



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 AM GMT

PDB ID : 2FSI  
Title : Complex SecA:ADP from Escherichia coli  
Authors : Papanikolau, Y.; Petratos, K.; Economou, A.  
Deposited on : 2006-01-23  
Resolution : 2.11 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

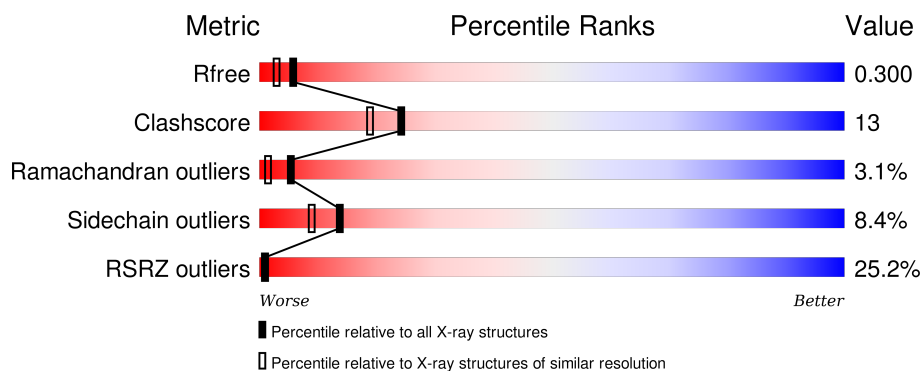
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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	853	<div> <div>15%</div> <div>60%</div> <div>18%</div> <div>•</div> <div>19%</div> </div>
1	B	853	<div> <div>28%</div> <div>52%</div> <div>27%</div> <div>7%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11936 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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5500	3445	971	1058	26			
1	B	748	Total	C	N	O	S	0	0	0
			5948	3730	1050	1138	30			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

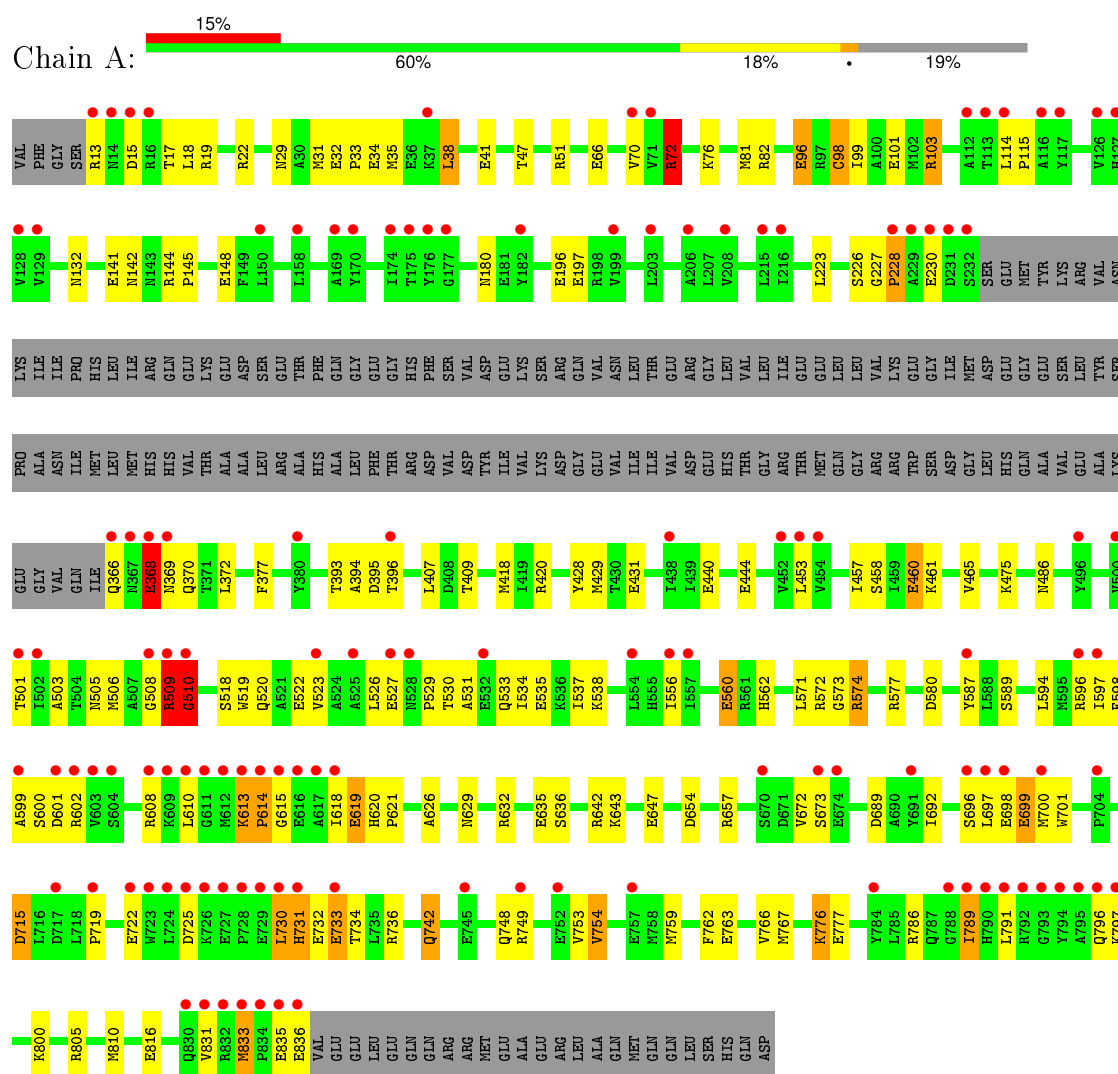
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total 179	O 179	0	0
3	B	255	Total 255	O 255	0	0

### 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: Preprotein translocase secA subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.56Å 90.43Å 163.29Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	19.85 – 2.11 19.84 – 2.11	Depositor EDS
% Data completeness (in resolution range)	90.6 (19.85-2.11) 90.6 (19.84-2.11)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.203 , 0.263 0.256 , 0.300	Depositor DCC
$R_{free}$ test set	5665 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.2	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 112860 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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	1.32	29/5590 (0.5%)	1.07	15/7542 (0.2%)
1	B	1.56	68/6045 (1.1%)	1.27	48/8154 (0.6%)
All	All	1.45	97/11635 (0.8%)	1.17	63/15696 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	GLU	CD-OE1	14.09	1.41	1.25
1	A	699	GLU	CD-OE2	12.11	1.39	1.25
1	A	697	LEU	C-O	11.52	1.45	1.23
1	A	98	CYS	CB-SG	-11.41	1.62	1.82
1	B	23	LYS	CE-NZ	11.33	1.77	1.49
1	B	71	VAL	CB-CG2	10.78	1.75	1.52
1	B	210	GLU	CG-CD	9.82	1.66	1.51
1	B	98	CYS	CB-SG	-8.88	1.67	1.82
1	B	385	GLU	CD-OE2	8.81	1.35	1.25
1	A	698	GLU	C-O	8.81	1.40	1.23
1	B	96	GLU	CD-OE1	8.61	1.35	1.25
1	B	385	GLU	CD-OE1	8.35	1.34	1.25
1	A	587	TYR	CE2-CZ	-8.13	1.27	1.38
1	B	117	TYR	CD2-CE2	-7.68	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLU	CD-OE2	7.56	1.33	1.25
1	B	801	GLN	N-CA	7.45	1.61	1.46
1	A	431	GLU	CD-OE1	7.45	1.33	1.25
1	B	103	ARG	CG-CD	7.37	1.70	1.51
1	B	380	TYR	CE2-CZ	-7.32	1.29	1.38
1	B	61	GLU	CD-OE1	7.28	1.33	1.25
1	B	68	PHE	CD2-CE2	7.23	1.53	1.39
1	B	635	GLU	CD-OE1	7.23	1.33	1.25
1	B	803	TYR	CD2-CE2	7.19	1.50	1.39
1	B	560	GLU	CG-CD	7.01	1.62	1.51
1	B	385	GLU	CG-CD	6.89	1.62	1.51
1	A	560	GLU	CD-OE1	6.78	1.33	1.25
1	A	696	SER	CB-OG	6.74	1.51	1.42
1	B	141	GLU	CG-CD	6.68	1.61	1.51
1	B	73	GLU	N-CA	6.57	1.59	1.46
1	B	394	ALA	CA-CB	6.57	1.66	1.52
1	A	141	GLU	CG-CD	6.55	1.61	1.51
1	B	56	LYS	CD-CE	6.54	1.67	1.51
1	B	46	LYS	CB-CG	-6.53	1.34	1.52
1	A	460	GLU	CB-CG	6.41	1.64	1.52
1	B	122	THR	C-O	-6.36	1.11	1.23
1	B	163	ALA	CA-CB	6.31	1.65	1.52
1	A	572	ARG	CB-CG	-6.29	1.35	1.52
1	B	572	ARG	CB-CG	-6.28	1.35	1.52
1	B	722	GLU	CD-OE1	6.28	1.32	1.25
1	B	76	LYS	CE-NZ	6.21	1.64	1.49
1	B	196	GLU	CB-CG	-6.15	1.40	1.52
1	B	202	LYS	CD-CE	6.10	1.66	1.51
1	A	460	GLU	CG-CD	6.09	1.61	1.51
1	A	626	ALA	CA-CB	-6.03	1.39	1.52
1	A	816	GLU	CB-CG	6.03	1.63	1.52
1	B	115	PRO	CG-CD	6.02	1.70	1.50
1	B	24	VAL	CB-CG2	5.98	1.65	1.52
1	B	560	GLU	CD-OE1	5.98	1.32	1.25
1	B	126	VAL	C-O	-5.98	1.11	1.23
1	B	665	GLU	CG-CD	5.96	1.60	1.51
1	B	106	GLU	CD-OE1	5.96	1.32	1.25
1	B	148	GLU	CG-CD	5.94	1.60	1.51
1	B	41	GLU	CG-CD	5.91	1.60	1.51
1	A	560	GLU	CG-CD	5.89	1.60	1.51
1	B	616	GLU	CB-CG	5.82	1.63	1.52
1	B	36	GLU	CB-CG	-5.79	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GLU	CG-CD	5.76	1.60	1.51
1	B	80	GLY	C-O	-5.75	1.14	1.23
1	B	173	ASP	CB-CG	5.75	1.63	1.51
1	B	578	GLN	CB-CG	5.73	1.68	1.52
1	A	503	ALA	CA-CB	-5.67	1.40	1.52
1	A	431	GLU	CD-OE2	5.66	1.31	1.25
1	B	444	GLU	CG-CD	5.62	1.60	1.51
1	A	96	GLU	CG-CD	-5.60	1.43	1.51
1	B	421	LYS	CE-NZ	5.57	1.62	1.49
1	B	656	ARG	CB-CG	5.55	1.67	1.52
1	B	149	PHE	CD2-CE2	-5.53	1.28	1.39
1	B	56	LYS	CE-NZ	5.53	1.62	1.49
1	B	496	TYR	CB-CG	-5.51	1.43	1.51
1	B	660	TYR	CD2-CE2	5.48	1.47	1.39
1	B	763	GLU	CG-CD	5.46	1.60	1.51
1	B	647	GLU	CD-OE2	5.43	1.31	1.25
1	B	58	GLU	CD-OE1	5.40	1.31	1.25
1	A	101	GLU	CD-OE2	5.39	1.31	1.25
1	A	560	GLU	CD-OE2	5.38	1.31	1.25
