



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 AM GMT

PDB ID : 2R4O  
Title : Crystal structure of the long-chain fatty acid transporter FadL mutant delta NPA  
Authors : Hearn, E.M.; Patel, D.R.; Lepore, B.W.; Indic, M.; van den Berg, B.  
Deposited on : 2007-08-31  
Resolution : 3.60 Å(reported)

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

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

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

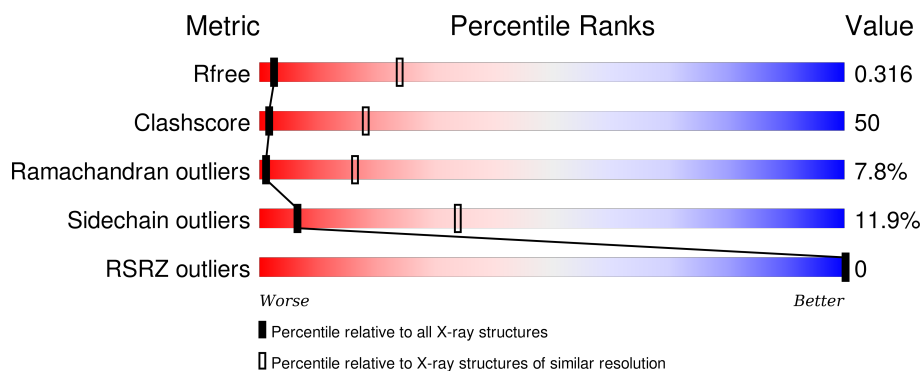
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

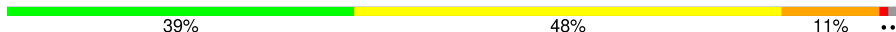

The reported resolution of this entry is 3.60 Å.

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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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

Mol	Chain	Length	Quality of chain
1	A	427	 39% 48% 11% ..
1	B	427	 40% 45% 12% ..

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	LDA	A	501	-	-	-	X
2	LDA	A	503	-	-	X	X
2	LDA	B	502	-	-	-	X
2	LDA	B	504	-	-	X	X

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6550 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.

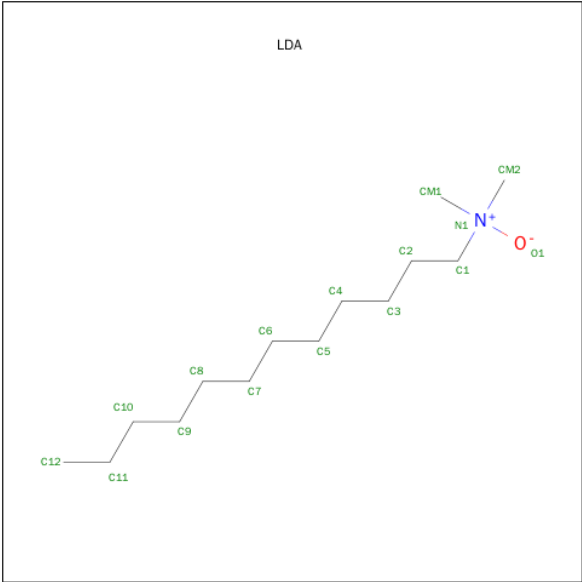
- Molecule 1 is a protein called Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3243	2049	551	637	6			
1	B	421	Total	C	N	O	S	0	0	0
			3243	2049	551	637	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	ASN	ENGINEERED	UNP P10384
A	34	GLY	PRO	ENGINEERED	UNP P10384
A	35	GLY	ALA	ENGINEERED	UNP P10384
A	197	THR	ILE	CONFLICT	UNP P10384
A	422	HIS	-	EXPRESSION TAG	UNP P10384
A	423	HIS	-	EXPRESSION TAG	UNP P10384
A	424	HIS	-	EXPRESSION TAG	UNP P10384
A	425	HIS	-	EXPRESSION TAG	UNP P10384
A	426	HIS	-	EXPRESSION TAG	UNP P10384
A	427	HIS	-	EXPRESSION TAG	UNP P10384
B	33	GLY	ASN	ENGINEERED	UNP P10384
B	34	GLY	PRO	ENGINEERED	UNP P10384
B	35	GLY	ALA	ENGINEERED	UNP P10384
B	197	THR	ILE	CONFLICT	UNP P10384
B	422	HIS	-	EXPRESSION TAG	UNP P10384
B	423	HIS	-	EXPRESSION TAG	UNP P10384
B	424	HIS	-	EXPRESSION TAG	UNP P10384
B	425	HIS	-	EXPRESSION TAG	UNP P10384
B	426	HIS	-	EXPRESSION TAG	UNP P10384
B	427	HIS	-	EXPRESSION TAG	UNP P10384

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).

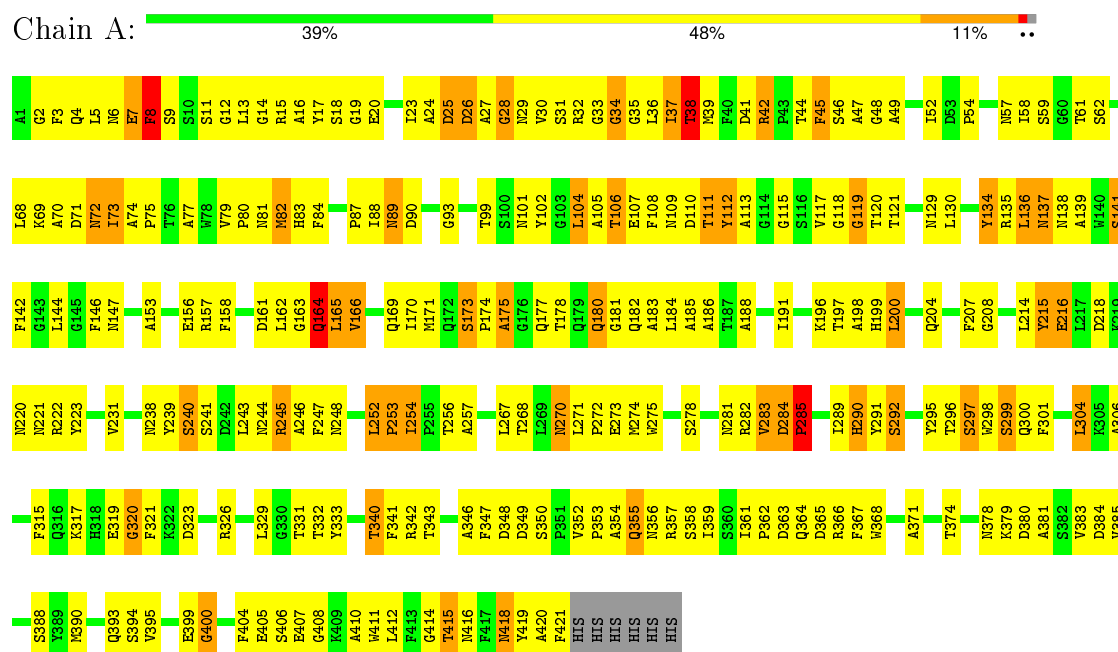


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

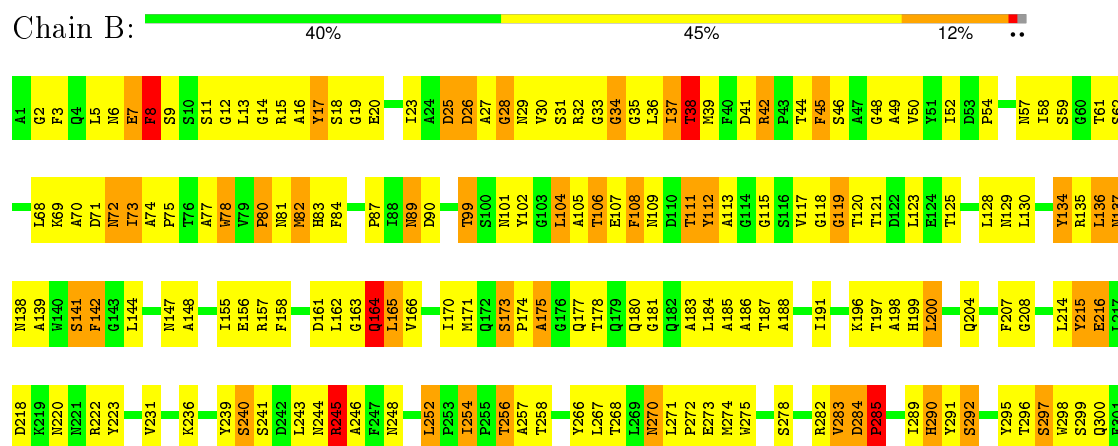
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Long-chain fatty acid transport protein



#### • Molecule 1: Long-chain fatty acid transport protein



D884	V885	S888	X889	X890	Q893	S894	V895	E899	G900	P901	Y902	Q903	P904	E905	S906	E907	G908	K909	A910	W911	L912	F913	G914	T915	W916	F917	W918	Y919	H920	F921	H922	H923	H924	H925	H926	H927	H928	H929	H930	H931	H932	H933	H934	H935	H936	H937	H938	H939	H940	H941	H942	H943	H944	H945	H946	H947	H948	H949	H950	H951	H952	H953	H954	H955	H956	H957	H958	H959	H960	H961	H962	H963	H964	H965	H966	H967	H968	A969	A970	A971	T972	Y973	M974	K975	D976	A977
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.05Å 146.62Å 151.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.60 41.54 – 3.58	Depositor EDS
% Data completeness (in resolution range)	98.7 (10.00-3.60) 98.4 (41.54-3.58)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 3.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.243 , 0.314 0.250 , 0.316	Depositor DCC
$R_{free}$ test set	1602 reflections (10.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.2	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 7.9	EDS
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 16838 reflections (0.012%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	6550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.47	0/3331	0.72	0/4533
1	B	0.48	0/3331	0.73	0/4533
All	All	0.48	0/6662	0.73	0/9066

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3243	0	3020	313	0
1	B	3243	0	3020	320	0
2	A	32	0	62	14	0
2	B	32	0	62	12	0
All	All	6550	0	6164	635	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 50.

