



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:08 PM UTC

PDB ID : 1F9W / pdb_00001f9w
Title : CRYSTAL STRUCTURES OF MUTANTS REVEAL A SIGNALLING
PATHWAY FOR ACTIVATION OF THE KINESIN MOTOR ATPASE
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Deposited on : 2000-07-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

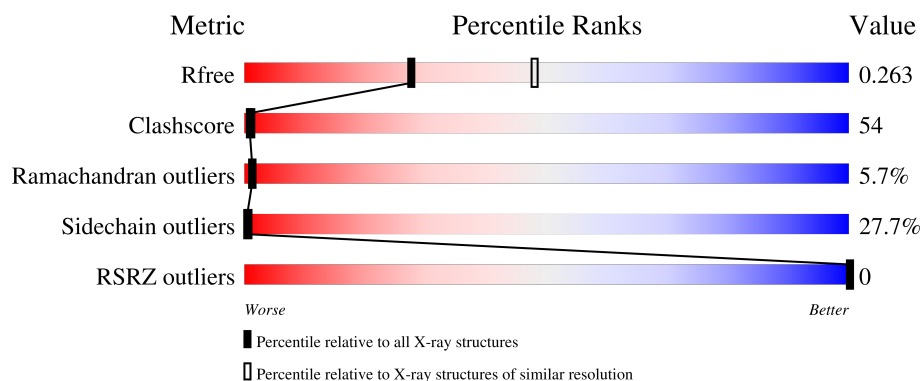
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

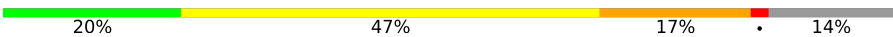
The reported resolution of this entry is 2.50 Å.

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	347	
1	B	347	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4935 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 KINESIN-LIKE PROTEIN KAR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2372	1487	415	461	9			
1	B	300	Total	C	N	O	S	0	0	0
			2372	1487	415	461	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	MET	LYS	engineered mutation	UNP P17119
A	631	ALA	GLU	engineered mutation	UNP P17119
B	383	MET	LYS	engineered mutation	UNP P17119
B	631	ALA	GLU	engineered mutation	UNP P17119

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

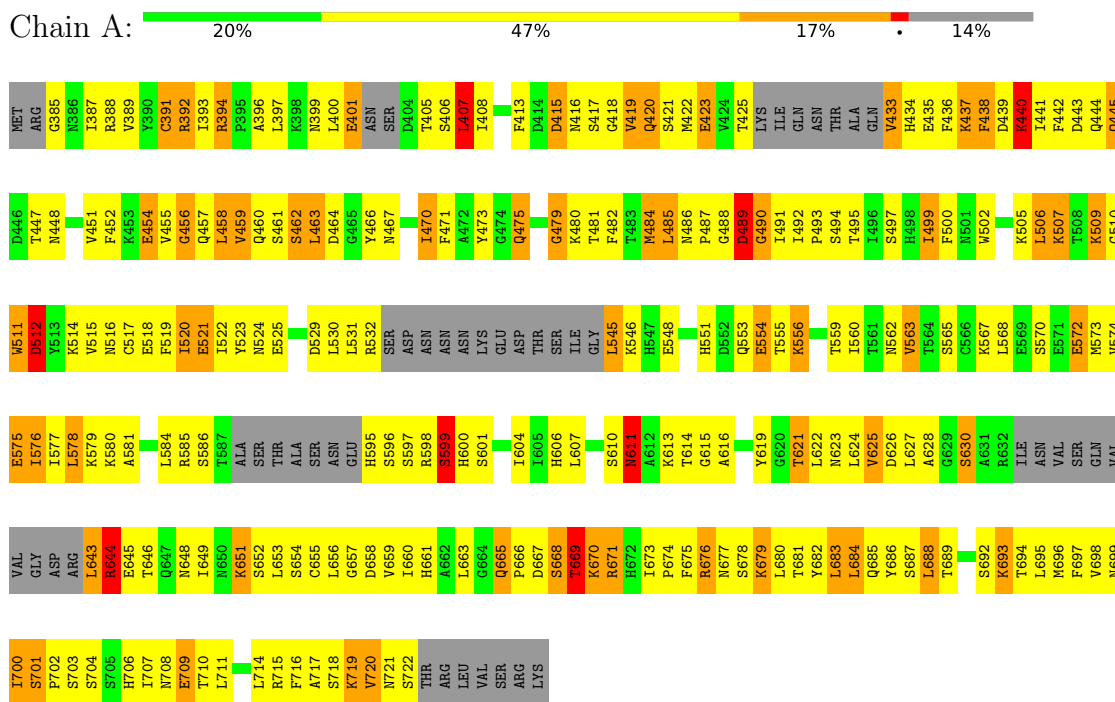
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	63	Total O 63 63	0	0
4	B	72	Total O 72 72	0	0

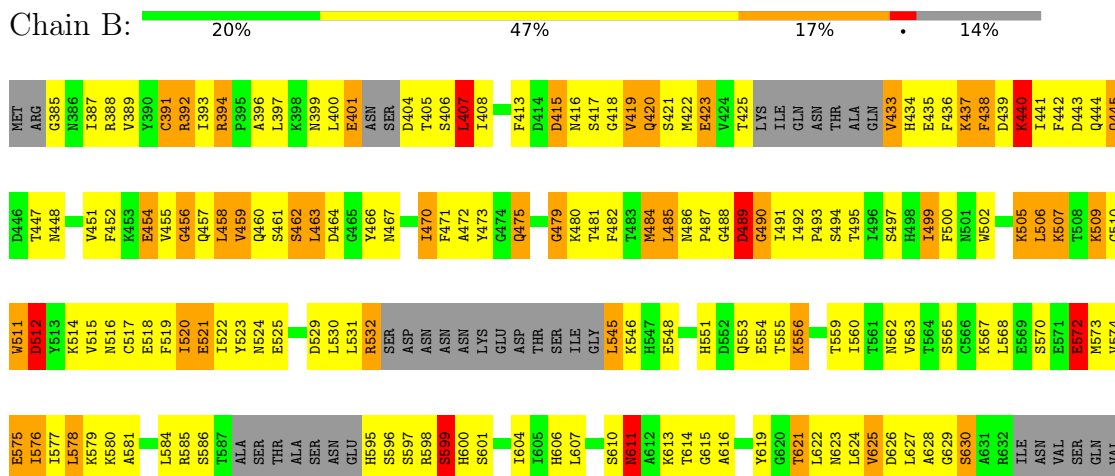
3 Residue-property plots

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

• Molecule 1: KINESIN-LIKE PROTEIN KAR3



• Molecule 1: KINESIN-LIKE PROTEIN KAR3



I700	VAL
S701	GLY
P702	ASP
S703	ARG
S704	L643
	L644
I707	S644
	S645
M708	T646
E709	G647
T710	N648
L711	L649
	L650
L714	K651
	S652
R715	L653
F716	S654
A717	G655
S718	L656
K719	G657
V720	D658
N721	V659
S722	I660
THR	H661
ARG	L662
LEU	L663
VAL	G664
SER	G665
ARG	P666
LYS	D667
	S668
S669	T669
	K670
K671	H671
L672	L672
	L673
P674	P674
F675	F675
R676	R676
M677	M677
S678	S678
K679	K679
	L680
L681	L681
V682	V682
L683	L683
L684	L684
G685	G685
V686	V686
S687	S687
L688	L688
T689	T689
S692	S692
	K693
T694	T694
L695	L695
M696	M696
F697	F697
V698	V698
V699	V699

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	62.89Å 62.89Å 153.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.6 (20.00-2.50) 89.6 (20.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.49Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.276 0.225 , 0.263	Depositor DCC
R_{free} test set	1802 reflections (9.78%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4935	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.60	0/2408	1.04	13/3245 (0.4%)
1	B	0.60	0/2408	1.04	14/3245 (0.4%)
All	All	0.60	0/4816	1.04	27/6490 (0.4%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	GLY	N-CA-C	7.26	125.45	115.00
1	A	687	SER	N-CA-C	-7.17	104.47	112.57
1	B	479	GLY	N-CA-C	6.90	124.94	115.00
1	B	645	GLU	N-CA-C	-6.82	104.06	112.38
1	A	645	GLU	N-CA-C	-6.72	104.18	112.38
1	B	687	SER	N-CA-C	-6.66	105.05	112.57
1	B	489	ASP	N-CA-C	6.52	119.65	111.24
1	B	625	VAL	N-CA-C	6.30	116.99	108.17
1	A	644	ARG	N-CA-C	-6.23	103.82	112.30
1	A	489	ASP	N-CA-C	6.11	119.12	111.24
1	A	625	VAL	N-CA-C	5.92	116.46	108.17
1	A	669	THR	N-CA-C	-5.89	104.94	111.71
1	B	644	ARG	N-CA-C	-5.88	104.30	112.30
1	B	669	THR	N-CA-C	-5.81	105.03	111.71
1	B	391	CYS	N-CA-C	-5.66	102.39	110.59
1	A	391	CYS	N-CA-C	-5.61	102.45	110.59
1	B	417	SER	N-CA-C	-5.59	106.16	112.87
1	B	668	SER	N-CA-C	-5.56	107.15	114.04
1	A	417	SER	N-CA-C	-5.54	106.22	112.87
1	A	599	SER	N-CA-C	5.28	116.30	108.86
1	A	668	SER	N-CA-C	-5.26	107.52	114.04
1	B	463	LEU	N-CA-C	-5.19	106.21	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	599	SER	N-CA-C	5.16	116.14	108.86
1	B	407	LEU	N-CA-C	-5.14	107.04	113.72
1	A	407	LEU	N-CA-C	-5.14	107.04	113.72
1	B	572	GLU	N-CA-C	-5.12	105.78	111.36
1	A	463	LEU	N-CA-C	-5.10	106.31	112.54

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	2372	0	2358	260	0
1	B	2372	0	2358	261	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	3	0
4	A	63	0	0	1	0
4	B	72	0	0	4	0
All	All	4935	0	4740	519	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 54.