1	B	72	ARG	CZ-NH1	-5.35	1.26	1.33
1	B	106	GLU	CD-OE2	5.34	1.31	1.25
1	B	416	ARG	N-CA	5.34	1.57	1.46
1	B	170	TYR	CD1-CE1	5.33	1.47	1.39
1	B	723	TRP	CB-CG	5.29	1.59	1.50
1	A	465	VAL	CB-CG1	-5.27	1.41	1.52
1	B	141	GLU	CD-OE1	5.27	1.31	1.25
1	B	665	GLU	CD-OE2	5.25	1.31	1.25
1	A	777	GLU	CG-CD	5.20	1.59	1.51
1	B	828	LYS	CE-NZ	5.20	1.62	1.49
1	B	816	GLU	CB-CG	5.19	1.62	1.52
1	A	41	GLU	CG-CD	5.14	1.59	1.51
1	B	727	GLU	CD-OE1	5.11	1.31	1.25
1	A	673	SER	CB-OG	-5.07	1.35	1.42
1	B	654	ASP	CG-OD1	5.06	1.36	1.25
1	A	196	GLU	CD-OE2	5.04	1.31	1.25
1	B	821	GLU	CG-CD	-5.04	1.44	1.51
1	B	37	LYS	N-CA	5.03	1.56	1.46
1	A	816	GLU	CG-CD	5.03	1.59	1.51
1	B	43	LEU	C-O	5.02	1.32	1.23
1	A	501	THR	C-O	-5.02	1.13	1.23
1	B	25	VAL	C-O	-5.01	1.13	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	B	167	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	657	ARG	NE-CZ-NH2	10.02	125.31	120.30
1	A	72	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	A	657	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	B	786	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	B	23	LYS	CD-CE-NZ	8.43	131.09	111.70
1	B	408	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	144	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	B	201	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	B	189	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	B	782	MET	CG-SD-CE	7.27	111.83	100.20
1	B	207	LEU	CB-CG-CD2	-7.18	98.79	111.00
1	B	801	GLN	N-CA-CB	7.09	123.36	110.60
1	B	53	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	540	ASP	CB-CG-OD2	7.01	124.61	118.30
1	B	786	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	A	72	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	B	97	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	B	102	MET	CG-SD-CE	-6.58	89.68	100.20
1	B	367	ASN	CB-CA-C	6.55	123.51	110.40
1	B	408	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	572	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	821	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	B	187	LEU	CB-CG-CD1	-6.33	100.24	111.00
1	B	723	TRP	CA-CB-CG	6.26	125.59	113.70
1	B	133	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	367	ASN	N-CA-CB	-5.98	99.83	110.60
1	B	167	ARG	CD-NE-CZ	5.89	131.85	123.60
1	B	540	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	367	ASN	N-CA-C	5.86	126.83	111.00
1	B	103	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	A	509	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	B	387	LEU	CA-CB-CG	5.79	128.60	115.30
1	A	654	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	A	689	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	810	MET	CG-SD-CE	-5.72	91.04	100.20
1	B	801	GLN	CB-CA-C	-5.70	99.00	110.40
1	A	805	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	173	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	805	ARG	CB-CA-C	-5.55	99.30	110.40
1	B	821	GLU	CB-CA-C	-5.53	99.35	110.40
1	A	657	ARG	NE-CZ-NH1	-5.47	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	800	LYS	C-N-CA	-5.43	108.11	121.70
1	B	572	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	77	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	85	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	656	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	779	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	418	MET	CG-SD-CE	5.21	108.54	100.20
1	A	38	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	189	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	475	LYS	CD-CE-NZ	-5.15	99.85	111.70
1	B	77	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	81	MET	CG-SD-CE	-5.14	91.98	100.20
1	B	682	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	420	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	649	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	53	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	805	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	801	GLN	CA-CB-CG	5.03	124.47	113.40
1	B	422	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	580	ASP	CB-CG-OD2	-5.03	113.78	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	510	GLY	Peptide
1	B	393	THR	Peptide
1	B	394	ALA	Peptide
1	B	791	LEU	Peptide
1	B	793	GLY	Peptide
1	B	794	TYR	Peptide

## 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	5500	0	5481	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5948	0	5946	203	0
2	A	27	0	12	0	0
2	B	27	0	12	4	0
3	A	179	0	0	11	0
3	B	255	0	0	34	0
All	All	11936	0	11451	298	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 13.

