
1:A:405:HIS:HB2	1:A:412:LEU:HD21	1.99	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:B:194:PRO:HG3	1:B:512:ARG:HD3	1.98	0.44
1:B:80:ASN:OD1	1:B:94:THR:HG21	2.17	0.44
1:A:568:ASP:HA	1:A:583:ARG:HG2	2.00	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:B:596:GLU:HA	1:B:597:PRO:HD2	1.73	0.44
1:B:516:LEU:HD11	1:B:563:MET:HE1	2.00	0.44
1:A:188:LYS:O	1:A:192:ALA:N	2.51	0.44
1:A:185:LEU:O	1:A:189:ARG:HG3	2.17	0.44
1:B:490:VAL:HG11	1:B:533:ILE:HD13	2.00	0.44
1:B:77:LEU:HD12	1:B:158:GLN:NE2	2.33	0.44
1:A:421:TYR:HA	1:A:733:MET:CE	2.47	0.44
1:B:125:THR:HA	1:B:180:THR:HA	2.00	0.44
1:A:8:THR:O	1:A:32:GLN:HG3	2.17	0.44
1:B:291:ARG:HH22	1:B:358:ALA:HB2	1.83	0.44
1:B:199:LYS:HG2	1:B:200:PRO:O	2.18	0.43
1:A:586:ASN:HD22	1:A:675:ARG:NH1	2.16	0.43
1:A:312:GLU:O	1:A:315:ASN:N	2.38	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:593:TYR:CZ	2:A:801:5S4:H22	2.53	0.43
1:A:62:VAL:HG21	1:A:103:ILE:HG22	2.00	0.43
1:A:174:LYS:HA	1:A:174:LYS:HD2	1.59	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:604:LEU:HD13	1:A:646:LEU:HD11	2.01	0.42
1:A:294:TYR:CD1	1:A:357:LEU:HD23	2.54	0.42
1:A:427:ASN:ND2	1:A:453:ASN:HB2	2.34	0.42
1:B:42:LEU:HA	1:B:42:LEU:HD12	1.75	0.42
1:B:94:THR:HG23	1:B:95:PRO:O	2.19	0.42
1:B:5:LEU:N	1:B:45:ILE:HD11	2.35	0.42
1:B:604:LEU:HD13	1:B:646:LEU:HD21	2.01	0.42
1:A:147:ASN:HB3	1:A:153:ILE:HG13	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:173:TYR:HB3	1:B:176:LEU:HD12	2.02	0.42
1:B:754:HIS:CE1	1:B:763:LEU:HD13	2.55	0.42
1:B:435:ILE:O	1:B:455:SER:OG	2.32	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:364:GLU:O	1:B:367:ASN:HB2	2.20	0.41
1:A:196:ARG:HA	1:A:196:ARG:HD3	1.84	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:630:TYR:OH	1:B:679:PRO:O	2.24	0.41
1:B:185:LEU:O	1:B:189:ARG:HG3	2.19	0.41
1:B:97:GLY:HA2	1:B:118:ILE:HG22	2.03	0.41
1:A:312:GLU:HG2	1:A:312:GLU:O	2.21	0.41
1:B:718:ILE:O	1:B:757:ILE:HB	2.21	0.41
1:B:294:TYR:OH	1:B:545:ARG:NH2	2.54	0.41
1:A:493:PHE:HB2	1:A:505:GLY:HA3	2.01	0.41
1:B:429:TYR:CZ	1:B:433:GLU:HG3	2.55	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:614:THR:O	1:A:630:TYR:HB2	2.21	0.40
1:A:96:LYS:HB2	1:A:118:ILE:O	2.21	0.40
1:B:440:LEU:HB2	1:B:445:ALA:HB2	2.02	0.40
1:A:667:LEU:HB3	1:A:672:LYS:O	2.21	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:B:194:PRO:HD3	1:B:512:ARG:HD3	2.03	0.40
1:A:612:LEU:N	1:A:632:VAL:HG12	2.36	0.40
1:B:5:LEU:HB2	1:B:45:ILE:HG12	2.03	0.40
1:A:97:GLY:HA2	1:A:118:ILE:HG22	2.03	0.40
1:A:617:ALA:O	1:A:618:LYS:HD2	2.22	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%)	56 76
1	B	764/776 (98%)	746 (98%)	16 (2%)	2 (0%)	46 66
All	All	1519/1552 (98%)	1488 (98%)	28 (2%)	3 (0%)	52 73

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%)	72	90
1	B	658/666 (99%)	639 (97%)	19 (3%)	50	75
All	All	1309/1332 (98%)	1280 (98%)	29 (2%)	60	83

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

Some 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 ⓘ

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 ⓘ

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	A	801	1	19,27,28	2.30	4 (21%)	24,36,39	1.75	5 (20%)
2	5S4	B	801	1	19,27,28	2.28	4 (21%)	24,36,39	1.43	4 (16%)

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	A	801	1	-	0/35/37/38	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5S4	B	801	1	-	0/35/37/38	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	5S4	C13-C14	2.54	1.56	1.51
2	B	801	5S4	C13-C14	2.70	1.56	1.51
2	B	801	5S4	C19-N18	4.33	1.42	1.33
2	A	801	5S4	C19-N18	4.60	1.43	1.33
2	B	801	5S4	C14-N15	4.65	1.44	1.33
2	A	801	5S4	C14-N15	4.66	1.44	1.33
2	B	801	5S4	C10-N11	6.39	1.46	1.33
2	A	801	5S4	C10-N11	6.40	1.46	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	5S4	O26-C14-C13	-2.28	118.01	121.97
2	A	801	5S4	C16-N15-C14	-2.06	118.71	122.79
2	B	801	5S4	C07-C05-C08	2.07	112.95	109.17
2	B	801	5S4	C12-N11-C10	2.08	126.80	122.62
2	B	801	5S4	C13-C14-N15	2.22	120.33	116.46
2	A	801	5S4	C13-C14-N15	2.83	121.38	116.46
2	A	801	5S4	C07-C05-C04	4.05	113.75	108.50
2	B	801	5S4	C12-C13-C14	4.56	120.04	112.22
2	A	801	5S4	C12-C13-C14	4.83	120.50	112.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

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, 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%) 7 8	59, 78, 135, 177	0
1	B	768/776 (98%)	0.62	54 (7%) 19 22	59, 78, 109, 154	0
All	All	1527/1552 (98%)	0.69	137 (8%) 12 13	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	4.4

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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	768	ALA	3.5
1	B	764	LEU	3.5
1	A	195	LYS	3.5
1	A	736	ILE	3.4
1	A	707	TRP	3.4
1	A	680	ASP	3.3
1	B	612	LEU	3.3
1	A	612	LEU	3.3
1	A	762	ARG	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	749	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	704	ALA	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	2.7
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	713	ILE	2.6
1	A	3	ARG	2.6
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	767	GLN	2.4
1	B	742	ILE	2.4
1	B	766	GLU	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	671	GLY	2.3
1	A	31	CYS	2.3
1	A	22	GLU	2.2
1	B	542	TYR	2.2
1	A	490	VAL	2.2
1	A	358	ALA	2.2
1	B	665	PHE	2.2
1	A	281	VAL	2.2
1	B	393	PHE	2.2
1	A	561	GLU	2.2
1	B	179	THR	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	A	190	LEU	2.1
1	A	397	GLY	2.1
1	B	683	ALA	2.1
1	A	655	ILE	2.1
1	B	745	SER	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	5S4	B	801	28/29	0.93	0.32	2.18	65,78,99,126	0
2	5S4	A	801	28/29	0.93	0.31	1.86	69,81,95,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.