All (635) 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:346:ALA:HB3	1:B:368:TRP:HB2	1.37	1.05
1:B:75:PRO:HD2	1:B:105:ALA:HB1	1.39	1.05
1:A:75:PRO:HD2	1:A:105:ALA:HB1	1.38	1.04
1:A:346:ALA:HB3	1:A:368:TRP:HB2	1.38	1.04
1:B:89:ASN:CG	1:B:90:ASP:H	1.64	1.00
1:B:252:LEU:HD12	1:B:252:LEU:H	1.27	0.97
1:B:134:TYR:HD2	1:B:135:ARG:N	1.62	0.97
1:A:134:TYR:HD2	1:A:135:ARG:N	1.65	0.95
1:A:19:GLY:N	1:A:292:SER:HB2	1.82	0.95
1:B:241:SER:HB3	1:B:257:ALA:HA	1.47	0.94
1:A:252:LEU:HD12	1:A:252:LEU:H	1.28	0.94
1:A:89:ASN:CG	1:A:90:ASP:H	1.71	0.93
1:A:357:ARG:NH1	1:A:395:VAL:HB	1.82	0.93
1:B:357:ARG:NH1	1:B:395:VAL:HB	1.83	0.92
1:A:289:ILE:HG13	1:A:331:THR:HG22	1.53	0.91
1:B:52:ILE:HG12	1:B:412:LEU:HD22	1.52	0.91
1:B:102:TYR:OH	1:B:272:PRO:HG2	1.72	0.90
1:B:52:ILE:HB	1:B:77:ALA:HB3	1.54	0.90
1:A:241:SER:HB3	1:A:257:ALA:HA	1.52	0.90
1:B:134:TYR:HD2	1:B:135:ARG:H	1.19	0.90
1:B:19:GLY:N	1:B:292:SER:HB2	1.87	0.89
1:B:289:ILE:HG13	1:B:331:THR:HG22	1.55	0.89
1:A:385:VAL:HG22	1:A:415:THR:HG23	1.54	0.88
1:A:134:TYR:HD2	1:A:135:ARG:H	1.22	0.88
1:B:75:PRO:CD	1:B:105:ALA:HB1	2.03	0.88
1:B:68:LEU:HD12	1:B:404:PHE:HE2	1.37	0.88
1:A:248:ASN:HD21	1:A:257:ALA:H	1.21	0.87
1:A:52:ILE:HB	1:A:77:ALA:HB3	1.57	0.87
1:A:75:PRO:CD	1:A:105:ALA:HB1	2.04	0.86
1:B:385:VAL:HG22	1:B:415:THR:HG23	1.55	0.86
1:A:157:ARG:C	1:A:197:THR:HG22	1.95	0.85
1:A:173:SER:O	1:A:175:ALA:N	2.08	0.85
1:A:38:THR:HG21	1:A:141:SER:HB3	1.57	0.85
1:B:173:SER:O	1:B:175:ALA:N	2.09	0.84
1:B:137:ASN:ND2	1:B:139:ALA:H	1.75	0.84
1:A:68:LEU:HD12	1:A:404:PHE:HE2	1.41	0.84
1:B:68:LEU:HD12	1:B:404:PHE:CE2	2.13	0.83
1:B:104:LEU:HA	2:B:502:LDA:H62	1.62	0.82
1:A:284:ASP:OD1	1:A:285:PRO:HD2	1.79	0.82
1:B:248:ASN:HD21	1:B:257:ALA:H	1.25	0.82
1:B:117:VAL:HG13	1:B:359:ILE:HD11	1.61	0.82
1:A:31:SER:O	1:A:32:ARG:HB3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HG12	1:A:412:LEU:HD22	1.61	0.81
1:A:73:ILE:O	1:A:75:PRO:HD3	1.79	0.81
1:B:31:SER:O	1:B:32:ARG:HB3	1.80	0.80
1:B:157:ARG:C	1:B:197:THR:HG22	2.01	0.80
1:B:267:LEU:HD23	1:B:268:THR:N	1.96	0.80
1:A:111:THR:O	1:A:112:TYR:HB3	1.83	0.79
1:A:28:GLY:HA2	1:A:83:HIS:CG	2.17	0.79
1:B:273:GLU:HG2	1:B:297:SER:OG	1.82	0.78
1:A:137:ASN:ND2	1:A:139:ALA:H	1.81	0.78
1:B:28:GLY:HA2	1:B:83:HIS:CG	2.18	0.78
1:A:267:LEU:HD23	1:A:268:THR:N	1.99	0.77
1:B:12:GLY:HA2	1:B:15:ARG:NH1	1.99	0.77
1:A:68:LEU:HD12	1:A:404:PHE:CE2	2.18	0.77
1:B:111:THR:O	1:B:112:TYR:HB3	1.85	0.76
1:B:72:ASN:HD22	1:B:73:ILE:N	1.83	0.76
1:A:104:LEU:HB2	2:A:501:LDA:H21	1.67	0.76
1:A:72:ASN:HD22	1:A:73:ILE:N	1.84	0.76
1:B:89:ASN:CG	1:B:90:ASP:N	2.35	0.75
1:B:200:LEU:HB3	2:B:504:LDA:H111	1.67	0.75
1:B:141:SER:C	1:B:142:PHE:HD2	1.89	0.75
1:B:134:TYR:CD2	1:B:135:ARG:N	2.52	0.75
1:B:73:ILE:O	1:B:75:PRO:HD3	1.87	0.75
1:A:273:GLU:HG2	1:A:297:SER:OG	1.86	0.75
1:A:75:PRO:HD2	1:A:105:ALA:CB	2.18	0.74
1:A:48:GLY:HA3	1:A:416:ASN:ND2	2.02	0.74
1:A:157:ARG:O	1:A:197:THR:HG22	1.88	0.74
1:B:157:ARG:O	1:B:197:THR:HG22	1.88	0.74
1:B:241:SER:CB	1:B:257:ALA:HA	2.18	0.73
1:A:156:GLU:OE1	1:A:196:LYS:HE2	1.88	0.73
1:A:317:LYS:NZ	2:A:503:LDA:HM23	2.04	0.73
1:A:296:THR:O	1:A:298:TRP:N	2.22	0.73
1:B:38:THR:HG21	1:B:141:SER:HB3	1.69	0.72
1:B:73:ILE:HG22	1:B:107:GLU:H	1.54	0.72
1:B:75:PRO:HD2	1:B:105:ALA:CB	2.19	0.72
1:A:102:TYR:OH	1:A:272:PRO:HG2	1.89	0.72
1:B:346:ALA:HB3	1:B:368:TRP:CB	2.15	0.72
1:A:23:ILE:HG12	1:A:23:ILE:O	1.90	0.72
1:A:346:ALA:HB3	1:A:368:TRP:CB	2.17	0.72
1:A:12:GLY:HA2	1:A:15:ARG:NH1	2.05	0.71
1:B:62:SER:CB	1:B:68:LEU:HD21	2.20	0.71
1:A:62:SER:CB	1:A:68:LEU:HD21	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TRP:O	1:A:412:LEU:HD23	1.91	0.71
1:A:270:ASN:N	1:A:270:ASN:HD22	1.89	0.70
1:A:134:TYR:CD2	1:A:135:ARG:N	2.55	0.70
1:A:58:ILE:HB	1:A:70:ALA:HB3	1.74	0.70
1:A:38:THR:HG21	1:A:141:SER:CB	2.22	0.70
1:B:48:GLY:HA3	1:B:416:ASN:ND2	2.05	0.70
1:B:73:ILE:HG22	1:B:107:GLU:N	2.07	0.70
1:A:248:ASN:ND2	1:A:257:ALA:H	1.90	0.69
1:A:37:ILE:O	1:A:39:MET:N	2.25	0.69
1:B:291:TYR:O	1:B:292:SER:HB2	1.92	0.69
1:A:89:ASN:CG	1:A:90:ASP:N	2.42	0.69
1:A:58:ILE:HD13	1:A:406:SER:HB2	1.75	0.69
1:B:199:HIS:O	1:B:239:TYR:HA	1.92	0.68
1:B:284:ASP:OD1	1:B:285:PRO:HD2	1.93	0.68
1:B:156:GLU:OE1	1:B:196:LYS:HE2	1.93	0.68
1:A:199:HIS:O	1:A:239:TYR:HA	1.93	0.68
1:A:248:ASN:HD21	1:A:257:ALA:N	1.90	0.68
1:B:200:LEU:N	1:B:200:LEU:HD12	2.09	0.68
1:B:384:ASP:HB2	1:B:416:ASN:HB2	1.74	0.68
1:B:166:VAL:O	1:B:170:ILE:HG13	1.93	0.68
1:A:46:SER:CB	1:A:418:ASN:HB3	2.24	0.67
1:B:420:ALA:C	1:B:421:PHE:HD2	1.96	0.67
1:B:248:ASN:HD21	1:B:256:THR:HA	1.59	0.67
1:B:267:LEU:HD23	1:B:267:LEU:C	2.14	0.67
1:A:358:SER:HB2	1:A:399:GLU:OE1	1.95	0.67
1:B:37:ILE:O	1:B:39:MET:N	2.28	0.67
1:B:214:LEU:HD12	1:B:215:TYR:N	2.10	0.67
1:B:38:THR:HG21	1:B:141:SER:CB	2.24	0.67
1:A:248:ASN:HD21	1:A:256:THR:HA	1.57	0.67
1:B:58:ILE:HB	1:B:70:ALA:HB3	1.76	0.67
1:B:46:SER:CB	1:B:418:ASN:HB3	2.25	0.67
1:A:141:SER:C	1:A:142:PHE:HD2	1.97	0.66
1:A:267:LEU:C	1:A:267:LEU:HD23	2.15	0.66
1:A:361:ILE:HD11	2:A:503:LDA:H21	1.75	0.66
1:A:220:ASN:HB3	1:A:282:ARG:HB3	1.76	0.66
1:A:102:TYR:CE1	1:A:271:LEU:HB3	2.31	0.66
1:B:220:ASN:HB3	1:B:282:ARG:HB3	1.77	0.66
1:A:166:VAL:O	1:A:170:ILE:HG13	1.94	0.66
1:A:252:LEU:CD1	1:A:252:LEU:H	2.04	0.66
1:A:200:LEU:N	1:A:200:LEU:HD12	2.12	0.65
1:A:243:LEU:HD13	1:A:254:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLY:O	1:B:35:GLY:N	2.28	0.65
1:A:7:GLU:O	1:A:9:SER:N	2.27	0.65