All (298) 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:71:VAL:CB	1:B:71:VAL:CG2	1.75	1.59
1:B:23:LYS:NZ	1:B:23:LYS:CE	1.77	1.44
1:A:538:LYS:HZ3	1:B:528:ASN:ND2	1.28	1.27
1:A:538:LYS:NZ	1:B:528:ASN:HD22	1.48	1.10
1:B:629:ASN:HD22	1:B:632:ARG:NH2	1.59	1.00
1:A:538:LYS:NZ	1:B:528:ASN:ND2	2.07	0.96
1:B:493:GLN:HG2	3:B:1068:HOH:O	1.66	0.96
1:B:395:ASP:HB2	3:B:1109:HOH:O	1.63	0.96
1:B:519:TRP:CH2	1:B:538:LYS:NZ	2.35	0.94
1:B:519:TRP:CZ2	1:B:538:LYS:NZ	2.37	0.92
1:A:577:ARG:HD3	3:A:1000:HOH:O	1.73	0.89
1:B:297:SER:O	1:B:303:ASN:ND2	2.06	0.87
1:B:800:LYS:O	1:B:801:GLN:HB2	1.75	0.86
1:B:17:THR:HG22	1:B:21:MET:HE2	1.58	0.85
1:B:598:PHE:O	1:B:600:SER:N	2.09	0.84
1:B:647:GLU:OE2	1:B:800:LYS:HE2	1.78	0.83
1:B:17:THR:HG22	1:B:21:MET:CE	2.09	0.82
1:A:732:GLU:OE2	1:A:736:ARG:NH1	2.12	0.82
1:A:531:ALA:O	1:A:534:ILE:HG13	1.80	0.81
1:B:33:PRO:O	1:B:37:LYS:HD3	1.81	0.81
1:B:518:SER:HA	3:B:1001:HOH:O	1.79	0.80
1:A:395:ASP:HA	3:A:927:HOH:O	1.83	0.79
1:A:598:PHE:O	1:A:600:SER:N	2.16	0.78
1:B:637:ARG:NH1	1:B:641:ILE:HD11	2.00	0.76
1:B:526:LEU:HD21	1:B:533:GLN:HE22	1.49	0.76
1:B:518:SER:CA	3:B:1001:HOH:O	2.33	0.76
1:A:753:VAL:HG21	1:A:833:MET:HE2	1.67	0.76
1:B:316:ALA:O	1:B:317:HIS:CG	2.40	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASP:CB	3:B:1109:HOH:O	2.25	0.74
1:B:103:ARG:HD3	3:B:914:HOH:O	1.86	0.74
1:B:521:ALA:O	1:B:524:ALA:N	2.18	0.73
1:A:618:ILE:O	1:A:619:GLU:HB2	1.88	0.72
1:B:800:LYS:O	1:B:801:GLN:CB	2.29	0.72
1:B:629:ASN:ND2	1:B:632:ARG:NH2	2.38	0.71
1:A:103:ARG:NH1	1:A:573:GLY:O	2.24	0.70
1:B:621:PRO:HG2	3:B:966:HOH:O	1.93	0.69
1:A:395:ASP:CG	1:A:396:THR:N	2.46	0.69
1:A:731:HIS:CE1	1:A:734:THR:HG23	2.28	0.69
1:B:71:VAL:CA	1:B:71:VAL:CG2	2.67	0.68
1:B:600:SER:HB3	1:B:603:VAL:HB	1.76	0.68
1:B:685:LYS:HE3	3:B:1135:HOH:O	1.93	0.68
1:B:395:ASP:CA	3:B:1109:HOH:O	2.41	0.67
1:B:788:GLY:CA	3:B:1137:HOH:O	2.43	0.66
1:A:530:THR:H	1:A:533:GLN:HE21	1.43	0.66
1:B:647:GLU:OE2	1:B:800:LYS:CE	2.44	0.65
1:B:114:LEU:HB2	1:B:115:PRO:CD	2.27	0.65
1:B:614:PRO:HA	3:B:1115:HOH:O	1.95	0.65
1:B:311:THR:O	1:B:315:ARG:HB2	1.96	0.64
1:B:238:ARG:NE	1:B:238:ARG:HA	2.12	0.64
1:B:282:ILE:CD1	1:B:286:LEU:HD13	2.28	0.64
1:A:508:GLY:O	1:A:510:GLY:N	2.31	0.63
1:B:37:LYS:CD	3:B:1125:HOH:O	2.47	0.63
1:B:71:VAL:CG2	1:B:71:VAL:CG1	2.72	0.63
1:A:742:GLN:HE21	1:A:742:GLN:HA	1.65	0.62
1:B:304:ILE:HG21	1:B:781:ALA:HB1	1.80	0.62
1:A:508:GLY:C	1:A:510:GLY:H	2.02	0.62
1:A:395:ASP:CG	1:A:396:THR:H	2.04	0.62
1:B:198:ARG:HH21	1:B:664:ASN:HD22	1.47	0.62
1:A:531:ALA:O	1:A:534:ILE:CG1	2.47	0.61
1:A:699:GLU:OE2	1:A:700:MET:CE	2.49	0.61
1:B:817:SER:O	1:B:821:GLU:CG	2.49	0.61
1:A:15:ASP:OD1	1:A:19:ARG:NH2	2.34	0.61
1:B:804:LYS:HE2	3:B:954:HOH:O	2.00	0.61
1:A:144:ARG:O	1:A:148:GLU:HG3	2.01	0.61
1:B:668:ASP:OD1	3:B:1147:HOH:O	2.16	0.61
1:A:520:GLN:CD	3:A:1029:HOH:O	2.39	0.60
1:B:114:LEU:HB2	1:B:115:PRO:HD3	1.84	0.60
1:A:29:ASN:OD1	1:A:72:ARG:NH1	2.32	0.60
1:B:144:ARG:HB3	1:B:145:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HD13	1:B:529:PRO:HG2	1.84	0.60
1:A:180:ASN:HD22	1:A:377:PHE:HZ	1.49	0.60
1:B:104:THR:HG21	1:B:577:ARG:CZ	2.32	0.60
1:B:228:PRO:O	1:B:230:GLU:HB2	2.02	0.59
1:B:11:GLY:O	1:B:16:ARG:HB2	2.02	0.59
1:B:657:ARG:HD3	3:B:1144:HOH:O	2.02	0.59
1:A:510:GLY:HA2	1:A:574:ARG:HH11	1.67	0.59
1:B:287:VAL:O	1:B:288:LYS:HG2	2.02	0.59
1:A:594:LEU:HG	1:A:597:ILE:HD13	1.84	0.59
1:B:742:GLN:O	1:B:745:GLU:HG2	2.02	0.59
1:B:316:ALA:O	1:B:317:HIS:CD2	2.55	0.59
1:B:657:ARG:HH21	1:B:657:ARG:HG3	1.68	0.58
1:B:233:SER:O	1:B:234:GLU:HB2	2.04	0.58
1:A:629:ASN:HD22	1:A:632:ARG:HH21	1.51	0.58
1:B:786:ARG:O	1:B:789:ILE:HB	2.04	0.58
1:B:395:ASP:HA	3:B:1109:HOH:O	2.01	0.58
1:B:198:ARG:HH21	1:B:664:ASN:ND2	2.02	0.58
1:B:509:ARG:O	1:B:577:ARG:NH2	2.35	0.58
1:B:392:GLY:O	1:B:394:ALA:HB3	2.03	0.58
1:A:519:TRP:CH2	1:A:538:LYS:HD3	2.39	0.58
1:A:227:GLY:HA3	1:A:372:LEU:HD21	1.85	0.57
1:B:146:LEU:O	1:B:149:PHE:HB3	2.04	0.57
1:B:304:ILE:CG2	1:B:781:ALA:HB1	2.34	0.57