All (519) 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:462:SER:HB2	1:B:607:LEU:HD12	1.31	1.10
1:A:668:SER:HA	1:A:671:ARG:HB3	1.32	1.08
1:B:394:ARG:HE	1:B:701:SER:HB2	1.15	1.07
1:A:462:SER:HB2	1:A:607:LEU:HD12	1.34	1.07
1:B:668:SER:HA	1:B:671:ARG:HB3	1.30	1.05
1:A:394:ARG:HE	1:A:701:SER:HB2	1.17	1.04
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:MET:HE2	1:A:577:ILE:HG13	1.50	0.91
1:B:560:ILE:HD11	1:B:683:LEU:HD21	1.52	0.91
1:B:394:ARG:HG3	1:B:394:ARG:HH11	1.36	0.91
1:A:560:ILE:HD11	1:A:683:LEU:HD21	1.53	0.90
1:B:573:MET:HE2	1:B:577:ILE:HG13	1.54	0.88
1:A:700:ILE:HG21	1:A:714:LEU:HD21	1.58	0.86
1:A:448:ASN:HD22	1:A:489:ASP:HB3	1.41	0.85
1:B:462:SER:HB2	1:B:607:LEU:CD1	2.05	0.85
1:B:698:VAL:HG21	1:B:717:ALA:HB2	1.59	0.85
1:A:462:SER:HB2	1:A:607:LEU:CD1	2.06	0.84
1:A:698:VAL:HG21	1:A:717:ALA:HB2	1.59	0.84
1:B:448:ASN:HD22	1:B:489:ASP:HB3	1.40	0.84
1:A:570:SER:OG	1:A:572:GLU:HG2	1.77	0.84
1:B:700:ILE:HG21	1:B:714:LEU:HD21	1.59	0.84
1:B:570:SER:OG	1:B:572:GLU:HG2	1.79	0.83
1:A:440:LYS:HD3	1:A:454:GLU:HG3	1.61	0.83
1:B:572:GLU:O	1:B:576:ILE:HD12	1.79	0.82
1:B:440:LYS:HD3	1:B:454:GLU:HG3	1.62	0.82
1:A:572:GLU:O	1:A:576:ILE:HD12	1.80	0.81
1:B:394:ARG:NE	1:B:701:SER:HB2	1.96	0.80
1:A:394:ARG:HE	1:A:701:SER:CB	1.94	0.80
1:B:521:GLU:HB3	1:B:530:LEU:HD11	1.64	0.79
1:B:521:GLU:OE1	1:B:599:SER:HB2	1.82	0.79
1:B:394:ARG:HE	1:B:701:SER:CB	1.92	0.79
1:B:419:VAL:HG23	1:B:420:GLN:N	1.98	0.79
1:B:458:LEU:HD23	1:B:459:VAL:N	1.98	0.79
1:A:524:ASN:HA	1:A:648:ASN:HD22	1.48	0.78
1:A:458:LEU:HD23	1:A:459:VAL:N	1.98	0.78
1:A:521:GLU:HB3	1:A:530:LEU:HD11	1.64	0.78
1:A:521:GLU:OE1	1:A:599:SER:HB2	1.84	0.78
1:B:394:ARG:HH11	1:B:394:ARG:CG	1.96	0.77
1:A:394:ARG:HH11	1:A:394:ARG:CG	1.96	0.77
1:B:425:THR:OG1	1:B:433:VAL:HG22	1.86	0.76
1:B:574:VAL:HG12	1:B:578:LEU:HD23	1.67	0.76
1:A:419:VAL:HG23	1:A:420:GLN:N	2.00	0.76
1:A:574:VAL:HG12	1:A:578:LEU:HD23	1.67	0.76
1:A:394:ARG:NE	1:A:701:SER:HB2	1.98	0.76
1:B:524:ASN:HA	1:B:648:ASN:HD22	1.49	0.75
1:A:459:VAL:HG12	1:A:622:LEU:CD2	2.18	0.74
1:A:425:THR:OG1	1:A:433:VAL:HG22	1.88	0.73
1:A:559:THR:HG22	1:A:560:ILE:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:THR:HG23	1:A:670:LYS:HG2	1.72	0.72
1:B:459:VAL:HG12	1:B:622:LEU:CD2	2.19	0.72
1:A:481:THR:HG21	1:A:585:ARG:O	1.90	0.72
1:B:669:THR:HG23	1:B:670:LYS:HG2	1.72	0.72
1:B:553:GLN:HA	1:B:686:TYR:OH	1.89	0.72
1:B:448:ASN:ND2	1:B:489:ASP:HB3	2.04	0.72
1:B:510:GLY:HA2	1:B:613:LYS:NZ	2.05	0.72
1:B:707:ILE:O	1:B:711:LEU:HG	1.89	0.72
1:A:448:ASN:ND2	1:A:489:ASP:HB3	2.04	0.71
1:A:553:GLN:HA	1:A:686:TYR:OH	1.88	0.71
1:A:510:GLY:HA2	1:A:613:LYS:NZ	2.06	0.71
1:A:715:ARG:O	1:A:719:LYS:HG2	1.91	0.70
1:B:481:THR:HG21	1:B:585:ARG:O	1.91	0.70
1:A:458:LEU:HD22	1:A:695:LEU:HD11	1.73	0.70
1:B:559:THR:HG22	1:B:560:ILE:H	1.55	0.70
1:A:524:ASN:HA	1:A:648:ASN:ND2	2.07	0.70
1:B:387:ILE:O	1:B:388:ARG:HD2	1.92	0.70
1:B:502:TRP:O	1:B:506:LEU:HD12	1.92	0.70
1:B:385:GLY:HA2	1:B:692:SER:O	1.91	0.69
1:A:707:ILE:O	1:A:711:LEU:HG	1.92	0.69
1:B:458:LEU:HD22	1:B:695:LEU:HD11	1.75	0.69
1:A:604:ILE:HG23	1:A:623:ASN:ND2	2.08	0.69
1:B:604:ILE:HG23	1:B:623:ASN:ND2	2.08	0.69
1:A:475:GLN:HB2	1:A:709:GLU:HG3	1.75	0.69
1:B:524:ASN:HA	1:B:648:ASN:ND2	2.07	0.69
1:A:442:PHE:CD2	1:A:451:VAL:HG22	2.29	0.68
1:A:502:TRP:O	1:A:506:LEU:HD12	1.93	0.68
1:A:387:ILE:O	1:A:388:ARG:HD2	1.93	0.68
1:B:413:PHE:HE1	1:B:415:ASP:HB3	1.59	0.68
1:B:475:GLN:HB2	1:B:709:GLU:HG3	1.76	0.68
1:B:397:LEU:H	1:B:401:GLU:CG	2.07	0.68
1:A:385:GLY:HA2	1:A:692:SER:O	1.93	0.68
1:A:600:HIS:CD2	1:A:680:LEU:HD22	2.29	0.68
1:A:519:PHE:HB3	1:A:531:LEU:HG	1.75	0.67
1:A:458:LEU:HD13	1:A:695:LEU:HD21	1.77	0.67
1:B:401:GLU:HA	1:B:703:SER:OG	1.95	0.67
1:A:401:GLU:HA	1:A:703:SER:OG	1.94	0.67
1:A:600:HIS:HD2	1:A:680:LEU:HD22	1.58	0.67
1:A:397:LEU:H	1:A:401:GLU:CG	2.07	0.67
1:B:715:ARG:O	1:B:719:LYS:HG2	1.95	0.67
1:A:413:PHE:HE1	1:A:415:ASP:HB3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:PHE:CD2	1:B:451:VAL:HG22	2.31	0.66
1:B:600:HIS:CD2	1:B:680:LEU:HD22	2.30	0.66
1:B:600:HIS:HD2	1:B:680:LEU:HD22	1.60	0.66
1:A:423:GLU:HG2	4:A:1127:HOH:O	1.95	0.66
1:B:458:LEU:HD13	1:B:695:LEU:HD21	1.78	0.66
1:A:407:LEU:HD11	1:A:704:SER:HB3	1.78	0.65
1:A:515:VAL:HG12	1:A:568:LEU:HB2	1.79	0.65
1:B:519:PHE:HB3	1:B:531:LEU:HG	1.77	0.65
1:B:545:LEU:HD23	4:B:1161:HOH:O	1.96	0.65
1:A:495:THR:HG22	1:A:499:ILE:HD12	1.78	0.65
1:B:473:TYR:HB2	1:B:627:LEU:HD12	1.78	0.65
1:B:667:ASP:CG	1:B:670:LYS:HG3	2.22	0.64
1:A:667:ASP:CG	1:A:670:LYS:HG3	2.22	0.64
1:A:684:LEU:HB2	1:A:688:LEU:HD12	1.80	0.64
1:A:408:ILE:HD12	1:A:408:ILE:H	1.62	0.64
1:A:473:TYR:HB2	1:A:627:LEU:HD12	1.78	0.64
1:B:392:ARG:NH2	3:B:999:ADP:HN62	1.96	0.64
1:B:408:ILE:HD12	1:B:408:ILE:H	1.63	0.64
1:A:522:ILE:HB	1:A:600:HIS:HB2	1.80	0.63
1:A:574:VAL:CG1	1:A:578:LEU:HD23	2.27	0.63
1:B:490:GLY:C	1:B:493:PRO:HD2	2.24	0.63
1:A:518:GLU:HG3	1:A:565:SER:HA	1.81	0.63
1:B:407:LEU:HD11	1:B:704:SER:HB3	1.80	0.63
1:B:684:LEU:HB2	1:B:688:LEU:HD12	1.81	0.63
1:B:455:VAL:O	1:B:457:GLN:N	2.32	0.63
1:B:515:VAL:HG12	1:B:568:LEU:HB2	1.81	0.63
1:A:698:VAL:HG21	1:A:717:ALA:CB	2.29	0.62
1:B:495:THR:HG22	1:B:499:ILE:HD12	1.79	0.62
1:B:574:VAL:CG1	1:B:578:LEU:HD23	2.28	0.62
1:B:574:VAL:O	1:B:578:LEU:HB2	1.99	0.62
1:B:389:VAL:O	1:B:438:PHE:HB3	1.99	0.62
1:B:522:ILE:HB	1:B:600:HIS:HB2	1.81	0.62
1:B:518:GLU:HG3	1:B:565:SER:HA	1.81	0.62
1:A:392:ARG:NH2	3:A:998:ADP:HN62	1.96	0.62
1:A:574:VAL:O	1:A:578:LEU:HB2	1.99	0.62
1:A:490:GLY:C	1:A:493:PRO:HD2	2.25	0.62
1:B:461:SER:O	1:B:464:ASP:HB2	2.00	0.62
1:A:457:GLN:NE2	1:A:460:GLN:HE21	1.96	0.62
1:A:461:SER:O	1:A:464:ASP:HB2	1.99	0.62
1:A:485:LEU:O	1:A:486:ASN:C	2.43	0.61
1:A:556:LYS:HG3	1:A:686:TYR:CE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:VAL:HG21	1:B:681:THR:HG21	1.82	0.61