1:B:384:ASP:O	1:B:415:THR:HA	1.97	0.65
1:B:215:TYR:HD2	1:B:216:GLU:N	1.93	0.65
1:B:23:ILE:O	1:B:23:ILE:HG12	1.96	0.65
1:B:104:LEU:HD11	1:B:121:THR:HG22	1.78	0.65
1:A:18:SER:O	1:A:290:HIS:HB2	1.96	0.65
1:A:304:LEU:HD21	2:A:503:LDA:H52	1.79	0.65
1:B:46:SER:HB2	1:B:418:ASN:HB3	1.78	0.65
1:B:62:SER:HB2	1:B:68:LEU:HD21	1.78	0.65
1:B:385:VAL:CG2	1:B:415:THR:HG23	2.24	0.65
1:B:390:MET:HE2	1:B:412:LEU:HD11	1.79	0.64
1:B:243:LEU:HD13	1:B:254:ILE:HD11	1.79	0.64
1:B:183:ALA:O	1:B:186:ALA:HB3	1.97	0.64
1:A:385:VAL:CG2	1:A:415:THR:HG23	2.27	0.64
1:A:388:SER:HB2	1:A:412:LEU:HB2	1.80	0.64
1:B:248:ASN:HD21	1:B:257:ALA:N	1.94	0.64
1:A:304:LEU:HD13	2:A:503:LDA:HM13	1.80	0.64
1:A:243:LEU:CD1	1:A:254:ILE:HD11	2.28	0.63
1:B:296:THR:O	1:B:298:TRP:N	2.31	0.63
1:A:107:GLU:O	1:A:108:PHE:HB2	1.98	0.63
1:B:388:SER:HB2	1:B:412:LEU:HB2	1.81	0.63
1:A:46:SER:HB2	1:A:418:ASN:HB3	1.81	0.63
1:B:81:ASN:HD21	1:B:416:ASN:HD21	1.47	0.63
1:A:215:TYR:HD2	1:A:216:GLU:N	1.97	0.63
1:B:73:ILE:H	1:B:73:ILE:HD12	1.64	0.63
1:A:62:SER:HB2	1:A:68:LEU:HD21	1.80	0.63
1:B:270:ASN:N	1:B:270:ASN:HD22	1.95	0.63
1:A:104:LEU:HD11	1:A:121:THR:HG22	1.81	0.62
1:A:117:VAL:HG13	1:A:359:ILE:HD11	1.81	0.62
1:A:326:ARG:HG3	1:A:348:ASP:HB3	1.80	0.62
1:A:33:GLY:O	1:A:35:GLY:N	2.33	0.62
1:A:248:ASN:ND2	1:A:256:THR:HA	2.15	0.62
1:B:30:VAL:HG13	1:B:31:SER:N	2.15	0.62
1:A:216:GLU:HB3	1:A:222:ARG:HG2	1.80	0.62
1:B:248:ASN:ND2	1:B:257:ALA:H	1.97	0.61
1:A:317:LYS:HZ1	2:A:503:LDA:HM23	1.62	0.61
1:B:420:ALA:O	1:B:421:PHE:HD2	1.82	0.61
1:B:18:SER:O	1:B:290:HIS:HB2	2.00	0.61
1:A:384:ASP:HB2	1:A:416:ASN:HB2	1.80	0.61
1:A:30:VAL:HG13	1:A:31:SER:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HA	1:B:165:LEU:CD1	2.30	0.61
1:A:183:ALA:O	1:A:186:ALA:HB3	2.00	0.61
1:A:57:ASN:HB2	1:A:407:GLU:HG3	1.82	0.61
1:B:137:ASN:ND2	1:B:137:ASN:C	2.53	0.61
1:A:291:TYR:O	1:A:292:SER:HB2	2.01	0.61
1:B:291:TYR:O	1:B:292:SER:CB	2.49	0.60
1:B:117:VAL:HG21	1:B:399:GLU:CD	2.22	0.60
1:A:241:SER:CB	1:A:257:ALA:HA	2.26	0.60
1:B:19:GLY:H	1:B:292:SER:HB2	1.66	0.60
1:B:248:ASN:ND2	1:B:256:THR:HA	2.15	0.60
1:B:48:GLY:HA3	1:B:416:ASN:HD22	1.66	0.60
1:B:32:ARG:O	1:B:32:ARG:HG2	2.00	0.60
1:B:107:GLU:O	1:B:108:PHE:HB2	2.01	0.60
1:A:105:ALA:O	1:A:106:THR:HB	2.01	0.60
1:A:304:LEU:HD22	2:A:503:LDA:HM13	1.84	0.60
1:B:222:ARG:C	1:B:223:TYR:CD1	2.75	0.60
1:B:135:ARG:O	1:B:136:LEU:C	2.40	0.60
1:A:19:GLY:H	1:A:292:SER:HB2	1.62	0.60
1:A:48:GLY:HA3	1:A:416:ASN:HD22	1.66	0.60
1:A:222:ARG:C	1:A:223:TYR:CD1	2.75	0.60
1:A:252:LEU:N	1:A:252:LEU:HD12	2.10	0.60
1:A:420:ALA:C	1:A:421:PHE:HD2	2.04	0.60
1:B:16:ALA:O	1:B:17:TYR:C	2.40	0.60
1:B:411:TRP:O	1:B:412:LEU:HD23	2.02	0.59
1:A:11:SER:HB3	1:A:384:ASP:OD1	2.02	0.59
1:A:384:ASP:O	1:A:415:THR:HA	2.02	0.59
1:B:7:GLU:CD	1:B:7:GLU:H	2.04	0.59
1:B:105:ALA:O	1:B:106:THR:HB	2.02	0.59
1:A:117:VAL:HG21	1:A:399:GLU:CD	2.23	0.59
1:A:41:ASP:O	1:A:87:PRO:HG3	2.02	0.59
1:A:385:VAL:HA	1:A:414:GLY:O	2.03	0.59
1:A:420:ALA:O	1:A:421:PHE:HD2	1.85	0.59
1:A:73:ILE:HG22	1:A:107:GLU:H	1.67	0.59
1:B:385:VAL:HA	1:B:414:GLY:O	2.02	0.59
1:B:7:GLU:O	1:B:9:SER:N	2.30	0.59
1:A:137:ASN:C	1:A:137:ASN:ND2	2.56	0.58
1:A:135:ARG:O	1:A:136:LEU:C	2.41	0.58
1:A:33:GLY:HA3	1:A:36:LEU:HD23	1.84	0.58
1:B:57:ASN:HB2	1:B:407:GLU:HG3	1.86	0.58
1:B:142:PHE:N	1:B:142:PHE:HD2	2.02	0.58
1:A:358:SER:CB	1:A:399:GLU:OE1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:C	1:A:39:MET:H	2.07	0.58
1:A:273:GLU:H	1:A:300:GLN:HE22	1.52	0.58
1:B:216:GLU:HB3	1:B:222:ARG:HG2	1.86	0.58
1:B:41:ASP:O	1:B:87:PRO:HG3	2.03	0.58
1:A:332:THR:HG23	1:A:341:PHE:O	2.03	0.58
1:A:72:ASN:HD22	1:A:73:ILE:H	1.50	0.58
1:B:142:PHE:N	1:B:142:PHE:CD2	2.71	0.58
1:B:326:ARG:HG3	1:B:348:ASP:HB3	1.86	0.57
1:B:361:ILE:HD11	2:B:504:LDA:O1	2.04	0.57
1:B:37:ILE:C	1:B:39:MET:H	2.08	0.57
1:A:214:LEU:HD12	1:A:215:TYR:N	2.19	0.57
1:B:359:ILE:HG12	1:B:399:GLU:OE2	2.04	0.57
1:B:252:LEU:HD12	1:B:252:LEU:N	2.08	0.57
1:A:73:ILE:H	1:A:73:ILE:HD12	1.69	0.57
1:B:352:VAL:HG21	1:B:357:ARG:HA	1.87	0.57
1:A:142:PHE:CD2	1:A:142:PHE:N	2.73	0.57
1:B:2:GLY:O	1:B:366:ARG:NH2	2.37	0.57
1:A:38:THR:OG1	1:A:135:ARG:NH1	2.37	0.57
1:A:13:LEU:HA	1:A:17:TYR:CZ	2.40	0.57
1:A:32:ARG:HG2	1:A:32:ARG:O	2.03	0.57
1:B:6:ASN:O	1:B:8:PHE:HD1	1.88	0.57
1:B:129:ASN:OD1	1:B:130:LEU:N	2.38	0.57
1:A:299:SER:OG	1:A:323:ASP:OD2	2.23	0.57
1:B:30:VAL:CG1	1:B:31:SER:N	2.68	0.56
1:A:162:LEU:HA	1:A:165:LEU:CD1	2.34	0.56
1:A:15:ARG:NH1	1:A:20:GLU:OE2	2.38	0.56
1:A:73:ILE:HG22	1:A:107:GLU:N	2.19	0.56
1:B:134:TYR:CD2	1:B:136:LEU:N	2.72	0.56
1:B:113:ALA:HB1	1:B:161:ASP:CG	2.25	0.56
1:A:378:ASN:C	1:A:380:ASP:H	2.08	0.56
1:B:50:VAL:O	1:B:78:TRP:O	2.23	0.56
1:A:25:ASP:O	1:A:26:ASP:CB	2.53	0.56
1:B:105:ALA:H	2:B:502:LDA:H51	1.70	0.56
1:A:88:ILE:HG13	1:A:93:GLY:HA2	1.88	0.56
1:B:52:ILE:HG12	1:B:412:LEU:CD2	2.32	0.56
1:B:358:SER:HB2	1:B:399:GLU:OE1	2.05	0.56
1:B:33:GLY:HA3	1:B:36:LEU:HD23	1.88	0.56
1:A:289:ILE:HG12	1:A:290:HIS:N	2.20	0.56
1:A:394:SER:OG	1:A:407:GLU:HB3	2.06	0.56
1:A:134:TYR:CD2	1:A:136:LEU:N	2.74	0.55
1:A:199:HIS:C	1:A:200:LEU:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:LEU:HA	1:B:165:LEU:HD13	1.89	0.55
1:A:355:GLN:CD	1:A:355:GLN:H	2.10	0.55
1:A:352:VAL:HG21	1:A:357:ARG:HA	1.88	0.55
1:B:117:VAL:HG22	1:B:117:VAL:O	2.06	0.55
1:B:58:ILE:HD13	1:B:406:SER:HB2	1.88	0.55
1:B:399:GLU:O	1:B:400:GLY:C	2.45	0.55
1:B:123:LEU:HB2	2:B:504:LDA:H31	1.88	0.55