1:B:394:ALA:HA	3:B:1002:HOH:O	2.05	0.57
1:B:16:ARG:NE	1:B:19:ARG:HH21	2.03	0.57
1:A:18:LEU:O	1:A:22:ARG:HG3	2.05	0.57
1:A:510:GLY:CA	1:A:574:ARG:NH1	2.68	0.56
1:B:81:MET:CE	2:B:901:ADP:C4	2.88	0.56
1:B:81:MET:HE2	2:B:901:ADP:C4	2.40	0.56
1:B:817:SER:O	1:B:821:GLU:HG2	2.06	0.56
1:A:72:ARG:HD2	1:A:82:ARG:HG2	1.86	0.56
1:B:245:HIS:HB2	3:B:1098:HOH:O	2.04	0.56
1:B:409:THR:HG23	3:B:912:HOH:O	2.03	0.56
1:A:395:ASP:N	3:A:927:HOH:O	2.38	0.56
1:A:519:TRP:O	1:A:522:GLU:HB2	2.05	0.56
1:B:102:MET:O	1:B:392:GLY:HA2	2.06	0.56
1:B:763:GLU:O	1:B:767:MET:HG3	2.06	0.56
1:B:37:LYS:HD2	3:B:1125:HOH:O	2.05	0.56
1:B:282:ILE:HD13	1:B:286:LEU:HD13	1.87	0.56
1:B:81:MET:HE2	2:B:901:ADP:N3	2.20	0.56
1:A:715:ASP:O	1:A:715:ASP:CG	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLU:OE2	1:B:395:ASP:N	2.39	0.55
1:B:518:SER:N	3:B:1049:HOH:O	2.39	0.55
1:B:691:TYR:O	1:B:693:PRO:HD3	2.06	0.55
1:B:738:ARG:O	1:B:742:GLN:HG2	2.06	0.55
1:A:754:VAL:CG1	1:A:759:MET:HG2	2.36	0.55
1:B:561:ARG:HB2	1:B:594:LEU:HD22	1.89	0.55
1:B:700:MET:HE3	3:B:1134:HOH:O	2.07	0.55
1:A:618:ILE:O	1:A:619:GLU:CB	2.55	0.55
1:B:11:GLY:O	1:B:16:ARG:CB	2.55	0.55
1:B:243:ILE:HD11	1:B:313:ALA:HB1	1.88	0.55
1:B:307:MET:O	1:B:311:THR:HG23	2.07	0.54
1:A:730:LEU:O	1:A:731:HIS:HB3	2.07	0.54
1:A:529:PRO:HA	1:A:533:GLN:NE2	2.21	0.54
1:A:614:PRO:HA	3:A:1064:HOH:O	2.08	0.53
1:B:727:GLU:HG2	1:B:730:LEU:HB3	1.90	0.53
1:B:308:HIS:CE1	1:B:784:TYR:CZ	2.97	0.53
1:B:518:SER:O	1:B:521:ALA:HB3	2.09	0.53
1:A:526:LEU:HD12	1:A:529:PRO:HB3	1.90	0.53
1:A:180:ASN:ND2	1:A:377:PHE:HZ	2.05	0.53
1:B:12:SER:HB2	1:B:15:ASP:OD2	2.09	0.53
1:B:392:GLY:O	1:B:394:ALA:CA	2.57	0.53
1:A:519:TRP:CZ2	1:A:538:LYS:HD3	2.45	0.52
1:A:731:HIS:NE2	1:A:733:GLU:HB3	2.25	0.52
1:A:429:MET:SD	1:A:608:ARG:HG2	2.49	0.52
1:B:17:THR:HG22	1:B:21:MET:HE1	1.89	0.52
1:A:457:ILE:HG22	1:A:562:HIS:CE1	2.44	0.52
1:B:99:ILE:HD12	1:B:211:VAL:HG11	1.92	0.52
1:B:789:ILE:O	1:B:789:ILE:HG22	2.10	0.52
1:B:14:ASN:HD21	1:B:411:VAL:H	1.58	0.51
1:B:526:LEU:HD21	1:B:533:GLN:NE2	2.22	0.51
1:A:535:GLU:HA	1:A:535:GLU:OE1	2.09	0.51
1:A:835:GLU:HG2	1:A:836:GLU:N	2.25	0.51
1:A:394:ALA:HB3	3:A:1006:HOH:O	2.10	0.51
1:B:757:GLU:HG3	3:B:1141:HOH:O	2.10	0.51
1:B:37:LYS:HD3	3:B:1125:HOH:O	2.07	0.51
1:B:759:MET:CE	1:B:762:PHE:HD2	2.24	0.51
1:A:731:HIS:HE1	1:A:734:THR:HG23	1.76	0.51
1:B:444:GLU:O	1:B:448:LYS:HG3	2.11	0.51
1:B:487:GLU:O	1:B:491:VAL:HG23	2.12	0.50
1:B:523:VAL:HG22	3:B:1096:HOH:O	2.11	0.50
1:B:618:ILE:O	1:B:619:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PRO:O	1:B:230:GLU:CB	2.59	0.50
1:B:302:ALA:HA	1:B:810:MET:HE3	1.93	0.50
1:A:461:LYS:HD2	1:A:560:GLU:OE2	2.12	0.50
1:B:789:ILE:O	1:B:789:ILE:CG2	2.59	0.50
1:B:104:THR:HG21	1:B:577:ARG:NH2	2.27	0.50
1:A:577:ARG:CD	3:A:1000:HOH:O	2.43	0.50
1:A:753:VAL:HG21	1:A:833:MET:CE	2.39	0.50
1:B:409:THR:CG2	3:B:912:HOH:O	2.59	0.50
1:B:522:GLU:HA	3:B:1003:HOH:O	2.12	0.50
1:B:771:LEU:HD23	1:B:771:LEU:C	2.32	0.50
1:A:786:ARG:O	1:A:789:ILE:HB	2.11	0.49
1:A:643:LYS:O	1:A:647:GLU:HG3	2.12	0.49
1:A:518:SER:HA	3:A:919:HOH:O	2.11	0.49
1:B:18:LEU:HD23	1:B:21:MET:HE3	1.93	0.49
1:B:691:TYR:OH	1:B:709:ARG:NH2	2.44	0.49
1:B:771:LEU:HD23	1:B:771:LEU:O	2.13	0.49
1:A:833:MET:HE2	1:A:833:MET:HA	1.94	0.49
1:B:833:MET:CB	1:B:834:PRO:HD2	2.42	0.49
1:B:657:ARG:CD	3:B:1144:HOH:O	2.59	0.49
1:B:688:ILE:HD11	1:B:739:ILE:HG21	1.95	0.49
1:A:486:ASN:HD21	1:B:132:ASN:HD21	1.61	0.49
1:B:105:GLY:O	1:B:578:GLN:NE2	2.43	0.48
1:B:712:ASN:C	1:B:828:LYS:HZ1	2.16	0.48
1:B:428:TYR:O	1:B:589:SER:HA	2.12	0.48
1:A:460:GLU:H	1:A:460:GLU:CD	2.16	0.48
1:A:223:LEU:HD21	1:A:377:PHE:CZ	2.49	0.48
1:B:759:MET:HE3	1:B:762:PHE:CD2	2.48	0.48
1:A:831:VAL:HG12	1:A:833:MET:HE3	1.96	0.48
1:B:282:ILE:HD11	1:B:298:LEU:HB3	1.95	0.48
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.46	0.48
1:B:306:LEU:O	1:B:309:HIS:HB2	2.14	0.48
1:B:648:TYR:CZ	1:B:800:LYS:HB2	2.49	0.48
1:A:76:LYS:HD2	1:A:82:ARG:HG3	1.96	0.48
1:A:132:ASN:HD21	1:B:486:ASN:HD21	1.61	0.48