1:A:458:LEU:HD23	1:A:459:VAL:HG22	1.81	0.61
1:A:458:LEU:HD12	1:A:693:LYS:HB3	1.83	0.61
1:B:676:ARG:HA	1:B:682:TYR:HB2	1.82	0.61
1:B:458:LEU:HD12	1:B:693:LYS:HB3	1.83	0.61
1:B:515:VAL:HG22	1:B:607:LEU:HD23	1.83	0.61
1:B:604:ILE:HG23	1:B:623:ASN:HD22	1.64	0.61
1:A:387:ILE:C	1:A:388:ARG:HD2	2.26	0.61
1:A:458:LEU:HD23	1:A:459:VAL:H	1.66	0.61
1:B:473:TYR:CE1	1:B:630:SER:HB2	2.36	0.61
1:B:698:VAL:HG21	1:B:717:ALA:CB	2.29	0.61
1:B:598:ARG:NH1	1:B:649:ILE:HD13	2.16	0.60
1:A:455:VAL:O	1:A:457:GLN:N	2.33	0.60
1:A:676:ARG:HA	1:A:682:TYR:HB2	1.83	0.60
1:B:490:GLY:O	1:B:493:PRO:HD2	2.02	0.60
1:B:485:LEU:O	1:B:486:ASN:C	2.43	0.60
1:A:389:VAL:HG11	1:A:717:ALA:HB1	1.83	0.60
1:B:457:GLN:NE2	1:B:460:GLN:HE21	1.98	0.60
1:B:387:ILE:C	1:B:388:ARG:HD2	2.26	0.60
1:A:473:TYR:CE1	1:A:630:SER:HB2	2.37	0.60
1:B:556:LYS:HG3	1:B:686:TYR:CE1	2.37	0.60
1:A:700:ILE:HD12	1:A:701:SER:O	2.02	0.60
1:B:545:LEU:HD22	1:B:546:LYS:H	1.66	0.60
1:A:471:PHE:O	1:A:697:PHE:HB2	2.01	0.59
1:A:545:LEU:HD22	1:A:546:LYS:H	1.66	0.59
1:B:458:LEU:HD23	1:B:459:VAL:HG22	1.84	0.59
1:A:694:THR:O	1:A:695:LEU:HD23	2.03	0.59
1:B:598:ARG:HD3	1:B:649:ILE:CD1	2.32	0.59
1:B:389:VAL:HG11	1:B:717:ALA:HB1	1.83	0.59
1:A:397:LEU:H	1:A:401:GLU:HG3	1.67	0.59
1:A:684:LEU:O	1:A:688:LEU:HD12	2.02	0.59
1:A:515:VAL:HG22	1:A:607:LEU:HD23	1.85	0.59
1:B:457:GLN:O	1:B:460:GLN:HG2	2.02	0.59
1:B:585:ARG:CZ	1:B:601:SER:HB3	2.33	0.59
1:A:457:GLN:O	1:A:460:GLN:HG2	2.02	0.59
1:A:604:ILE:HG23	1:A:623:ASN:HD22	1.66	0.59
1:A:585:ARG:CZ	1:A:601:SER:HB3	2.32	0.58
1:B:458:LEU:HD23	1:B:459:VAL:H	1.66	0.58
1:A:700:ILE:HG21	1:A:714:LEU:CD2	2.30	0.58
1:A:389:VAL:O	1:A:438:PHE:HB3	2.04	0.58
1:A:601:SER:OG	1:A:626:ASP:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:ILE:HG21	1:B:714:LEU:CD2	2.32	0.58
1:A:521:GLU:OE1	1:A:599:SER:CB	2.51	0.58
1:B:471:PHE:O	1:B:697:PHE:HB2	2.03	0.58
1:A:598:ARG:HD3	1:A:649:ILE:CD1	2.33	0.58
1:A:698:VAL:CG2	1:A:717:ALA:HB2	2.32	0.57
1:B:598:ARG:HD3	1:B:649:ILE:HD11	1.85	0.57
1:B:673:ILE:HB	1:B:675:PHE:CE2	2.39	0.57
1:A:545:LEU:HD21	1:B:572:GLU:HB2	1.87	0.57
1:B:510:GLY:HA2	1:B:613:LYS:HZ2	1.68	0.57
1:B:521:GLU:OE1	1:B:599:SER:CB	2.50	0.57
1:A:598:ARG:NH1	1:A:649:ILE:HD13	2.20	0.57
1:B:684:LEU:O	1:B:688:LEU:HD12	2.04	0.57
1:B:694:THR:O	1:B:695:LEU:HD23	2.04	0.57
1:A:490:GLY:O	1:A:493:PRO:HD2	2.04	0.57
1:A:413:PHE:CE1	1:A:415:ASP:HB3	2.40	0.56
1:A:684:LEU:C	1:A:688:LEU:HD12	2.30	0.56
1:B:481:THR:CG2	1:B:585:ARG:HB2	2.35	0.56
1:B:668:SER:CA	1:B:671:ARG:HB3	2.21	0.56
1:A:416:ASN:C	1:A:418:GLY:H	2.14	0.56
1:B:397:LEU:H	1:B:401:GLU:HG3	1.68	0.56
1:B:644:ARG:C	1:B:646:THR:N	2.64	0.56
1:B:700:ILE:HD12	1:B:701:SER:O	2.05	0.56
1:B:585:ARG:NH1	1:B:601:SER:HB3	2.21	0.56
1:B:719:LYS:HG3	1:B:720:VAL:N	2.21	0.56
1:A:585:ARG:NH1	1:A:601:SER:HB3	2.20	0.56
1:B:392:ARG:NH2	3:B:999:ADP:N6	2.54	0.56
1:B:416:ASN:C	1:B:418:GLY:N	2.63	0.56
1:B:601:SER:OG	1:B:626:ASP:HB3	2.04	0.56
1:A:523:TYR:HB2	1:A:599:SER:HB3	1.86	0.56
1:A:572:GLU:HB2	1:B:545:LEU:HD21	1.88	0.56
1:A:704:SER:HA	1:A:707:ILE:HG12	1.88	0.56
1:A:392:ARG:NH2	3:A:998:ADP:N6	2.54	0.55
1:A:407:LEU:HD12	1:A:407:LEU:H	1.72	0.55
1:A:644:ARG:C	1:A:646:THR:N	2.63	0.55
1:A:659:VAL:HG21	1:A:681:THR:HG21	1.88	0.55
1:A:480:LYS:HA	1:A:699:ASN:ND2	2.22	0.55
1:B:407:LEU:HD12	1:B:407:LEU:H	1.71	0.55
1:A:719:LYS:HG3	1:A:720:VAL:N	2.22	0.55
1:A:599:SER:O	1:A:628:ALA:HB2	2.07	0.55
1:B:393:ILE:HD12	1:B:393:ILE:H	1.72	0.55
1:B:684:LEU:C	1:B:688:LEU:HD12	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:SER:HA	1:B:707:ILE:HG12	1.88	0.55
1:A:511:TRP:HA	1:A:611:ASN:HB2	1.89	0.55
1:A:715:ARG:HA	1:A:718:SER:OG	2.06	0.55
1:B:391:CYS:HB3	1:B:441:ILE:HG23	1.86	0.55
1:B:480:LYS:HA	1:B:699:ASN:ND2	2.22	0.55
1:A:481:THR:CG2	1:A:585:ARG:HB2	2.37	0.54
1:B:437:LYS:O	1:B:437:LYS:HG3	2.07	0.54
1:B:523:TYR:HB2	1:B:599:SER:HB3	1.88	0.54
1:A:393:ILE:HD12	1:A:393:ILE:H	1.73	0.54
1:A:704:SER:HA	1:A:707:ILE:HD11	1.89	0.54
1:B:416:ASN:C	1:B:418:GLY:H	2.14	0.54
1:B:599:SER:O	1:B:628:ALA:HB2	2.08	0.54
1:B:698:VAL:CG2	1:B:717:ALA:HB2	2.33	0.54
1:A:704:SER:HA	1:A:707:ILE:CG1	2.38	0.54
1:B:667:ASP:OD2	1:B:670:LYS:HG3	2.08	0.54
1:A:598:ARG:HD3	1:A:649:ILE:HD11	1.88	0.54
1:B:679:LYS:O	1:B:683:LEU:HB2	2.08	0.54
1:B:394:ARG:HG3	1:B:394:ARG:NH1	2.13	0.54
1:A:448:ASN:HB2	1:A:489:ASP:CG	2.33	0.54
1:A:673:ILE:HB	1:A:675:PHE:CE2	2.41	0.54
1:B:704:SER:HA	1:B:707:ILE:CG1	2.38	0.54
1:B:397:LEU:H	1:B:401:GLU:HG2	1.72	0.54
1:B:461:SER:O	1:B:464:ASP:N	2.40	0.54
1:A:397:LEU:H	1:A:401:GLU:HG2	1.73	0.53
1:A:667:ASP:OD2	1:A:670:LYS:HG3	2.09	0.53
1:B:715:ARG:HA	1:B:718:SER:OG	2.07	0.53
1:A:416:ASN:C	1:A:418:GLY:N	2.63	0.53
1:A:394:ARG:HH12	1:A:397:LEU:HD11	1.73	0.53
1:B:413:PHE:CE1	1:B:415:ASP:HB3	2.40	0.53
1:A:559:THR:HG22	1:A:560:ILE:N	2.23	0.53
1:A:679:LYS:O	1:A:683:LEU:HB2	2.08	0.53
1:B:487:PRO:C	1:B:489:ASP:H	2.15	0.53
1:A:648:ASN:O	1:A:651:LYS:HB3	2.09	0.53
1:B:448:ASN:HB2	1:B:489:ASP:CG	2.34	0.53
1:B:572:GLU:O	1:B:576:ILE:CD1	2.56	0.53
1:A:510:GLY:HA2	1:A:613:LYS:HZ3	1.73	0.53
1:B:422:MET:HB3	1:B:441:ILE:CD1	2.39	0.53
1:A:401:GLU:HA	1:A:703:SER:CB	2.39	0.52
1:A:500:PHE:CE1	1:A:574:VAL:HG21	2.44	0.52
1:A:559:THR:O	1:A:560:ILE:HG13	2.10	0.52
1:B:521:GLU:HB3	1:B:530:LEU:CD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:HIS:ND1	1:B:619:TYR:OH	2.37	0.52
1:B:704:SER:HA	1:B:707:ILE:HD11	1.90	0.52
1:A:391:CYS:HB3	1:A:441:ILE:HG23	1.90	0.52
1:B:394:ARG:HH12	1:B:397:LEU:HD11	1.74	0.52
1:A:521:GLU:HB3	1:A:530:LEU:CD1	2.37	0.52
1:A:422:MET:HB3	1:A:441:ILE:CD1	2.39	0.52
1:B:443:ASP:HB3	1:B:445:GLN:NE2	2.25	0.52
1:B:573:MET:HE3	1:B:573:MET:HA	1.91	0.52
1:A:518:GLU:OE1	1:A:606:HIS:NE2	2.38	0.52
1:B:500:PHE:CE1	1:B:574:VAL:HG21	2.43	0.52
1:A:437:LYS:HG3	1:A:437:LYS:O	2.10	0.52