1:B:113:ALA:HA	1:B:161:ASP:H	1.71	0.55
1:A:274:MET:HG3	1:A:295:TYR:O	2.06	0.55
1:A:117:VAL:O	1:A:359:ILE:HD11	2.06	0.55
1:B:239:TYR:CG	1:B:240:SER:N	2.74	0.55
1:B:25:ASP:O	1:B:26:ASP:CB	2.55	0.55
1:B:111:THR:O	1:B:112:TYR:CB	2.55	0.55
1:A:135:ARG:HG2	1:A:135:ARG:O	2.07	0.55
1:B:243:LEU:CD1	1:B:254:ILE:HD11	2.36	0.55
1:B:72:ASN:HD22	1:B:73:ILE:H	1.53	0.55
1:B:394:SER:OG	1:B:407:GLU:HB3	2.07	0.54
1:A:13:LEU:HB2	1:A:17:TYR:OH	2.06	0.54
1:A:52:ILE:HG23	1:A:412:LEU:CD2	2.36	0.54
1:B:52:ILE:HG21	2:B:502:LDA:HM11	1.89	0.54
1:A:142:PHE:HD2	1:A:142:PHE:N	2.05	0.54
1:A:291:TYR:O	1:A:292:SER:CB	2.55	0.54
1:B:354:ALA:HA	1:B:357:ARG:HG3	1.89	0.54
1:B:25:ASP:OD1	1:B:25:ASP:O	2.25	0.54
1:A:129:ASN:OD1	1:A:130:LEU:N	2.40	0.54
1:A:378:ASN:O	1:A:380:ASP:N	2.41	0.54
1:B:54:PRO:HG2	1:B:74:ALA:O	2.07	0.54
1:A:104:LEU:CD1	1:A:104:LEU:C	2.75	0.54
1:A:19:GLY:CA	1:A:292:SER:HB2	2.36	0.54
1:B:289:ILE:HG12	1:B:290:HIS:N	2.22	0.54
1:A:30:VAL:CG1	1:A:31:SER:N	2.70	0.54
1:B:214:LEU:HD12	1:B:215:TYR:H	1.71	0.54
1:B:11:SER:HB3	1:B:384:ASP:OD1	2.08	0.54
1:B:218:ASP:OD1	1:B:220:ASN:N	2.37	0.54
1:A:113:ALA:HA	1:A:161:ASP:H	1.72	0.54
1:A:162:LEU:O	1:A:165:LEU:HD12	2.08	0.54
1:B:28:GLY:O	1:B:30:VAL:N	2.35	0.54
1:A:111:THR:O	1:A:112:TYR:CB	2.53	0.54
1:B:191:ILE:N	1:B:191:ILE:HD12	2.23	0.54
1:A:74:ALA:HA	1:A:105:ALA:HB1	1.91	0.53
1:A:58:ILE:CD1	1:A:406:SER:HB2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:HB1	1:A:161:ASP:CG	2.29	0.53
1:A:59:SER:OG	1:A:405:GLU:HB3	2.09	0.53
1:A:52:ILE:HG23	1:A:412:LEU:HD21	1.89	0.53
1:B:137:ASN:HD22	1:B:137:ASN:C	2.12	0.53
1:A:28:GLY:O	1:A:30:VAL:N	2.34	0.53
1:B:378:ASN:C	1:B:380:ASP:H	2.12	0.53
1:B:13:LEU:HA	1:B:17:TYR:CZ	2.44	0.53
1:B:102:TYR:CE1	1:B:271:LEU:HB3	2.44	0.53
1:A:117:VAL:HG22	1:A:117:VAL:O	2.08	0.53
1:B:17:TYR:HA	1:B:20:GLU:CD	2.30	0.52
1:B:181:GLY:O	1:B:185:ALA:N	2.32	0.52
1:A:162:LEU:HA	1:A:165:LEU:HD13	1.92	0.52
1:B:274:MET:HG3	1:B:295:TYR:O	2.09	0.52
1:B:61:THR:CA	1:B:68:LEU:HD23	2.40	0.52
1:B:273:GLU:H	1:B:300:GLN:HE22	1.58	0.52
1:B:319:GLU:O	1:B:320:GLY:C	2.48	0.52
1:A:2:GLY:O	1:A:366:ARG:NH2	2.42	0.52
1:A:161:ASP:O	1:A:164:GLN:HB2	2.10	0.52
1:B:243:LEU:O	1:B:257:ALA:HB1	2.10	0.52
1:A:107:GLU:O	1:A:119:GLY:O	2.28	0.52
1:B:38:THR:OG1	1:B:135:ARG:NH1	2.42	0.52
1:A:16:ALA:O	1:A:17:TYR:C	2.48	0.52
1:B:130:LEU:C	1:B:130:LEU:HD23	2.30	0.52
1:A:14:GLY:HA3	1:A:342:ARG:HD2	1.92	0.52
1:B:14:GLY:HA3	1:B:342:ARG:HD2	1.92	0.52
1:B:349:ASP:OD1	1:B:365:ASP:OD1	2.28	0.52
1:B:147:ASN:HB2	1:B:208:GLY:O	2.09	0.52
1:B:135:ARG:HG2	1:B:135:ARG:O	2.10	0.52
1:A:239:TYR:CG	1:A:240:SER:N	2.78	0.51
1:A:349:ASP:OD1	1:A:365:ASP:OD1	2.27	0.51
1:A:399:GLU:O	1:A:400:GLY:C	2.48	0.51
1:B:191:ILE:HG22	1:B:191:ILE:O	2.11	0.51
1:B:364:GLN:O	1:B:365:ASP:C	2.48	0.51
1:A:185:ALA:O	1:A:188:ALA:HB3	2.10	0.51
1:A:353:PRO:HB2	1:A:355:GLN:NE2	2.26	0.51
1:B:49:ALA:HA	1:B:80:PRO:HA	1.91	0.51
1:A:54:PRO:HG2	1:A:74:ALA:O	2.10	0.51
1:A:130:LEU:HD23	1:A:130:LEU:C	2.31	0.51
1:A:19:GLY:N	1:A:292:SER:CB	2.66	0.51
1:B:15:ARG:HG3	1:B:15:ARG:HH11	1.75	0.51
1:A:61:THR:CA	1:A:68:LEU:HD23	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:N	1:A:161:ASP:OD1	2.41	0.51
1:A:191:ILE:HD12	1:A:191:ILE:N	2.26	0.51
1:A:354:ALA:HA	1:A:357:ARG:HG3	1.92	0.51
1:A:23:ILE:O	1:A:23:ILE:HG23	2.10	0.51
1:B:204:GLN:NE2	1:B:204:GLN:HA	2.26	0.51
1:A:19:GLY:H	1:A:292:SER:CB	2.23	0.51
1:B:52:ILE:HG23	1:B:412:LEU:HD21	1.92	0.50
1:A:104:LEU:HD12	1:A:104:LEU:C	2.32	0.50
1:A:61:THR:C	1:A:68:LEU:HD23	2.32	0.50
1:A:37:ILE:C	1:A:39:MET:N	2.65	0.50
1:A:191:ILE:O	1:A:191:ILE:HG22	2.11	0.50
1:B:136:LEU:CD2	1:B:137:ASN:N	2.74	0.50
1:B:358:SER:CB	1:B:399:GLU:OE1	2.58	0.50
1:A:273:GLU:CG	1:A:297:SER:OG	2.58	0.50
1:A:317:LYS:HZ2	2:A:503:LDA:HM23	1.76	0.50
1:A:381:ALA:HA	1:A:418:ASN:O	2.11	0.50
1:B:19:GLY:H	1:B:292:SER:CB	2.25	0.50
1:A:6:ASN:O	1:A:8:PHE:HD1	1.94	0.50
1:A:204:GLN:NE2	1:A:204:GLN:HA	2.27	0.50
1:B:117:VAL:O	1:B:359:ILE:HD11	2.11	0.50
1:A:104:LEU:O	1:A:104:LEU:HD12	2.12	0.50
1:A:218:ASP:OD1	1:A:220:ASN:N	2.43	0.50
1:B:120:THR:HG22	1:B:121:THR:N	2.26	0.50
1:B:161:ASP:O	1:B:164:GLN:HB2	2.12	0.50
1:B:104:LEU:HD11	1:B:121:THR:CG2	2.41	0.49
1:B:199:HIS:C	1:B:200:LEU:HD12	2.32	0.49
1:A:81:ASN:HD21	1:A:416:ASN:HD21	1.58	0.49
1:B:282:ARG:O	1:B:283:VAL:C	2.50	0.49
1:B:378:ASN:O	1:B:380:ASP:N	2.44	0.49
1:A:359:ILE:O	1:A:362:PRO:HD3	2.12	0.49
1:B:104:LEU:CD1	1:B:104:LEU:C	2.81	0.49
1:B:381:ALA:HA	1:B:418:ASN:O	2.11	0.49
1:B:252:LEU:HD13	1:B:254:ILE:CG2	2.43	0.49
1:A:181:GLY:O	1:A:185:ALA:N	2.39	0.49
1:A:11:SER:CB	1:A:26:ASP:OD1	2.61	0.49
1:B:27:ALA:HB2	1:B:44:THR:HB	1.95	0.49
1:B:420:ALA:C	1:B:421:PHE:CD2	2.83	0.49
1:B:215:TYR:C	1:B:215:TYR:CD2	2.86	0.49
1:A:49:ALA:HA	1:A:80:PRO:HA	1.94	0.49
1:A:25:ASP:O	1:A:26:ASP:CG	2.51	0.49
1:B:68:LEU:HD22	1:B:68:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASP:N	1:B:161:ASP:OD1	2.44	0.49
1:B:52:ILE:HG23	1:B:412:LEU:CD2	2.43	0.49
1:A:120:THR:HG22	1:A:121:THR:N	2.28	0.49
1:B:89:ASN:ND2	1:B:90:ASP:H	2.10	0.49
1:A:353:PRO:HB2	1:A:355:GLN:OE1	2.13	0.49
1:A:329:LEU:C	1:A:329:LEU:HD23	2.33	0.49
1:A:290:HIS:ND1	1:A:290:HIS:N	2.61	0.48
1:B:62:SER:N	1:B:68:LEU:CD2	2.76	0.48
1:B:162:LEU:O	1:B:165:LEU:HD12	2.13	0.48
1:B:273:GLU:CG	1:B:297:SER:OG	2.57	0.48
1:B:119:GLY:HA3	1:B:157:ARG:HA	1.96	0.48
2:B:504:LDA:H41	2:B:504:LDA:HM11	1.95	0.48
1:B:359:ILE:HA	1:B:362:PRO:HG3	1.95	0.48
1:B:31:SER:O	1:B:32:ARG:CB	2.56	0.48