1:A:372:LEU:HD22	1:A:776:LYS:NZ	2.29	0.47
1:B:237:LYS:HA	1:B:240:ASN:HB2	1.96	0.47
1:B:526:LEU:HD11	1:B:533:GLN:NE2	2.29	0.47
1:B:230:GLU:HB3	1:B:231:ASP:O	2.15	0.47
1:B:14:ASN:ND2	1:B:411:VAL:H	2.12	0.47
1:B:302:ALA:HA	1:B:810:MET:CE	2.45	0.47
1:A:47:THR:O	1:A:51:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LYS:O	1:B:465:VAL:HG12	2.15	0.47
1:B:757:GLU:O	1:B:761:HIS:HD2	1.98	0.47
1:B:237:LYS:NZ	1:B:241:LYS:HD2	2.30	0.47
1:B:817:SER:O	1:B:821:GLU:HG3	2.15	0.47
1:B:713:ASP:C	1:B:828:LYS:NZ	2.69	0.47
1:B:287:VAL:O	1:B:287:VAL:HG13	2.15	0.46
1:B:284:GLU:O	1:B:287:VAL:HB	2.15	0.46
1:A:538:LYS:HZ3	1:B:528:ASN:HD22	0.59	0.46
1:A:510:GLY:HA2	1:A:574:ARG:NH1	2.29	0.46
1:B:730:LEU:O	1:B:731:HIS:HB2	2.15	0.46
1:A:458:SER:HB2	1:A:460:GLU:OE2	2.16	0.46
1:B:81:MET:HE1	2:B:901:ADP:C4	2.51	0.46
1:A:132:ASN:HD21	1:B:486:ASN:ND2	2.14	0.46
1:B:680:ARG:O	1:B:684:PHE:HB2	2.16	0.46
1:B:720:ILE:HG22	1:B:724:LEU:HG	1.98	0.46
1:A:613:LYS:HA	1:A:614:PRO:HD2	1.84	0.46
1:A:457:ILE:HA	1:A:505:ASN:OD1	2.15	0.46
1:B:508:GLY:O	1:B:510:GLY:N	2.48	0.46
1:B:71:VAL:O	1:B:71:VAL:HG12	2.16	0.45
1:A:508:GLY:O	1:A:509:ARG:HG2	2.16	0.45
1:A:368:GLU:N	1:A:368:GLU:CD	2.70	0.45
1:B:742:GLN:O	1:B:746:VAL:HG23	2.16	0.45
1:A:571:LEU:O	1:A:574:ARG:HB2	2.17	0.45
1:B:243:ILE:N	1:B:244:PRO:HD2	2.31	0.45
1:A:642:ARG:NH1	3:A:942:HOH:O	2.48	0.45
1:B:144:ARG:O	1:B:148:GLU:HB2	2.17	0.45
1:B:712:ASN:O	1:B:828:LYS:NZ	2.49	0.45
1:B:377:PHE:CD1	3:B:981:HOH:O	2.68	0.45
1:B:246:LEU:CD1	1:B:314:LEU:HD22	2.47	0.45
1:A:699:GLU:OE2	1:A:700:MET:HE1	2.17	0.45
1:A:227:GLY:N	1:A:370:GLN:O	2.50	0.45
1:A:518:SER:CA	3:A:919:HOH:O	2.64	0.45
1:B:589:SER:OG	1:B:592:ASP:OD2	2.27	0.45
1:B:732:GLU:O	1:B:735:LEU:HG	2.16	0.45
1:B:312:ALA:O	1:B:316:ALA:HB2	2.17	0.45
1:B:282:ILE:HG13	1:B:299:TYR:CE2	2.52	0.45
1:B:718:LEU:O	1:B:720:ILE:N	2.48	0.45
1:A:763:GLU:O	1:A:767:MET:HG3	2.17	0.45
1:B:230:GLU:OE1	1:B:368:GLU:O	2.36	0.44
1:B:239:VAL:O	1:B:242:ILE:HG22	2.17	0.44
1:B:430:THR:OG1	1:B:433:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ILE:O	1:B:404:ILE:HG22	2.18	0.44
1:B:60:LEU:O	1:B:63:LEU:HB2	2.16	0.44
1:B:392:GLY:O	1:B:394:ALA:CB	2.66	0.44
1:B:440:GLU:O	1:B:444:GLU:HG3	2.18	0.44
1:B:202:LYS:NZ	3:B:1081:HOH:O	2.50	0.44
1:B:518:SER:C	3:B:1001:HOH:O	2.54	0.44
1:B:718:LEU:HB3	1:B:723:TRP:CZ2	2.53	0.44
1:B:697:LEU:H	1:B:697:LEU:HD12	1.82	0.44
1:B:693:PRO:O	1:B:696:SER:HB2	2.18	0.43
1:B:594:LEU:HG	1:B:597:ILE:HD13	2.01	0.43
1:B:718:LEU:O	1:B:720:ILE:HD12	2.19	0.43
1:B:735:LEU:C	1:B:735:LEU:HD12	2.38	0.43
1:B:593:ALA:O	1:B:595:MET:N	2.51	0.43
1:B:11:GLY:O	1:B:16:ARG:HG2	2.19	0.43
1:A:754:VAL:HG11	1:A:759:MET:HG2	2.00	0.43
1:A:66:GLU:O	1:A:70:VAL:HG23	2.19	0.43
1:B:679:ILE:O	1:B:683:VAL:HG23	2.19	0.43
1:B:796:GLN:O	1:B:798:ASP:N	2.51	0.43
1:B:392:GLY:O	1:B:394:ALA:N	2.52	0.43
1:A:620:HIS:HA	1:A:621:PRO:HD2	1.76	0.43
1:B:718:LEU:HB3	1:B:723:TRP:HZ2	1.83	0.43
1:B:788:GLY:CA	1:B:792:ARG:CG	2.97	0.43
1:B:311:THR:O	1:B:315:ARG:CB	2.66	0.43
1:B:745:GLU:HG3	1:B:749:ARG:NH2	2.33	0.43
1:B:788:GLY:O	1:B:792:ARG:CG	2.67	0.42
1:A:719:PRO:HB2	1:A:722:GLU:HB2	2.01	0.42
1:B:103:ARG:HG2	1:B:393:THR:OG1	2.19	0.42
1:A:699:GLU:OE2	1:A:700:MET:HE2	2.18	0.42
1:B:507:ALA:O	3:B:1136:HOH:O	2.22	0.42
1:A:33:PRO:O	1:A:34:GLU:C	2.57	0.42
1:A:519:TRP:CH2	1:A:538:LYS:HE2	2.54	0.42
1:B:530:THR:HG22	1:B:533:GLN:HG3	2.00	0.42
1:B:12:SER:HB2	1:B:15:ASP:OD1	2.19	0.42
1:A:35:MET:HA	1:A:38:LEU:HD13	2.01	0.42
1:A:594:LEU:O	1:A:597:ILE:HG12	2.20	0.42
1:A:428:TYR:O	1:A:589:SER:HA	2.19	0.42
1:A:114:LEU:HB2	1:A:115:PRO:CD	2.50	0.42
1:B:228:PRO:O	1:B:230:GLU:N	2.53	0.42
1:B:692:ILE:HG21	1:B:732:GLU:HG3	2.01	0.42
1:B:187:LEU:HD21	1:B:375:ILE:HB	2.01	0.42
1:A:228:PRO:O	1:A:230:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:N	1:B:115:PRO:HD2	2.35	0.41
1:B:242:ILE:HD11	1:B:246:LEU:HD21	2.02	0.41
1:A:762:PHE:O	1:A:766:VAL:HG23	2.20	0.41
1:A:142:ASN:O	1:A:145:PRO:HD2	2.20	0.41
1:B:103:ARG:HD2	1:B:104:THR:N	2.35	0.41