1:A:492:ILE:HB	1:A:493:PRO:HD3	1.92	0.52
1:A:644:ARG:C	1:A:646:THR:H	2.16	0.51
1:A:572:GLU:H	1:A:572:GLU:CD	2.16	0.51
1:B:511:TRP:HA	1:B:611:ASN:HB2	1.90	0.51
1:B:559:THR:HG22	1:B:560:ILE:N	2.24	0.51
1:B:559:THR:O	1:B:560:ILE:HG13	2.10	0.51
1:B:599:SER:C	1:B:628:ALA:HB2	2.35	0.51
1:B:644:ARG:C	1:B:646:THR:H	2.17	0.51
1:A:610:SER:OG	1:A:611:ASN:N	2.42	0.51
1:B:481:THR:HG21	1:B:585:ARG:HB2	1.92	0.51
1:A:443:ASP:HB3	1:A:445:GLN:NE2	2.26	0.51
1:A:458:LEU:CD1	1:A:693:LYS:HB3	2.41	0.51
1:B:663:LEU:HD21	1:B:689:THR:HG22	1.93	0.51
1:A:487:PRO:C	1:A:489:ASP:H	2.18	0.51
1:A:517:CYS:HA	1:A:604:ILE:O	2.11	0.51
1:B:458:LEU:CD1	1:B:693:LYS:HB3	2.41	0.51
1:B:572:GLU:CD	1:B:572:GLU:H	2.18	0.51
1:B:610:SER:OG	1:B:611:ASN:N	2.42	0.51
1:A:668:SER:CA	1:A:671:ARG:HB3	2.23	0.51
1:B:455:VAL:O	1:B:456:GLY:C	2.54	0.51
1:B:487:PRO:O	1:B:489:ASP:N	2.39	0.51
1:A:545:LEU:HD13	1:A:562:ASN:HB3	1.93	0.50
1:B:648:ASN:O	1:B:651:LYS:HB3	2.11	0.50
1:A:599:SER:C	1:A:628:ALA:HB2	2.36	0.50
1:A:457:GLN:HE21	1:A:460:GLN:HE21	1.57	0.50
1:A:573:MET:HA	1:A:573:MET:HE3	1.92	0.50
1:A:495:THR:O	1:A:499:ILE:HB	2.11	0.50
1:B:545:LEU:HD13	1:B:562:ASN:HB3	1.93	0.50
1:A:455:VAL:O	1:A:456:GLY:C	2.54	0.50
1:A:704:SER:O	1:A:707:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLU:HA	1:B:703:SER:CB	2.41	0.49
1:A:423:GLU:HA	1:A:434:HIS:O	2.12	0.49
1:B:467:ASN:HA	1:B:621:THR:O	2.12	0.49
1:B:520:ILE:HG22	1:B:529:ASP:HA	1.94	0.49
1:A:459:VAL:HG12	1:A:622:LEU:HD23	1.94	0.49
1:A:510:GLY:HA2	1:A:613:LYS:HZ2	1.76	0.49
1:B:649:ILE:HG22	1:B:653:LEU:HD12	1.94	0.49
1:B:704:SER:O	1:B:707:ILE:HG12	2.13	0.49
1:B:423:GLU:HA	1:B:434:HIS:O	2.13	0.49
1:A:419:VAL:HG11	1:A:437:LYS:HE3	1.95	0.49
1:A:479:GLY:HA2	3:A:998:ADP:H8	1.78	0.49
1:A:663:LEU:HD21	1:A:689:THR:HG22	1.95	0.49
1:B:394:ARG:CD	1:B:701:SER:HA	2.42	0.49
1:A:438:PHE:CD2	1:A:438:PHE:N	2.80	0.49
1:B:517:CYS:HA	1:B:604:ILE:O	2.13	0.49
1:B:655:CYS:O	1:B:659:VAL:HG23	2.13	0.49
1:A:704:SER:HA	1:A:707:ILE:CD1	2.43	0.48
1:B:495:THR:O	1:B:499:ILE:HB	2.12	0.48
1:B:458:LEU:HD12	1:B:693:LYS:CG	2.44	0.48
1:A:649:ILE:HG22	1:A:653:LEU:HD12	1.96	0.48
1:B:704:SER:HA	1:B:707:ILE:CD1	2.44	0.48
1:A:520:ILE:HG22	1:A:529:ASP:HA	1.94	0.48
1:B:419:VAL:HG11	1:B:437:LYS:HE3	1.94	0.48
1:B:439:ASP:O	1:B:440:LYS:CB	2.61	0.48
1:A:467:ASN:HA	1:A:621:THR:O	2.13	0.48
1:B:611:ASN:OD1	1:B:613:LYS:HB2	2.13	0.48
1:B:479:GLY:C	1:B:699:ASN:HD22	2.22	0.48
1:B:560:ILE:HD12	4:B:1210:HOH:O	2.12	0.48
1:B:611:ASN:CG	1:B:611:ASN:O	2.57	0.48
1:B:492:ILE:HB	1:B:493:PRO:HD3	1.95	0.48
1:A:458:LEU:HD12	1:A:693:LYS:CG	2.43	0.48
1:A:482:PHE:O	1:A:486:ASN:HB2	2.14	0.48
1:B:440:LYS:HG2	1:B:442:PHE:CE1	2.49	0.48
1:B:457:GLN:HE21	1:B:460:GLN:HE21	1.60	0.48
1:B:568:LEU:HD22	1:B:574:VAL:HG22	1.96	0.48
1:A:479:GLY:C	1:A:699:ASN:HD22	2.22	0.48
1:B:660:ILE:O	1:B:661:HIS:C	2.57	0.48
1:A:572:GLU:CD	1:A:572:GLU:N	2.72	0.47
1:B:479:GLY:HA2	3:B:999:ADP:H8	1.79	0.47
1:B:492:ILE:HG12	1:B:624:LEU:CD1	2.44	0.47
1:B:644:ARG:HD3	1:B:644:ARG:HA	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:SER:O	1:A:464:ASP:N	2.44	0.47
1:A:470:ILE:CG2	1:A:484:MET:HE1	2.44	0.47
1:A:481:THR:HG21	1:A:585:ARG:HB2	1.96	0.47
1:A:470:ILE:HG13	1:A:624:LEU:CD2	2.44	0.47
1:A:655:CYS:O	1:A:659:VAL:HG23	2.14	0.47
1:B:389:VAL:HG21	1:B:721:ASN:HB2	1.95	0.47
1:A:394:ARG:CD	1:A:701:SER:HA	2.43	0.47
1:A:439:ASP:O	1:A:440:LYS:CB	2.62	0.47
1:A:606:HIS:ND1	1:A:619:TYR:OH	2.40	0.47
1:A:644:ARG:HD3	1:A:644:ARG:HA	1.55	0.47
1:A:611:ASN:OD1	1:A:613:LYS:HB2	2.14	0.47
1:B:598:ARG:HH11	1:B:649:ILE:CD1	2.28	0.47
1:B:656:LEU:HD21	1:B:696:MET:HE1	1.97	0.47
1:A:568:LEU:HD22	1:A:574:VAL:HG22	1.96	0.47
1:A:660:ILE:O	1:A:661:HIS:C	2.58	0.47
1:A:394:ARG:HD3	1:A:702:PRO:HD3	1.97	0.47
1:B:518:GLU:OE1	1:B:606:HIS:NE2	2.39	0.47
1:A:421:SER:HA	1:A:436:PHE:O	2.15	0.46
1:A:456:GLY:C	1:A:459:VAL:HG23	2.40	0.46
1:A:611:ASN:CG	1:A:611:ASN:O	2.57	0.46
1:B:421:SER:HA	1:B:436:PHE:O	2.14	0.46
1:B:545:LEU:CD2	1:B:546:LYS:H	2.28	0.46
1:B:711:LEU:O	1:B:715:ARG:HB2	2.16	0.46
1:A:719:LYS:HG3	1:A:720:VAL:H	1.81	0.46
1:B:510:GLY:HA3	1:B:613:LYS:HD3	1.97	0.46
1:B:611:ASN:O	1:B:615:GLY:N	2.47	0.46
1:A:389:VAL:HG21	1:A:721:ASN:HB2	1.96	0.46
1:A:492:ILE:HG12	1:A:624:LEU:CD1	2.45	0.46
1:B:510:GLY:HA2	1:B:613:LYS:HZ3	1.80	0.46
1:A:595:HIS:C	1:A:597:SER:N	2.74	0.46
1:A:394:ARG:HG3	1:A:394:ARG:NH1	2.12	0.46
1:B:517:CYS:HB2	1:B:604:ILE:O	2.15	0.46
1:A:512:ASP:OD1	1:A:512:ASP:C	2.59	0.46
1:A:611:ASN:O	1:A:615:GLY:N	2.49	0.46
1:A:684:LEU:HB2	1:A:688:LEU:CD1	2.45	0.46
1:B:500:PHE:HE1	1:B:574:VAL:HG21	1.81	0.46
1:A:572:GLU:O	1:A:576:ILE:CD1	2.57	0.46
1:B:394:ARG:HD3	1:B:702:PRO:HD3	1.97	0.46
1:A:555:THR:O	1:A:556:LYS:HB2	2.16	0.46
1:A:656:LEU:HD21	1:A:696:MET:HE1	1.98	0.46
1:B:482:PHE:O	1:B:486:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:CD2	1:A:546:LYS:H	2.29	0.46
1:A:711:LEU:O	1:A:715:ARG:HB2	2.16	0.46
1:B:456:GLY:C	1:B:459:VAL:HG23	2.40	0.46
1:A:440:LYS:HG2	1:A:442:PHE:CE1	2.51	0.46
1:B:438:PHE:CD2	1:B:438:PHE:N	2.81	0.46
1:B:472:ALA:O	1:B:480:LYS:HD2	2.16	0.46
1:B:595:HIS:C	1:B:597:SER:N	2.74	0.46
1:A:452:PHE:CD1	1:A:494:SER:HB2	2.51	0.45
1:A:573:MET:HG3	1:A:577:ILE:HD12	1.97	0.45
1:B:470:ILE:CG2	1:B:484:MET:HE1	2.45	0.45
1:A:422:MET:HB3	1:A:441:ILE:HD12	1.98	0.45
1:B:715:ARG:HA	1:B:718:SER:HG	1.81	0.45
1:A:625:VAL:HG12	1:A:627:LEU:HD23	1.99	0.45
1:B:401:GLU:N	1:B:401:GLU:OE2	2.49	0.45
1:B:445:GLN:H	1:B:445:GLN:HG3	1.42	0.45
1:B:452:PHE:CD1	1:B:494:SER:HB2	2.52	0.45
1:B:572:GLU:CD	1:B:572:GLU:N	2.74	0.45
1:B:455:VAL:C	1:B:457:GLN:N	2.74	0.45
1:A:413:PHE:HE1	1:A:415:ASP:CB	2.29	0.45
1:B:709:GLU:CD	1:B:709:GLU:O	2.60	0.45
1:A:401:GLU:N	1:A:401:GLU:OE2	2.50	0.45
1:A:654:SER:O	1:A:658:ASP:OD2	2.35	0.45
1:A:480:LYS:N	1:A:699:ASN:HD22	2.14	0.44
1:B:510:GLY:CA	1:B:613:LYS:HD3	2.46	0.44