1:B:181:GLY:HA2	1:B:184:LEU:HB3	1.94	0.48
1:A:221:ASN:ND2	1:A:281:ASN:HD22	2.11	0.48
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.78	0.48
1:A:200:LEU:HD21	1:A:315:PHE:CD2	2.49	0.48
1:A:25:ASP:O	1:A:25:ASP:OD1	2.31	0.48
1:A:364:GLN:NE2	1:A:408:GLY:HA3	2.29	0.48
1:B:59:SER:OG	1:B:405:GLU:HB3	2.14	0.48
1:B:239:TYR:OH	1:B:256:THR:O	2.21	0.48
1:B:11:SER:CB	1:B:26:ASP:OD1	2.62	0.48
1:B:364:GLN:NE2	1:B:408:GLY:HA3	2.29	0.48
1:B:245:ARG:NH2	1:B:258:THR:O	2.46	0.48
1:B:37:ILE:C	1:B:39:MET:N	2.65	0.48
1:B:304:LEU:HD21	2:B:504:LDA:HM11	1.96	0.48
1:A:105:ALA:O	1:A:121:THR:O	2.31	0.48
1:B:252:LEU:HB2	1:B:254:ILE:HG22	1.96	0.48
1:B:137:ASN:HD21	1:B:139:ALA:H	1.59	0.48
1:A:137:ASN:C	1:A:137:ASN:HD22	2.17	0.48
1:B:74:ALA:HA	1:B:105:ALA:HB1	1.96	0.47
1:A:215:TYR:CD2	1:A:215:TYR:C	2.85	0.47
1:A:147:ASN:HB2	1:A:208:GLY:O	2.13	0.47
1:B:19:GLY:N	1:B:292:SER:CB	2.69	0.47
1:A:270:ASN:N	1:A:270:ASN:ND2	2.60	0.47
1:A:5:LEU:HB3	1:A:7:GLU:HG2	1.95	0.47
1:B:185:ALA:O	1:B:188:ALA:HB3	2.15	0.47
1:B:14:GLY:HA3	1:B:342:ARG:CD	2.45	0.47
1:B:109:ASN:C	1:B:111:THR:H	2.18	0.47
1:A:6:ASN:O	1:A:7:GLU:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:N	1:B:7:GLU:CD	2.67	0.47
1:A:31:SER:O	1:A:32:ARG:CB	2.54	0.47
1:A:7:GLU:H	1:A:7:GLU:CD	2.17	0.47
1:A:340:THR:HB	1:A:374:THR:HB	1.97	0.47
1:B:346:ALA:CB	1:B:368:TRP:HB2	2.25	0.47
1:A:105:ALA:H	2:A:501:LDA:C2	2.28	0.47
1:B:290:HIS:N	1:B:290:HIS:ND1	2.63	0.47
1:A:158:PHE:HA	1:A:197:THR:H	1.80	0.47
1:A:36:LEU:O	1:A:37:ILE:C	2.53	0.47
1:A:45:PHE:CD1	1:A:45:PHE:C	2.87	0.47
1:A:74:ALA:HA	1:A:105:ALA:CB	2.45	0.47
1:B:61:THR:C	1:B:68:LEU:HD23	2.35	0.47
1:A:297:SER:HA	1:A:323:ASP:OD2	2.15	0.47
1:A:359:ILE:HA	1:A:362:PRO:HG3	1.95	0.47
1:A:364:GLN:O	1:A:365:ASP:C	2.53	0.47
1:B:340:THR:HB	1:B:374:THR:HB	1.97	0.47
1:A:26:ASP:C	1:A:26:ASP:OD2	2.53	0.47
1:B:30:VAL:O	1:B:34:GLY:N	2.42	0.47
1:A:118:GLY:O	1:A:119:GLY:C	2.54	0.46
1:A:356:ASN:O	1:A:357:ARG:C	2.54	0.46
1:B:120:THR:CG2	1:B:121:THR:N	2.78	0.46
1:A:79:VAL:HG22	2:A:501:LDA:H112	1.96	0.46
1:A:353:PRO:HB2	1:A:355:GLN:HE22	1.79	0.46
1:A:136:LEU:CD2	1:A:137:ASN:N	2.79	0.46
1:B:19:GLY:CA	1:B:292:SER:HB2	2.45	0.46
1:B:352:VAL:HG11	1:B:363:ASP:HB3	1.97	0.46
1:A:115:GLY:C	1:A:117:VAL:N	2.67	0.46
1:A:319:GLU:O	1:A:320:GLY:C	2.52	0.46
1:B:105:ALA:O	1:B:121:THR:O	2.33	0.46
1:B:196:LYS:HD3	1:B:199:HIS:HB2	1.95	0.46
1:A:62:SER:N	1:A:68:LEU:CD2	2.79	0.46
1:A:68:LEU:HD22	1:A:68:LEU:N	2.31	0.46
1:A:367:PHE:O	1:A:390:MET:HA	2.16	0.46
1:A:361:ILE:HD11	2:A:503:LDA:HM21	1.97	0.46
1:B:356:ASN:O	1:B:357:ARG:C	2.54	0.46
1:B:223:TYR:HA	1:B:278:SER:O	2.16	0.46
1:B:244:ASN:O	1:B:246:ALA:N	2.49	0.46
1:B:156:GLU:O	1:B:157:ARG:HD3	2.16	0.46
1:A:104:LEU:HD11	1:A:121:THR:CG2	2.45	0.46
1:B:399:GLU:O	1:B:400:GLY:O	2.34	0.46
1:A:181:GLY:HA2	1:A:184:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:SER:OG	1:B:323:ASP:OD2	2.34	0.46
1:A:106:THR:HG22	1:A:106:THR:O	2.16	0.46
1:A:162:LEU:O	1:A:163:GLY:C	2.54	0.46
1:A:134:TYR:CE2	1:A:136:LEU:HA	2.51	0.45
1:B:48:GLY:O	1:B:81:ASN:N	2.40	0.45
1:B:136:LEU:HD22	1:B:137:ASN:HB3	1.97	0.45
1:B:101:ASN:O	1:B:102:TYR:CG	2.69	0.45
1:B:267:LEU:HD23	1:B:268:THR:CA	2.47	0.45
1:B:162:LEU:O	1:B:163:GLY:C	2.54	0.45
1:A:15:ARG:HD3	1:A:290:HIS:HE2	1.82	0.45
1:B:359:ILE:O	1:B:362:PRO:HD3	2.17	0.45
1:B:6:ASN:O	1:B:7:GLU:C	2.55	0.45
1:A:34:GLY:O	1:A:37:ILE:HG13	2.17	0.45
1:A:30:VAL:O	1:A:34:GLY:N	2.43	0.45
1:A:14:GLY:HA3	1:A:342:ARG:CD	2.47	0.45
1:B:69:LYS:HE2	1:B:71:ASP:OD1	2.17	0.45
1:B:155:ILE:HD11	2:B:504:LDA:H61	1.99	0.45
1:A:4:GLN:HA	1:A:102:TYR:CD2	2.51	0.45
1:B:302:GLN:NE2	1:B:320:GLY:HA2	2.31	0.45
1:A:109:ASN:C	1:A:111:THR:H	2.19	0.45
1:A:282:ARG:O	1:A:283:VAL:C	2.55	0.45
1:B:104:LEU:C	1:B:104:LEU:HD12	2.38	0.45
1:B:239:TYR:O	1:B:240:SER:CB	2.65	0.45
1:A:73:ILE:HG21	1:A:108:PHE:CD1	2.52	0.45
1:B:135:ARG:HG3	1:B:135:ARG:HH11	1.82	0.45
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.82	0.45
1:B:239:TYR:O	1:B:240:SER:HB3	2.16	0.44
1:A:347:PHE:CG	1:A:348:ASP:N	2.85	0.44
1:A:164:GLN:O	1:A:165:LEU:C	2.56	0.44
1:B:352:VAL:CG1	1:B:363:ASP:HB3	2.48	0.44
1:A:57:ASN:O	1:A:406:SER:HA	2.16	0.44
1:A:136:LEU:HD22	1:A:137:ASN:HB3	2.00	0.44
1:A:352:VAL:HG11	1:A:363:ASP:HB3	1.99	0.44
1:B:25:ASP:O	1:B:26:ASP:CG	2.56	0.44
1:B:81:ASN:O	1:B:82:MET:HB2	2.18	0.44
1:B:236:LYS:HD3	1:B:266:TYR:CE2	2.53	0.44
1:B:156:GLU:HA	1:B:198:ALA:O	2.18	0.44
1:A:120:THR:CG2	1:A:121:THR:N	2.80	0.44
1:A:346:ALA:CB	1:A:368:TRP:HB2	2.27	0.44
1:B:26:ASP:OD2	1:B:26:ASP:C	2.55	0.44
1:B:109:ASN:O	1:B:111:THR:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TYR:CE2	1:B:136:LEU:HA	2.53	0.44
1:A:304:LEU:HD13	2:A:503:LDA:CM1	2.48	0.44
1:A:102:TYR:CG	1:A:271:LEU:HD22	2.52	0.44
1:B:164:GLN:O	1:B:165:LEU:C	2.57	0.44
1:A:348:ASP:O	1:A:348:ASP:OD2	2.35	0.44
1:B:266:TYR:HB2	1:B:307:THR:HG23	2.00	0.44
1:B:332:THR:HG23	1:B:341:PHE:O	2.17	0.44
1:A:178:THR:C	1:A:180:GLN:N	2.71	0.44
1:A:119:GLY:HA3	1:A:157:ARG:HA	2.00	0.43
1:B:15:ARG:NH1	1:B:20:GLU:OE2	2.51	0.43
1:B:178:THR:C	1:B:180:GLN:N	2.71	0.43
1:A:223:TYR:HA	1:A:278:SER:O	2.18	0.43
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.83	0.43
1:A:352:VAL:CG1	1:A:363:ASP:HB3	2.49	0.43
1:A:267:LEU:HD12	1:A:306:ALA:HB2	2.00	0.43
1:B:282:ARG:HG3	1:B:282:ARG:O	2.17	0.43
1:A:165:LEU:O	1:A:166:VAL:C	2.56	0.43
1:B:353:PRO:HB2	1:B:355:GLN:NE2	2.32	0.43
1:B:129:ASN:OD1	1:B:129:ASN:C	2.56	0.43