1:A:99:ILE:HD11	1:A:407:LEU:HD13	2.02	0.41
1:B:179:ASN:HB2	1:B:377:PHE:CE1	2.54	0.41
1:B:672:VAL:O	1:B:672:VAL:HG12	2.21	0.41
1:B:788:GLY:HA3	3:B:1137:HOH:O	2.14	0.41
1:B:534:ILE:O	1:B:535:GLU:C	2.57	0.41
1:A:31:MET:CE	1:A:66:GLU:HG2	2.51	0.41
1:B:282:ILE:CD1	1:B:286:LEU:CD1	2.98	0.41
1:B:150:LEU:HA	1:B:150:LEU:HD23	1.95	0.41
1:A:395:ASP:CA	3:A:927:HOH:O	2.55	0.41
1:B:523:VAL:CG2	3:B:1096:HOH:O	2.69	0.41
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.93	0.41
1:B:750:LYS:HD2	1:B:829:VAL:HG13	2.03	0.41
1:A:440:GLU:O	1:A:444:GLU:HG3	2.21	0.41
1:A:598:PHE:C	1:A:600:SER:N	2.75	0.40
1:B:103:ARG:CD	1:B:104:THR:N	2.85	0.40
1:B:723:TRP:HB2	1:B:724:LEU:HD23	2.04	0.40
1:B:701:TRP:N	1:B:701:TRP:CD1	2.87	0.40
1:A:453:LEU:HB3	1:A:556:ILE:HD13	2.03	0.40
1:A:692:ILE:HG23	1:A:701:TRP:CD1	2.57	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	687/853 (80%)	639 (93%)	36 (5%)	12 (2%)	<b>11</b> <b>5</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	742/853 (87%)	657 (88%)	53 (7%)	32 (4%)	3 1
All	All	1429/1706 (84%)	1296 (91%)	89 (6%)	44 (3%)	5 1

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	A	599	ALA
1	A	614	PRO
1	B	229	ALA
1	B	289	GLU
1	B	292	MET
1	B	293	ASP
1	B	368	GLU
1	B	394	ALA
1	B	599	ALA
1	B	614	PRO
1	B	729	GLU
1	B	741	ALA
1	B	797	LYS
1	B	834	PRO
1	A	509	ARG
1	A	601	ASP
1	A	602	ARG
1	B	302	ALA
1	B	509	ARG
1	B	510	GLY
1	B	594	LEU
1	B	740	LEU
1	B	796	GLN
1	A	619	GLU
1	B	317	HIS
1	B	395	ASP
1	B	481	ALA
1	B	719	PRO
1	B	731	HIS
1	A	613	LYS
1	A	789	ILE
1	B	287	VAL
1	B	835	GLU
1	A	228	PRO
1	A	510	GLY

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Mol	Chain	Res	Type
1	B	232	SER
1	B	619	GLU
1	B	789	ILE
1	B	790	HIS
1	B	798	ASP
1	A	615	GLY
1	B	698	GLU
1	B	704	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	586/728 (80%)	548 (94%)	38 (6%)	21	17
1	B	635/728 (87%)	571 (90%)	64 (10%)	9	5
All	All	1221/1456 (84%)	1119 (92%)	102 (8%)	14	9

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	17	THR
1	A	72	ARG
1	A	96	GLU
1	A	98	CYS
1	A	103	ARG
1	A	226	SER
1	A	366	GLN
1	A	368	GLU
1	A	369	ASN
1	A	393	THR
1	A	409	THR
1	A	475	LYS
1	A	506	MET
1	A	523	VAL

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Mol	Chain	Res	Type
1	A	527	GLU
1	A	537	ILE
1	A	574	ARG
1	A	596	ARG
1	A	610	LEU
1	A	635	GLU
1	A	636	SER
1	A	672	VAL
1	A	715	ASP
1	A	725	ASP
1	A	730	LEU
1	A	731	HIS
1	A	733	GLU
1	A	742	GLN
1	A	748	GLN
1	A	749	ARG
1	A	754	VAL
1	A	776	LYS
1	A	791	LEU
1	A	796	GLN
1	A	797	LYS
1	A	800	LYS
1	A	833	MET
1	B	16	ARG
1	B	38	LEU
1	B	102	MET
1	B	103	ARG
1	B	210	GLU
1	B	225	ILE
1	B	226	SER
1	B	231	ASP
1	B	237	LYS
1	B	241	LYS
1	B	242	ILE
1	B	281	LEU
1	B	282	ILE
1	B	284	GLU
1	B	285	LEU
1	B	286	LEU
1	B	288	LYS
1	B	294	GLU
1	B	306	LEU

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Mol	Chain	Res	Type
1	B	310	VAL
1	B	368	GLU
1	B	393	THR
1	B	409	THR
1	B	416	ARG
1	B	429	MET
1	B	509	ARG
1	B	518	SER
1	B	520	GLN
1	B	523	VAL
1	B	526	LEU
1	B	530	THR
1	B	535	GLU
1	B	536	LYS
1	B	606	MET
1	B	607	MET
1	B	609	LYS
1	B	614	PRO
1	B	632	ARG
1	B	637	ARG
1	B	643	LYS
1	B	657	ARG
1	B	679	ILE
1	B	696	SER
1	B	703	ILE
1	B	707	GLN
1	B	711	LYS
1	B	718	LEU
1	B	723	TRP
1	B	724	LEU
1	B	725	ASP
1	B	726	LYS
1	B	727	GLU
1	B	729	GLU
1	B	730	LEU
1	B	733	GLU
1	B	735	LEU
1	B	749	ARG
1	B	769	GLN
1	B	779	LEU
1	B	792	ARG
1	B	796	GLN

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Mol	Chain	Res	Type
1	B	800	LYS
1	B	831	VAL
1	B	833	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	484	HIS
1	A	486	ASN
1	A	533	GLN
1	A	542	GLN
1	A	629	ASN
1	A	662	GLN
1	A	742	GLN
1	A	761	HIS
1	B	14	ASN
1	B	180	ASN
1	B	240	ASN
1	B	303	ASN
1	B	308	HIS
1	B	317	HIS
1	B	369	ASN
1	B	484	HIS
1	B	486	ASN
1	B	520	GLN
1	B	528	ASN
1	B	545	HIS
1	B	629	ASN
1	B	638	ASN
1	B	664	ASN
1	B	731	HIS
1	B	742	GLN
1	B	761	HIS
1	B	769	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates 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	ADP	A	900	-	22,29,29	1.35	3 (13%)	27,45,45	2.30	5 (18%)