1:B:719:LYS:HG3	1:B:720:VAL:H	1.81	0.44
1:A:510:GLY:HA3	1:A:613:LYS:HD3	2.00	0.44
1:A:598:ARG:HH11	1:A:649:ILE:CD1	2.31	0.44
1:B:459:VAL:HG12	1:B:622:LEU:HD23	1.95	0.44
1:A:510:GLY:CA	1:A:613:LYS:HD3	2.48	0.44
1:A:445:GLN:H	1:A:445:GLN:HG3	1.41	0.44
1:A:509:LYS:C	1:A:511:TRP:H	2.26	0.44
1:B:470:ILE:HG13	1:B:624:LEU:CD2	2.47	0.44
1:A:570:SER:HB2	1:A:572:GLU:OE2	2.18	0.44
1:A:394:ARG:CG	1:A:394:ARG:NH1	2.66	0.44
1:A:573:MET:HE2	1:A:577:ILE:CG1	2.35	0.44
1:A:717:ALA:O	1:A:718:SER:C	2.61	0.44
1:B:512:ASP:OD1	1:B:512:ASP:C	2.60	0.44
1:A:487:PRO:O	1:A:489:ASP:N	2.41	0.44
1:A:509:LYS:HB3	1:A:509:LYS:HE3	1.73	0.44
1:B:598:ARG:HH11	1:B:649:ILE:HD13	1.82	0.44
1:B:676:ARG:C	1:B:678:SER:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLN:OE1	1:A:502:TRP:NE1	2.50	0.44
1:B:509:LYS:C	1:B:511:TRP:H	2.26	0.44
1:A:438:PHE:HE1	1:A:717:ALA:HB3	1.83	0.43
1:A:643:LEU:HB3	1:A:644:ARG:H	1.52	0.43
1:A:674:PRO:HB2	1:A:677:ASN:CG	2.44	0.43
1:A:709:GLU:CD	1:A:709:GLU:O	2.61	0.43
1:B:506:LEU:O	1:B:507:LYS:C	2.60	0.43
1:B:578:LEU:HD13	1:B:578:LEU:HA	1.79	0.43
1:B:684:LEU:HB2	1:B:688:LEU:CD1	2.46	0.43
1:A:676:ARG:C	1:A:678:SER:H	2.25	0.43
1:A:716:PHE:CD1	1:A:717:ALA:N	2.87	0.43
1:B:458:LEU:HD12	1:B:693:LYS:CB	2.48	0.43
1:B:460:GLN:OE1	1:B:502:TRP:NE1	2.50	0.43
1:B:716:PHE:CD1	1:B:717:ALA:N	2.86	0.43
1:A:455:VAL:C	1:A:457:GLN:N	2.75	0.43
1:A:458:LEU:HD12	1:A:693:LYS:HG2	2.00	0.43
1:A:517:CYS:HB2	1:A:604:ILE:O	2.18	0.43
1:B:438:PHE:HE1	1:B:717:ALA:HB3	1.84	0.43
1:A:710:THR:HG22	1:A:714:LEU:HD11	2.00	0.43
1:B:389:VAL:HG12	1:B:438:PHE:HD1	1.83	0.43
1:A:394:ARG:HE	1:A:701:SER:CA	2.31	0.43
1:A:570:SER:CB	1:A:572:GLU:HG2	2.47	0.43
1:B:570:SER:HB2	1:B:572:GLU:OE2	2.18	0.43
1:A:448:ASN:HD22	1:A:490:GLY:N	2.16	0.43
1:B:555:THR:O	1:B:556:LYS:HB2	2.19	0.43
1:B:621:THR:CG2	1:B:623:ASN:HD21	2.31	0.43
1:B:625:VAL:HG12	1:B:627:LEU:HD23	2.00	0.43
1:B:707:ILE:O	1:B:711:LEU:CG	2.63	0.43
1:A:506:LEU:O	1:A:507:LYS:C	2.60	0.43
1:B:480:LYS:N	1:B:699:ASN:HD22	2.16	0.43
1:B:573:MET:HG3	1:B:577:ILE:HD12	2.00	0.43
1:A:458:LEU:HD12	1:A:693:LYS:CB	2.47	0.43
1:A:393:ILE:HD13	1:A:443:ASP:HA	2.00	0.43
1:A:551:HIS:CE1	1:A:685:GLN:HG2	2.54	0.43
1:B:462:SER:HA	1:B:466:TYR:O	2.19	0.43
1:B:708:ASN:HD22	1:B:708:ASN:HA	1.58	0.42
1:B:393:ILE:HD13	1:B:443:ASP:HA	2.01	0.42
1:A:457:GLN:NE2	1:A:460:GLN:NE2	2.66	0.42
1:A:485:LEU:HD21	1:A:581:ALA:HB3	2.01	0.42
1:B:668:SER:C	1:B:671:ARG:H	2.27	0.42
1:A:470:ILE:HG13	1:A:624:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:PHE:HE1	1:A:574:VAL:HG21	1.82	0.42
1:A:554:GLU:HB2	1:A:555:THR:H	1.69	0.42
1:B:716:PHE:CD1	1:B:716:PHE:C	2.98	0.42
1:B:422:MET:HB3	1:B:441:ILE:HD12	2.02	0.42
1:B:509:LYS:HB3	1:B:509:LYS:HE3	1.72	0.42
1:B:710:THR:HG22	1:B:714:LEU:HD11	2.00	0.42
1:A:394:ARG:HD3	1:A:701:SER:HA	2.01	0.42
1:A:574:VAL:CG1	1:A:578:LEU:CD2	2.97	0.42
1:B:551:HIS:CE1	1:B:685:GLN:HG2	2.55	0.42
1:B:570:SER:CB	1:B:572:GLU:HG2	2.48	0.42
1:A:671:ARG:HE	1:A:671:ARG:HB2	1.39	0.42
1:A:655:CYS:SG	1:A:678:SER:HB2	2.60	0.42
1:A:716:PHE:CD1	1:A:716:PHE:C	2.98	0.42
1:B:394:ARG:HE	1:B:701:SER:CA	2.31	0.42
1:B:654:SER:O	1:B:658:ASP:OD2	2.37	0.42
1:B:717:ALA:O	1:B:718:SER:C	2.62	0.42
1:B:457:GLN:O	1:B:460:GLN:CG	2.67	0.41
1:B:559:THR:C	1:B:560:ILE:HG13	2.44	0.41
1:B:437:LYS:O	1:B:437:LYS:CG	2.68	0.41
1:B:573:MET:HE3	1:B:576:ILE:HB	2.03	0.41
1:A:389:VAL:HG12	1:A:438:PHE:HD1	1.84	0.41
1:A:560:ILE:CG2	1:A:563:VAL:HG21	2.51	0.41
1:A:656:LEU:O	1:A:657:GLY:C	2.63	0.41
1:B:394:ARG:HD3	1:B:701:SER:HA	2.01	0.41
1:B:458:LEU:HD12	1:B:693:LYS:HG2	2.03	0.41
1:B:505:LYS:HD2	4:B:1133:HOH:O	2.20	0.41
1:B:663:LEU:C	1:B:665:GLN:H	2.28	0.41
1:A:683:LEU:HD22	1:A:683:LEU:O	2.21	0.41
1:B:404:ASP:N	4:B:1138:HOH:O	2.53	0.41
1:B:448:ASN:HD22	1:B:490:GLY:N	2.18	0.41
1:B:532:ARG:O	1:B:532:ARG:HG3	2.19	0.41
1:A:575:GLU:O	1:A:579:LYS:HB2	2.20	0.41
1:A:462:SER:HA	1:A:466:TYR:O	2.20	0.41
1:A:507:LYS:C	1:A:509:LYS:H	2.28	0.41
1:B:407:LEU:HD13	1:B:707:ILE:HG13	2.02	0.41
1:B:667:ASP:OD1	1:B:670:LYS:HG3	2.21	0.41
1:A:663:LEU:C	1:A:665:GLN:H	2.29	0.41
1:B:507:LYS:C	1:B:509:LYS:H	2.28	0.41
1:B:581:ALA:HA	1:B:584:LEU:HD12	2.03	0.41
1:A:407:LEU:HD13	1:A:707:ILE:HG13	2.03	0.41
1:A:457:GLN:O	1:A:460:GLN:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:THR:C	1:A:560:ILE:HG13	2.46	0.41
1:A:610:SER:O	1:A:611:ASN:CB	2.68	0.41
1:B:663:LEU:HD13	1:B:688:LEU:O	2.21	0.41
1:B:575:GLU:O	1:B:579:LYS:HB2	2.20	0.41
1:A:573:MET:HE3	1:A:576:ILE:HB	2.03	0.40
1:B:708:ASN:HA	1:B:711:LEU:HD12	2.03	0.40
1:B:574:VAL:CG1	1:B:578:LEU:CD2	2.97	0.40
1:B:674:PRO:HB2	1:B:677:ASN:CG	2.46	0.40
1:A:425:THR:OG1	1:A:433:VAL:CG2	2.65	0.40
1:A:507:LYS:C	1:A:509:LYS:N	2.80	0.40
1:A:581:ALA:HA	1:A:584:LEU:HD12	2.02	0.40
1:A:614:THR:HG22	1:A:614:THR:O	2.22	0.40
1:B:439:ASP:O	1:B:440:LYS:HB2	2.22	0.40
1:B:614:THR:HG22	1:B:614:THR:O	2.21	0.40
1:A:668:SER:C	1:A:671:ARG:H	2.29	0.40
1:B:470:ILE:HG13	1:B:624:LEU:HD22	2.04	0.40
1:A:475:GLN:HE22	1:A:706:HIS:HB3	1.87	0.40
1:A:598:ARG:HH11	1:A:649:ILE:HD13	1.85	0.40
1:B:663:LEU:HG	1:B:673:ILE:HD13	2.03	0.40
1:B:683:LEU:HD22	1:B:683:LEU:O	2.21	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	288/347 (83%)	233 (81%)	39 (14%)	16 (6%)	1	1
1	B	288/347 (83%)	233 (81%)	38 (13%)	17 (6%)	1	1
All	All	576/694 (83%)	466 (81%)	77 (13%)	33 (6%)	1	1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	THR
1	A	415	ASP
1	A	420	GLN
1	A	440	LYS
1	A	511	TRP
1	A	611	ASN
1	B	405	THR
1	B	415	ASP
1	B	420	GLN
1	B	440	LYS
1	B	511	TRP
1	B	611	ASN
1	A	396	ALA
1	A	419	VAL
1	A	438	PHE
1	A	456	GLY
1	A	490	GLY
1	A	512	ASP
1	A	525	GLU
1	A	666	PRO
1	B	396	ALA
1	B	419	VAL
1	B	438	PHE
1	B	456	GLY
1	B	490	GLY
1	B	512	ASP
1	B	525	GLU
1	B	666	PRO
1	A	616	ALA
1	B	488	GLY
1	B	616	ALA
1	A	488	GLY
1	B	629	GLY