1:A:135:ARG:NH1	1:A:135:ARG:HG3	2.33	0.43
1:B:28:GLY:O	1:B:83:HIS:CD2	2.72	0.43
1:B:162:LEU:O	1:B:166:VAL:HG23	2.18	0.43
1:B:49:ALA:CB	1:B:80:PRO:HA	2.49	0.43
1:A:350:SER:OG	1:A:352:VAL:HG12	2.18	0.43
1:B:25:ASP:O	1:B:26:ASP:HB3	2.17	0.43
1:A:3:PHE:HD1	1:A:3:PHE:O	2.01	0.43
1:A:25:ASP:O	1:A:26:ASP:HB3	2.18	0.43
1:B:418:ASN:N	1:B:418:ASN:OD1	2.52	0.43
1:A:156:GLU:HA	1:A:198:ALA:O	2.19	0.43
1:B:353:PRO:HB2	1:B:355:GLN:HE22	1.83	0.43
1:A:253:PRO:O	1:A:254:ILE:C	2.57	0.43
1:B:347:PHE:CG	1:B:348:ASP:N	2.86	0.43
1:B:236:LYS:HD3	1:B:266:TYR:CZ	2.53	0.43
1:B:104:LEU:O	1:B:104:LEU:HD12	2.19	0.43
1:B:68:LEU:N	1:B:68:LEU:CD2	2.81	0.43
1:B:62:SER:N	1:B:68:LEU:HD21	2.34	0.43
1:A:267:LEU:HD23	1:A:268:THR:CA	2.49	0.43
1:A:165:LEU:O	1:A:169:GLN:N	2.44	0.43
1:B:23:ILE:O	1:B:23:ILE:HG23	2.19	0.43
1:A:104:LEU:HD13	1:A:105:ALA:O	2.19	0.42
1:B:134:TYR:CE2	1:B:136:LEU:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASN:C	1:B:111:THR:N	2.72	0.42
1:A:45:PHE:CD1	1:A:46:SER:N	2.87	0.42
1:B:8:PHE:HB2	1:B:99:THR:CG2	2.48	0.42
1:B:3:PHE:HD1	1:B:3:PHE:O	2.02	0.42
1:A:343:THR:HA	1:A:371:ALA:HA	2.00	0.42
1:A:352:VAL:O	1:A:352:VAL:HG13	2.20	0.42
1:B:115:GLY:C	1:B:117:VAL:N	2.70	0.42
1:A:161:ASP:O	1:A:162:LEU:C	2.58	0.42
1:A:129:ASN:C	1:A:129:ASN:OD1	2.57	0.42
1:A:69:LYS:HE2	1:A:71:ASP:OD1	2.18	0.42
1:B:297:SER:HA	1:B:323:ASP:OD2	2.18	0.42
1:A:267:LEU:CD2	1:A:268:THR:N	2.78	0.42
1:B:73:ILE:N	1:B:73:ILE:HD12	2.32	0.42
1:B:36:LEU:O	1:B:37:ILE:C	2.57	0.42
1:A:185:ALA:O	1:A:186:ALA:C	2.57	0.42
1:B:30:VAL:CG1	1:B:31:SER:H	2.32	0.42
1:B:329:LEU:HD23	1:B:329:LEU:C	2.39	0.42
1:A:48:GLY:O	1:A:81:ASN:N	2.44	0.42
1:B:267:LEU:HD12	1:B:306:ALA:HB2	2.02	0.42
1:B:185:ALA:O	1:B:186:ALA:C	2.58	0.42
1:B:107:GLU:O	1:B:119:GLY:O	2.37	0.42
1:B:186:ALA:O	1:B:187:THR:C	2.57	0.42
2:B:504:LDA:H41	2:B:504:LDA:CM1	2.49	0.42
1:B:175:ALA:HA	1:B:178:THR:HG23	2.02	0.42
1:A:101:ASN:O	1:A:102:TYR:CG	2.73	0.42
1:A:215:TYR:HD2	1:A:215:TYR:C	2.22	0.42
1:B:5:LEU:HB3	1:B:7:GLU:HG2	2.00	0.42
1:B:158:PHE:N	1:B:158:PHE:CD1	2.87	0.42
1:A:158:PHE:N	1:A:197:THR:HG22	2.35	0.42
1:B:15:ARG:CG	1:B:15:ARG:HH11	2.31	0.42
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.84	0.42
1:B:346:ALA:HB3	1:B:368:TRP:CG	2.54	0.42
1:B:368:TRP:CE2	1:B:390:MET:SD	3.13	0.42
1:A:273:GLU:H	1:A:300:GLN:NE2	2.17	0.42
1:A:418:ASN:OD1	1:A:418:ASN:N	2.52	0.42
1:B:245:ARG:HB3	1:B:245:ARG:HE	1.78	0.42
1:B:125:THR:O	1:B:125:THR:HG22	2.20	0.42
1:B:128:LEU:HB2	1:B:148:ALA:HB3	2.02	0.42
1:A:301:PHE:HD2	1:A:321:PHE:CD1	2.38	0.42
1:B:401:PRO:HD2	1:B:402:TYR:CE1	2.55	0.42
1:B:106:THR:O	1:B:106:THR:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:THR:OG1	1:B:112:TYR:N	2.50	0.41
1:A:361:ILE:CD1	2:A:503:LDA:HM21	2.50	0.41
1:B:181:GLY:O	1:B:184:LEU:HB3	2.20	0.41
1:A:146:PHE:CZ	1:A:207:PHE:HD1	2.38	0.41
1:B:118:GLY:O	1:B:119:GLY:C	2.58	0.41
1:B:15:ARG:HD3	1:B:290:HIS:HE2	1.85	0.41
1:A:381:ALA:HB2	1:A:419:TYR:HD1	1.84	0.41
1:B:200:LEU:HB3	2:B:504:LDA:H92	2.02	0.41
1:B:267:LEU:CD2	1:B:268:THR:N	2.78	0.41
1:B:57:ASN:O	1:B:406:SER:HA	2.19	0.41
1:A:137:ASN:HD21	1:A:139:ALA:H	1.64	0.41
1:A:45:PHE:HE1	1:A:47:ALA:HB2	1.84	0.41
1:B:45:PHE:CD1	1:B:45:PHE:C	2.92	0.41
1:B:367:PHE:O	1:B:390:MET:HA	2.21	0.41
1:A:368:TRP:CE2	1:A:390:MET:SD	3.14	0.41
1:A:57:ASN:HB2	1:A:407:GLU:CG	2.47	0.41
1:B:266:TYR:CD1	1:B:266:TYR:N	2.89	0.41
1:A:378:ASN:C	1:A:380:ASP:N	2.72	0.41
1:B:353:PRO:HB2	1:B:355:GLN:OE1	2.21	0.41
1:B:252:LEU:HD13	1:B:254:ILE:HG23	2.02	0.41
1:B:54:PRO:HA	1:B:410:ALA:CB	2.50	0.41
1:A:158:PHE:CD2	1:A:196:LYS:HA	2.56	0.41
1:A:383:VAL:HA	1:A:416:ASN:O	2.21	0.41
1:A:420:ALA:C	1:A:421:PHE:CD2	2.90	0.41
1:A:333:TYR:HB3	1:A:341:PHE:HB2	2.03	0.41
1:A:239:TYR:O	1:A:240:SER:CB	2.69	0.41
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.84	0.41
1:A:111:THR:OG1	1:A:112:TYR:N	2.53	0.41
1:B:304:LEU:CD2	2:B:504:LDA:HM11	2.50	0.41
1:A:24:ALA:HB2	1:A:36:LEU:HD12	2.03	0.41
1:B:267:LEU:C	1:B:267:LEU:CD2	2.84	0.41
1:B:161:ASP:O	1:B:162:LEU:C	2.59	0.41
1:B:270:ASN:N	1:B:270:ASN:ND2	2.66	0.41
1:A:110:ASP:C	1:A:110:ASP:OD2	2.58	0.41
1:A:27:ALA:HB2	1:A:44:THR:HB	2.02	0.41
1:A:15:ARG:O	1:A:16:ALA:C	2.59	0.41
1:A:200:LEU:N	1:A:200:LEU:CD1	2.82	0.41
1:A:239:TYR:OH	1:A:256:THR:O	2.29	0.41
1:B:307:THR:OG1	1:B:308:SER:N	2.54	0.41
1:B:207:PHE:N	1:B:207:PHE:CD2	2.88	0.41
1:B:135:ARG:NH1	1:B:135:ARG:HG3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:O	1:A:82:MET:HB2	2.21	0.40
1:B:358:SER:C	1:B:360:SER:N	2.74	0.40
1:B:298:TRP:C	1:B:300:GLN:N	2.72	0.40
1:A:153:ALA:CB	2:A:503:LDA:H81	2.51	0.40
1:A:28:GLY:O	1:A:83:HIS:CD2	2.74	0.40
1:A:221:ASN:ND2	1:A:281:ASN:ND2	2.70	0.40
1:B:393:GLN:CA	1:B:393:GLN:HE21	2.33	0.40
1:B:339:TRP:CE2	1:B:375:TYR:HD1	2.39	0.40
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.89	0.40
1:A:54:PRO:HA	1:A:410:ALA:CB	2.51	0.40
1:A:364:GLN:NE2	1:A:408:GLY:N	2.69	0.40
1:B:333:TYR:HB3	1:B:341:PHE:HB2	2.02	0.40
1:B:343:THR:HA	1:B:371:ALA:HA	2.03	0.40
1:A:200:LEU:HA	1:A:238:ASN:O	2.21	0.40
1:A:243:LEU:O	1:A:257:ALA:HB1	2.21	0.40
1:B:385:VAL:HG13	1:B:414:GLY:O	2.21	0.40
1:B:175:ALA:HA	1:B:178:THR:CG2	2.51	0.40
1:A:353:PRO:HB2	1:A:355:GLN:CD	2.42	0.40
1:A:244:ASN:O	1:A:246:ALA:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/427 (98%)	320 (76%)	67 (16%)	32 (8%)	1	17
1	B	419/427 (98%)	321 (77%)	65 (16%)	33 (8%)	1	16
All	All	838/854 (98%)	641 (76%)	132 (16%)	65 (8%)	1	16