2	ADP	B	901	-	22,29,29	1.68	3 (13%)	27,45,45	2.48	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	ADP	A	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	901	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ADP	PA-O1A	-2.74	1.41	1.51
2	A	900	ADP	C5-C4	2.23	1.45	1.40
2	A	900	ADP	C2-N3	2.62	1.36	1.32
2	B	901	ADP	C5-C4	3.33	1.48	1.40
2	A	900	ADP	O4'-C1'	4.03	1.46	1.41
2	B	901	ADP	O4'-C1'	5.31	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ADP	N3-C2-N1	-8.83	122.13	128.89
2	B	901	ADP	N3-C2-N1	-6.91	123.60	128.89
2	B	901	ADP	O3A-PA-O5'	-6.60	85.43	102.94
2	A	900	ADP	O3A-PA-O5'	-4.37	91.34	102.94
2	B	901	ADP	C4'-O4'-C1'	-3.04	106.38	109.72
2	B	901	ADP	PA-O3A-PB	-2.82	123.22	132.67
2	B	901	ADP	O2B-PB-O1B	-2.53	102.42	110.58
2	A	900	ADP	O3B-PB-O1B	-2.52	102.45	110.58
2	A	900	ADP	O2B-PB-O1B	2.45	118.47	110.58
2	B	901	ADP	O2A-PA-O3A	2.67	117.22	105.09
2	B	901	ADP	O3B-PB-O2B	3.47	120.58	107.38
2	B	901	ADP	N6-C6-N1	3.52	126.77	119.20
2	A	900	ADP	C4'-O4'-C1'	3.54	113.61	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ADP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	691/853 (81%)	0.98	124 (17%) <b>2</b> <b>2</b>	30, 44, 75, 88	0
1	B	748/853 (87%)	1.70	239 (31%) <b>1</b> <b>1</b>	28, 46, 77, 98	0
All	All	1439/1706 (84%)	1.36	363 (25%) <b>1</b> <b>1</b>	28, 45, 76, 98	0

All (363) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	794	TYR	12.7
1	B	795	ALA	11.0
1	B	247	ILE	10.9
1	B	291	ILE	10.9
1	B	318	ALA	10.7
1	B	280	VAL	10.1
1	B	615	GLY	9.8
1	A	229	ALA	9.2
1	B	791	LEU	8.9
1	A	794	TYR	8.8
1	A	791	LEU	8.7
1	B	834	PRO	8.4
1	B	244	PRO	8.2
1	B	314	LEU	8.1
1	B	793	GLY	8.0
1	B	236	TYR	8.0
1	B	697	LEU	8.0
1	B	836	GLU	7.9
1	B	728	PRO	7.9
1	B	835	GLU	7.7
1	A	232	SER	7.6
1	B	833	MET	7.3
1	A	728	PRO	7.1
1	B	700	MET	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	695	GLN	7.0
1	B	229	ALA	7.0
1	A	836	GLU	6.9
1	B	614	PRO	6.9
1	A	231	ASP	6.8
1	A	795	ALA	6.8
1	B	231	ASP	6.8
1	B	233	SER	6.8
1	B	295	GLY	6.7
1	B	704	PRO	6.7
1	B	299	TYR	6.7
1	A	835	GLU	6.7
1	B	12	SER	6.7
1	B	292	MET	6.6
1	A	792	ARG	6.6
1	B	248	ARG	6.6
1	B	249	GLN	6.6
1	B	294	GLU	6.6
1	B	245	HIS	6.5
1	B	317	HIS	6.4
1	B	315	ARG	6.4
1	B	235	MET	6.4
1	A	616	GLU	6.4
1	B	796	GLN	6.4
1	A	230	GLU	6.3
1	A	615	GLY	6.3
1	B	731	HIS	6.3
1	B	696	SER	6.2
1	B	730	LEU	6.1
1	B	242	ILE	6.0
1	B	618	ILE	5.9
1	B	290	GLY	5.9
1	B	237	LYS	5.9
1	B	723	TRP	5.9
1	B	234	GLU	5.9
1	B	725	ASP	5.8
1	B	790	HIS	5.8
1	A	790	HIS	5.7
1	B	241	LYS	5.7
1	B	71	VAL	5.7
1	A	614	PRO	5.6
1	A	367	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	718	LEU	5.5
1	A	731	HIS	5.5
1	B	240	ASN	5.5
1	B	11	GLY	5.4
1	B	507	ALA	5.4
1	B	508	GLY	5.4
1	A	228	PRO	5.4
1	A	834	PRO	5.4
1	B	301	PRO	5.4
1	A	784	TYR	5.4
1	A	723	TRP	5.4
1	A	602	ARG	5.4
1	B	789	ILE	5.2
1	A	14	ASN	5.2
1	B	510	GLY	5.2
1	B	238	ARG	5.2
1	A	525	ALA	5.1
1	B	797	LYS	5.1
1	B	719	PRO	5.0
1	B	289	GLU	5.0
1	A	789	ILE	5.0
1	B	117	TYR	5.0
1	B	531	ALA	5.0
1	B	602	ARG	4.9
1	B	729	GLU	4.9
1	B	182	TYR	4.9
1	B	726	LYS	4.9
1	B	603	VAL	4.9
1	A	604	SER	4.9
1	B	703	ILE	4.9
1	B	699	GLU	4.9
1	B	368	GLU	4.8
1	B	232	SER	4.7
1	B	174	ILE	4.7
1	A	788	GLY	4.6
1	A	15	ASP	4.6
1	B	312	ALA	4.6
1	B	114	LEU	4.6
1	B	722	GLU	4.6
1	B	313	ALA	4.6
1	A	368	GLU	4.6
1	B	282	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	239	VAL	4.6
1	B	128	VAL	4.5
1	B	243	ILE	4.5
1	B	126	VAL	4.5
1	B	830	GLN	4.5
1	B	293	ASP	4.4
1	B	724	LEU	4.4
1	B	727	GLU	4.4
1	A	369	ASN	4.3
1	B	170	TYR	4.3
1	B	175	THR	4.3
1	A	13	ARG	4.2
1	B	113	THR	4.2
1	B	528	ASN	4.2
1	A	557	ILE	4.2
1	B	68	PHE	4.1
1	B	316	ALA	4.0
1	B	146	LEU	4.0
1	B	532	GLU	4.0
1	A	532	GLU	4.0
1	A	71	VAL	4.0
1	B	281	LEU	4.0
1	B	70	VAL	4.0
1	B	118	LEU	4.0
1	A	527	GLU	4.0
1	A	796	GLN	4.0
1	A	366	GLN	3.9
1	B	509	ARG	3.9
1	A	182	TYR	3.9
1	B	177	GLY	3.9
1	B	74	ALA	3.9
1	B	147	PHE	3.9
1	B	738	ARG	3.9
1	B	287	VAL	3.9
1	B	556	ILE	3.8
1	A	793	GLY	3.8
1	B	156	ILE	3.8
1	B	607	MET	3.8
1	A	726	LYS	3.8