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	274/316 (87%)	198 (72%)	76 (28%)	0	1
1	B	274/316 (87%)	198 (72%)	76 (28%)	0	1
All	All	548/632 (87%)	396 (72%)	152 (28%)	0	1

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ARG
1	A	394	ARG
1	A	399	ASN
1	A	400	LEU
1	A	401	GLU
1	A	406	SER
1	A	407	LEU
1	A	423	GLU
1	A	433	VAL
1	A	435	GLU
1	A	437	LYS
1	A	440	LYS
1	A	444	GLN
1	A	445	GLN
1	A	447	THR
1	A	454	GLU
1	A	458	LEU
1	A	459	VAL
1	A	462	SER
1	A	463	LEU
1	A	470	ILE
1	A	475	GLN
1	A	484	MET
1	A	485	LEU
1	A	489	ASP
1	A	491	ILE
1	A	497	SER
1	A	499	ILE
1	A	505	LYS
1	A	506	LEU
1	A	507	LYS
1	A	509	LYS
1	A	512	ASP
1	A	514	LYS
1	A	516	ASN

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Mol	Chain	Res	Type
1	A	520	ILE
1	A	521	GLU
1	A	532	ARG
1	A	545	LEU
1	A	548	GLU
1	A	554	GLU
1	A	556	LYS
1	A	563	VAL
1	A	567	LYS
1	A	572	GLU
1	A	575	GLU
1	A	576	ILE
1	A	578	LEU
1	A	580	LYS
1	A	586	SER
1	A	596	SER
1	A	599	SER
1	A	611	ASN
1	A	621	THR
1	A	630	SER
1	A	643	LEU
1	A	644	ARG
1	A	651	LYS
1	A	652	SER
1	A	665	GLN
1	A	669	THR
1	A	670	LYS
1	A	671	ARG
1	A	676	ARG
1	A	679	LYS
1	A	683	LEU
1	A	684	LEU
1	A	688	LEU
1	A	693	LYS
1	A	700	ILE
1	A	701	SER
1	A	708	ASN
1	A	709	GLU
1	A	719	LYS
1	A	720	VAL
1	A	722	SER
1	B	392	ARG