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	34	GLY
1	A	38	THR
1	A	136	LEU
1	A	292	SER
1	A	297	SER
1	B	7	GLU
1	B	8	PHE
1	B	25	ASP
1	B	26	ASP
1	B	34	GLY
1	B	38	THR
1	B	136	LEU
1	B	292	SER
1	B	297	SER
1	A	25	ASP
1	A	26	ASP
1	A	119	GLY
1	A	164	GLN
1	A	174	PRO
1	A	175	ALA
1	A	283	VAL
1	A	320	GLY
1	A	400	GLY
1	B	119	GLY
1	B	164	GLN
1	B	174	PRO
1	B	175	ALA
1	B	283	VAL
1	B	320	GLY
1	B	379	LYS
1	B	400	GLY
1	A	29	ASN
1	A	82	MET
1	A	285	PRO
1	A	379	LYS
1	B	29	ASN
1	B	82	MET
1	B	240	SER
1	B	245	ARG
1	A	240	SER
1	A	245	ARG

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Mol	Chain	Res	Type
1	B	37	ILE
1	B	112	TYR
1	B	285	PRO
1	B	378	ASN
1	A	106	THR
1	A	112	TYR
1	A	247	PHE
1	B	17	TYR
1	B	78	TRP
1	B	106	THR
1	B	256	THR
1	A	37	ILE
1	A	180	GLN
1	A	254	ILE
1	B	108	PHE
1	A	28	GLY
1	B	231	VAL
1	A	166	VAL
1	B	28	GLY
1	A	253	PRO
1	B	254	ILE
1	A	231	VAL