1	B	709	ARG	3.8
1	B	121	LEU	3.8
1	B	283	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	129	VAL	3.8
1	B	831	VAL	3.8
1	B	284	GLU	3.8
1	A	700	MET	3.7
1	B	792	ARG	3.7
1	B	367	ASN	3.7
1	B	519	TRP	3.7
1	B	176	TYR	3.7
1	B	89	LEU	3.7
1	B	610	LEU	3.7
1	A	729	GLU	3.7
1	A	832	ARG	3.7
1	A	612	MET	3.6
1	A	597	ILE	3.6
1	B	116	ALA	3.6
1	B	554	LEU	3.6
1	A	176	TYR	3.6
1	B	674	GLU	3.6
1	B	67	ALA	3.6
1	B	694	PRO	3.6
1	A	454	VAL	3.6
1	B	526	LEU	3.5
1	A	37	LYS	3.5
1	B	832	ARG	3.5
1	B	111	THR	3.5
1	A	617	ALA	3.5
1	A	508	GLY	3.5
1	B	288	LYS	3.5
1	B	611	GLY	3.5
1	A	603	VAL	3.5
1	B	616	GLU	3.4
1	A	175	THR	3.4
1	B	120	ALA	3.4
1	A	16	ARG	3.4
1	B	608	ARG	3.4
1	A	797	LYS	3.4
1	B	702	ASP	3.4
1	B	158	LEU	3.4
1	B	69	ALA	3.4
1	B	206	ALA	3.4
1	B	369	ASN	3.4
1	A	510	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	100	ALA	3.4
1	B	720	ILE	3.4
1	A	528	ASN	3.3
1	B	246	LEU	3.3
1	B	734	THR	3.3
1	B	708	GLU	3.3
1	A	697	LEU	3.3
1	B	557	ILE	3.2
1	B	717	ASP	3.2
1	A	453	LEU	3.2
1	A	730	LEU	3.2
1	B	733	GLU	3.2
1	B	707	GLN	3.2
1	A	618	ILE	3.2
1	A	452	VAL	3.2
1	B	394	ALA	3.2
1	A	113	THR	3.2
1	A	554	LEU	3.2
1	A	613	LYS	3.2
1	B	157	ASN	3.2
1	A	170	TYR	3.2
1	B	88	LEU	3.2
1	B	205	TYR	3.1
1	B	617	ALA	3.1
1	B	90	GLY	3.1
1	B	429	MET	3.1
1	B	745	GLU	3.1
1	B	601	ASP	3.1
1	A	128	VAL	3.1
1	B	186	TYR	3.0
1	A	70	VAL	3.0
1	B	93	VAL	3.0
1	B	606	MET	3.0
1	B	749	ARG	3.0
1	A	177	GLY	3.0
1	B	705	GLY	3.0
1	A	496	TYR	3.0
1	B	207	LEU	3.0
1	B	183	GLY	3.0
1	B	228	PRO	3.0
1	A	596	ARG	3.0
1	A	501	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	211	VAL	3.0
1	A	117	TYR	3.0
1	B	502	ILE	3.0
1	A	215	LEU	3.0
1	B	110	LEU	2.9
1	A	114	LEU	2.9
1	B	453	LEU	2.9
1	B	178	THR	2.9
1	B	91	GLY	2.9
1	A	396	THR	2.9
1	B	735	LEU	2.9
1	B	208	VAL	2.9
1	A	745	GLU	2.9
1	A	438	ILE	2.9
1	B	150	LEU	2.9
1	A	704	PRO	2.9
1	B	597	ILE	2.8
1	B	199	VAL	2.8
1	B	701	TRP	2.8
1	B	692	ILE	2.8
1	A	126	VAL	2.8
1	A	717	ASP	2.8
1	A	670	SER	2.8
1	B	605	GLY	2.8
1	A	127	HIS	2.7
1	B	136	ALA	2.7
1	A	833	MET	2.7
1	A	722	GLU	2.7
1	B	127	HIS	2.7
1	B	86	VAL	2.7
1	B	670	SER	2.7
1	B	99	ILE	2.7
1	A	727	GLU	2.7
1	B	154	VAL	2.6
1	B	389	GLY	2.6
1	A	725	ASP	2.6
1	A	523	VAL	2.6
1	A	724	LEU	2.6
1	A	509	ARG	2.6
1	A	608	ARG	2.6
1	B	285	LEU	2.6
1	B	596	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	375	ILE	2.6
1	B	737	GLU	2.6
1	B	87	GLN	2.6
1	B	478	VAL	2.6
1	B	452	VAL	2.5
1	B	691	TYR	2.5
1	A	206	ALA	2.5
1	B	588	LEU	2.5
1	A	719	PRO	2.5
1	B	714	PHE	2.5
1	B	447	ALA	2.5
1	A	733	GLU	2.5
1	B	523	VAL	2.5
1	A	116	ALA	2.5
1	A	609	LYS	2.5
1	B	115	PRO	2.5
1	B	200	GLN	2.5
1	B	303	ASN	2.4
1	A	502	ILE	2.4
1	A	556	ILE	2.4
1	A	587	TYR	2.4
1	B	152	LEU	2.4
1	B	215	LEU	2.4
1	A	169	ALA	2.4
1	B	503	ALA	2.4
1	B	63	LEU	2.4
1	B	94	LEU	2.4
1	B	752	GLU	2.3
1	B	530	THR	2.3
1	B	706	LEU	2.3
1	A	150	LEU	2.3
1	A	158	LEU	2.3
1	A	610	LEU	2.3
1	B	203	LEU	2.3
1	B	820	TYR	2.3
1	A	611	GLY	2.3
1	A	752	GLU	2.3
1	B	380	TYR	2.3
1	B	405	TYR	2.3
1	B	598	PHE	2.3
1	B	684	PHE	2.3
1	A	830	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	390	MET	2.3
1	A	112	ALA	2.3
1	B	388	ALA	2.3
1	A	601	ASP	2.3
1	A	674	GLU	2.3
1	B	586	PHE	2.3
1	B	711	LYS	2.3
1	A	831	VAL	2.3
1	B	64	ILE	2.3
1	B	187	LEU	2.3
1	B	214	ILE	2.2
1	B	721	ALA	2.2
1	B	412	VAL	2.2
1	B	712	ASN	2.2
1	A	129	VAL	2.2
1	A	208	VAL	2.2
1	B	575	SER	2.2
1	B	112	ALA	2.2
1	B	587	TYR	2.2
1	B	404	ILE	2.2
1	B	559	THR	2.2
1	B	682	ASP	2.2
1	B	65	PRO	2.2
1	B	83	HIS	2.1
1	A	380	TYR	2.1
1	A	599	ALA	2.1
1	A	749	ARG	2.1
1	A	203	LEU	2.1
1	B	103	ARG	2.1
1	A	691	TYR	2.1
1	A	199	VAL	2.1
1	A	500	VAL	2.1
1	B	75	SER	2.1
1	A	696	SER	2.1
1	A	698	GLU	2.1
1	A	216	ILE	2.1
1	B	230	GLU	2.1
1	A	673	SER	2.1
1	B	119	ASN	2.0
1	B	387	LEU	2.0
1	B	92	MET	2.0
1	B	172	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	637	ARG	2.0
1	A	757	GLU	2.0
1	A	174	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	A	900	27/27	0.96	0.11	-0.81	33,46,49,50	0
2	ADP	B	901	27/27	0.96	0.12	-1.17	24,34,39,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.