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Mol	Chain	Res	Type
1	B	394	ARG
1	B	399	ASN
1	B	400	LEU
1	B	401	GLU
1	B	406	SER
1	B	407	LEU
1	B	423	GLU
1	B	433	VAL
1	B	435	GLU
1	B	437	LYS
1	B	440	LYS
1	B	444	GLN
1	B	445	GLN
1	B	447	THR
1	B	454	GLU
1	B	458	LEU
1	B	459	VAL
1	B	462	SER
1	B	463	LEU
1	B	470	ILE
1	B	475	GLN
1	B	484	MET
1	B	485	LEU
1	B	489	ASP
1	B	491	ILE
1	B	497	SER
1	B	499	ILE
1	B	505	LYS
1	B	506	LEU
1	B	507	LYS
1	B	509	LYS
1	B	512	ASP
1	B	514	LYS
1	B	516	ASN
1	B	520	ILE
1	B	521	GLU
1	B	532	ARG
1	B	545	LEU
1	B	548	GLU
1	B	554	GLU
1	B	556	LYS
1	B	563	VAL

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Mol	Chain	Res	Type
1	B	567	LYS
1	B	572	GLU
1	B	575	GLU
1	B	576	ILE
1	B	578	LEU
1	B	580	LYS
1	B	586	SER
1	B	596	SER
1	B	599	SER
1	B	611	ASN
1	B	621	THR
1	B	630	SER
1	B	643	LEU
1	B	644	ARG
1	B	651	LYS
1	B	652	SER
1	B	665	GLN
1	B	669	THR
1	B	670	LYS
1	B	671	ARG
1	B	676	ARG
1	B	679	LYS
1	B	683	LEU
1	B	684	LEU
1	B	688	LEU
1	B	693	LYS
1	B	700	ILE
1	B	701	SER
1	B	708	ASN
1	B	709	GLU
1	B	719	LYS
1	B	720	VAL
1	B	722	SER

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

Mol	Chain	Res	Type
1	A	416	ASN
1	A	448	ASN
1	A	457	GLN
1	A	475	GLN
1	A	486	ASN

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Mol	Chain	Res	Type
1	A	516	ASN
1	A	526	ASN
1	A	617	HIS
1	A	623	ASN
1	A	677	ASN
1	A	685	GLN
1	A	699	ASN
1	A	708	ASN
1	A	721	ASN
1	B	416	ASN
1	B	448	ASN
1	B	457	GLN
1	B	475	GLN
1	B	486	ASN
1	B	516	ASN
1	B	526	ASN
1	B	617	HIS
1	B	623	ASN
1	B	665	GLN
1	B	677	ASN
1	B	685	GLN
1	B	699	ASN
1	B	708	ASN
1	B	721	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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$
3	ADP	B	999	2	28,29,29	1.56	4 (14%)	43,45,45	1.96	7 (16%)
3	ADP	A	998	2	28,29,29	1.48	4 (14%)	43,45,45	1.94	7 (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
3	ADP	B	999	2	-	5/16/32/32	0/3/3/3
3	ADP	A	998	2	-	5/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	ADP	C5-N7	-4.93	1.30	1.39
3	A	998	ADP	C5-N7	-4.50	1.30	1.39
3	B	999	ADP	C4-N9	-3.04	1.31	1.37
3	A	998	ADP	C4-N9	-2.90	1.31	1.37
3	B	999	ADP	C8-N9	-2.49	1.33	1.37
3	A	998	ADP	C8-N9	-2.26	1.33	1.37
3	B	999	ADP	PB-O2B	2.18	1.62	1.54
3	A	998	ADP	PA-O3A	-2.17	1.57	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	ADP	N3-C2-N1	-6.62	118.56	128.58
3	A	998	ADP	N3-C2-N1	-6.51	118.72	128.58
3	B	999	ADP	C5-C4-N3	-5.43	119.24	126.72
3	A	998	ADP	C5-C4-N3	-5.41	119.27	126.72
3	B	999	ADP	C2-N3-C4	4.57	123.00	111.83
3	A	998	ADP	C2-N3-C4	4.44	122.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	ADP	N3-C4-N9	3.91	133.82	127.17
3	A	998	ADP	N3-C4-N9	3.80	133.63	127.17
3	A	998	ADP	C4-C5-N7	-3.03	107.12	110.58
3	A	998	ADP	C5-N7-C8	2.99	108.16	103.45
3	B	999	ADP	C5-N7-C8	2.97	108.11	103.45
3	B	999	ADP	C4-C5-N7	-2.89	107.28	110.58
3	A	998	ADP	N9-C8-N7	-2.87	109.86	113.94
3	B	999	ADP	N9-C8-N7	-2.86	109.88	113.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	998	ADP	C5'-O5'-PA-O1A
3	A	998	ADP	C5'-O5'-PA-O2A
3	A	998	ADP	C5'-O5'-PA-O3A
3	B	999	ADP	C5'-O5'-PA-O1A
3	B	999	ADP	C5'-O5'-PA-O2A
3	B	999	ADP	C5'-O5'-PA-O3A
3	A	998	ADP	C3'-C4'-C5'-O5'
3	B	999	ADP	C3'-C4'-C5'-O5'
3	A	998	ADP	O4'-C4'-C5'-O5'
3	B	999	ADP	O4'-C4'-C5'-O5'