### 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	329/335 (98%)	290 (88%)	39 (12%)	6	34
1	B	329/335 (98%)	290 (88%)	39 (12%)	6	34
All	All	658/670 (98%)	580 (88%)	78 (12%)	6	34

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE

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Mol	Chain	Res	Type
1	A	38	THR
1	A	42	ARG
1	A	45	PHE
1	A	72	ASN
1	A	73	ILE
1	A	84	PHE
1	A	89	ASN
1	A	99	THR
1	A	104	LEU
1	A	111	THR
1	A	134	TYR
1	A	137	ASN
1	A	138	ASN
1	A	141	SER
1	A	144	LEU
1	A	164	GLN
1	A	165	LEU
1	A	171	MET
1	A	173	SER
1	A	177	GLN
1	A	182	GLN
1	A	200	LEU
1	A	215	TYR
1	A	216	GLU
1	A	245	ARG
1	A	252	LEU
1	A	270	ASN
1	A	275	TRP
1	A	284	ASP
1	A	285	PRO
1	A	290	HIS
1	A	299	SER
1	A	304	LEU
1	A	340	THR
1	A	355	GLN
1	A	393	GLN
1	A	415	THR
1	A	418	ASN
1	B	8	PHE
1	B	38	THR
1	B	42	ARG
1	B	45	PHE

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Mol	Chain	Res	Type
1	B	72	ASN
1	B	73	ILE
1	B	80	PRO
1	B	84	PHE
1	B	89	ASN
1	B	99	THR
1	B	104	LEU
1	B	111	THR
1	B	134	TYR
1	B	137	ASN
1	B	138	ASN
1	B	141	SER
1	B	142	PHE
1	B	144	LEU
1	B	164	GLN
1	B	165	LEU
1	B	171	MET
1	B	173	SER
1	B	177	GLN
1	B	200	LEU
1	B	215	TYR
1	B	216	GLU
1	B	245	ARG
1	B	252	LEU
1	B	270	ASN
1	B	275	TRP
1	B	284	ASP
1	B	285	PRO
1	B	290	HIS
1	B	304	LEU
1	B	340	THR
1	B	355	GLN
1	B	393	GLN
1	B	415	THR
1	B	418	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	72	ASN
1	A	81	ASN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	189	ASN
1	A	194	ASN
1	A	204	GLN
1	A	248	ASN
1	A	270	ASN
1	A	281	ASN
1	A	300	GLN
1	A	302	GLN
1	A	356	ASN
1	A	393	GLN
1	A	416	ASN
1	B	29	ASN
1	B	72	ASN
1	B	81	ASN
1	B	137	ASN
1	B	204	GLN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	300	GLN
1	B	302	GLN
1	B	316	GLN
1	B	356	ASN
1	B	393	GLN
1	B	416	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 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	LDA	A	501	-	15,15,15	3.52	2 (13%)	16,17,17	2.43	5 (31%)
2	LDA	A	503	-	15,15,15	3.77	2 (13%)	16,17,17	2.09	3 (18%)
2	LDA	B	502	-	15,15,15	3.75	2 (13%)	16,17,17	2.17	5 (31%)
2	LDA	B	504	-	15,15,15	4.14	2 (13%)	16,17,17	2.04	6 (37%)

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	LDA	A	501	-	-	0/13/13/13	0/0/0/0
2	LDA	A	503	-	-	0/13/13/13	0/0/0/0
2	LDA	B	502	-	-	0/13/13/13	0/0/0/0
2	LDA	B	504	-	-	0/13/13/13	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	LDA	O1-N1	-15.29	1.25	1.39
2	B	502	LDA	O1-N1	-13.79	1.26	1.39
2	A	503	LDA	O1-N1	-13.42	1.26	1.39
2	A	501	LDA	O1-N1	-12.91	1.27	1.39
2	A	503	LDA	CM2-N1	-4.80	1.42	1.49
2	B	504	LDA	CM2-N1	-4.12	1.43	1.49
2	B	502	LDA	CM2-N1	-3.87	1.43	1.49
2	A	501	LDA	CM2-N1	-3.60	1.43	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LDA	CM2-N1-CM1	-6.70	101.28	108.83
2	A	503	LDA	CM2-N1-CM1	-5.92	102.15	108.83
2	B	502	LDA	CM2-N1-CM1	-5.15	103.02	108.83
2	B	504	LDA	CM2-N1-CM1	-4.77	103.45	108.83
2	B	502	LDA	CM1-N1-C1	-2.40	102.04	109.77
2	B	504	LDA	C6-C5-C4	-2.34	102.47	114.53
2	B	504	LDA	C9-C8-C7	-2.33	102.51	114.53
2	A	501	LDA	CM1-N1-C1	-2.30	102.37	109.77
2	B	502	LDA	C9-C8-C7	-2.26	102.83	114.53
2	B	504	LDA	CM1-N1-C1	-2.09	103.03	109.77
2	A	501	LDA	C9-C8-C7	-2.08	103.79	114.53
2	A	503	LDA	O1-N1-CM2	2.67	112.62	109.05
2	B	504	LDA	O1-N1-CM2	2.72	112.70	109.05
2	B	502	LDA	O1-N1-CM2	3.05	113.13	109.05
2	A	501	LDA	O1-N1-CM2	3.31	113.47	109.05
2	A	503	LDA	O1-N1-C1	3.38	114.08	110.27
2	B	504	LDA	O1-N1-C1	3.42	114.13	110.27
2	B	502	LDA	O1-N1-C1	4.31	115.12	110.27
2	A	501	LDA	O1-N1-C1	4.50	115.33	110.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LDA	3	0
2	A	503	LDA	11	0
2	B	502	LDA	3	0
2	B	504	LDA	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	421/427 (98%)	-0.53	0 100 100	0, 8, 41, 69	0
1	B	421/427 (98%)	-0.53	0 100 100	0, 7, 38, 79	0
All	All	842/854 (98%)	-0.53	0 100 100	0, 7, 40, 79	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	LDA	B	502	16/16	0.86	0.35	5.74	8,8,8,8	0
2	LDA	A	503	16/16	0.84	0.40	4.37	8,8,8,8	0
2	LDA	B	504	16/16	0.90	0.39	3.14	8,8,8,8	0
2	LDA	A	501	16/16	0.83	0.32	2.55	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.