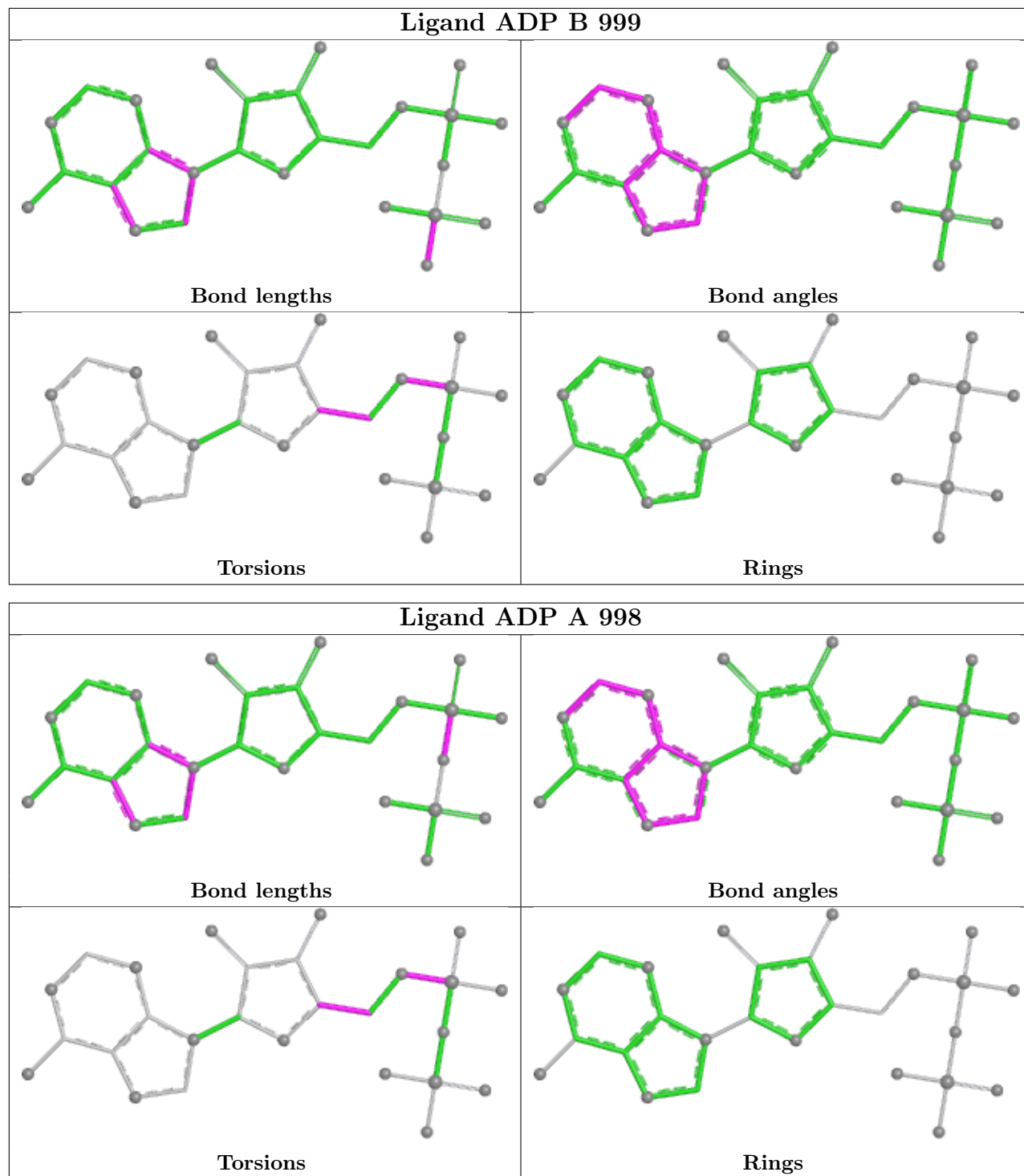
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	ADP	3	0
3	A	998	ADP	3	0

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

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	300/347 (86%)	-1.38	0 100 100	16, 41, 75, 86	0
1	B	300/347 (86%)	-1.38	0 100 100	14, 41, 76, 84	0
All	All	600/694 (86%)	-1.38	0 100 100	14, 41, 76, 86	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

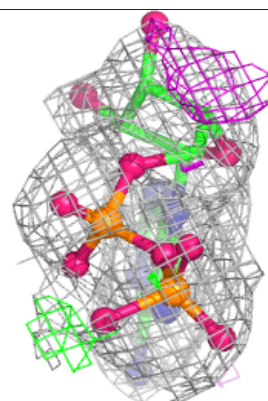
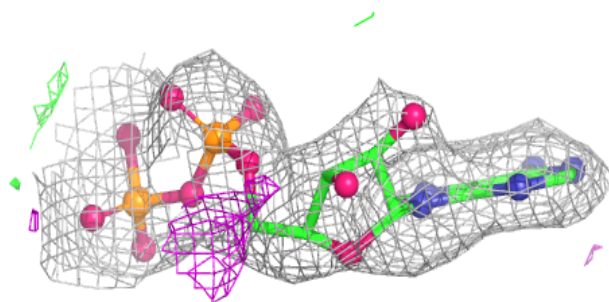
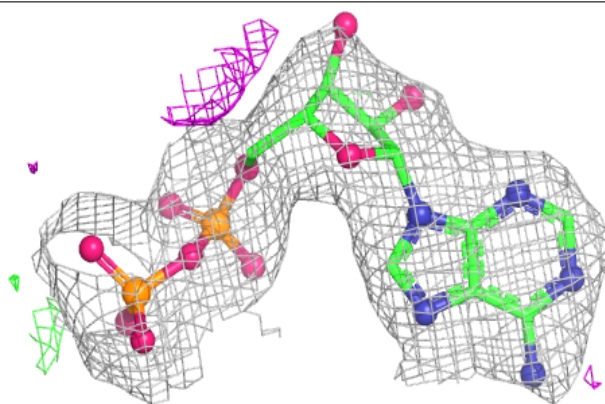
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	996	1/1	0.98	0.07	36,36,36,36	0
2	MG	B	997	1/1	0.99	0.07	38,38,38,38	0
3	ADP	A	998	27/27	0.99	0.03	27,42,53,57	0
3	ADP	B	999	27/27	0.99	0.03	28,40,55,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

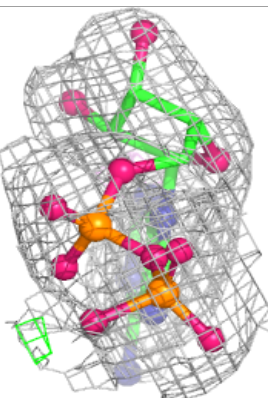
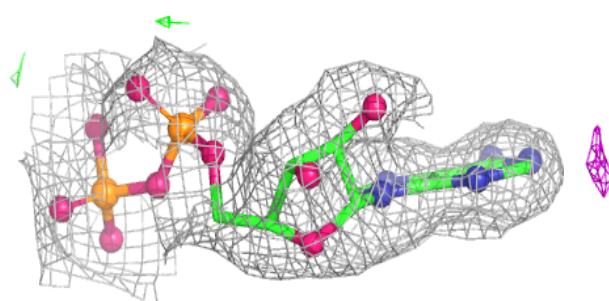
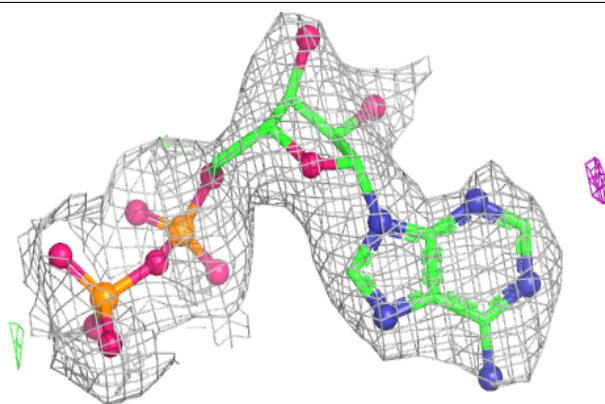
Electron density around ADP A 998:

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



Electron density around ADP B 999:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.