Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:43 AM GMT

PDB ID	:	3BXZ
Title	:	Crystal structure of the isolated DEAD motor domains from Escherichia coli SecA
Authors	:	Nithianantham, S.; Namjoshi, S.; Shilton, B.H.
Deposited on	:	2008-01-15
Resolution	:	3.00 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

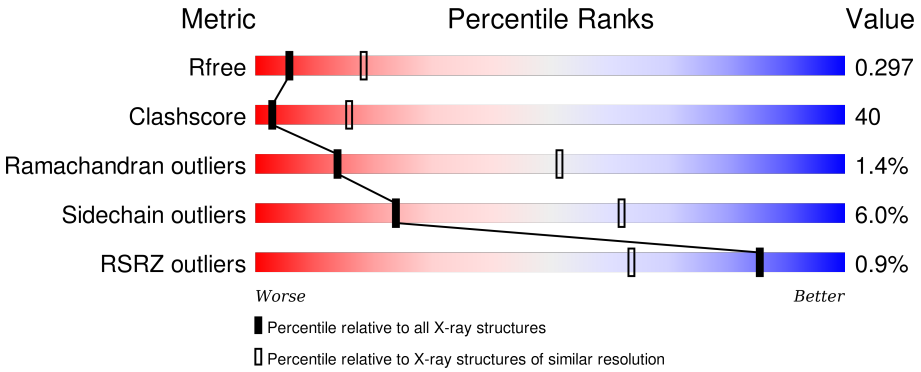
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	471	% 37% 52% · 7%
1	B	471	% 39% 51% · 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7106 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 subunit secA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3420	2143	608	655	14			
1	B	440	Total	C	N	O	S	0	0	0
			3439	2154	613	657	15			

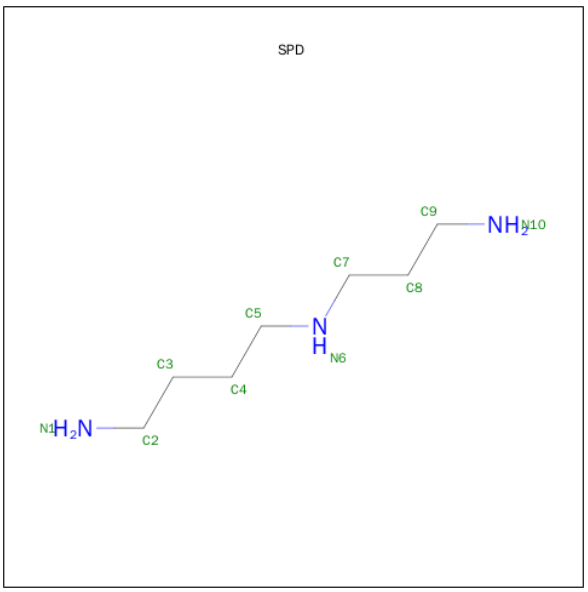
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P10408
A	0	HIS	-	EXPRESSION TAG	UNP P10408
A	1	HIS	-	EXPRESSION TAG	UNP P10408
A	2	HIS	-	EXPRESSION TAG	UNP P10408
A	3	HIS	-	EXPRESSION TAG	UNP P10408
A	4	HIS	-	EXPRESSION TAG	UNP P10408
A	5	HIS	-	EXPRESSION TAG	UNP P10408
A	368	ALA	GLU	ENGINEERED	UNP P10408
B	-1	MET	-	EXPRESSION TAG	UNP P10408
B	0	HIS	-	EXPRESSION TAG	UNP P10408
B	1	HIS	-	EXPRESSION TAG	UNP P10408
B	2	HIS	-	EXPRESSION TAG	UNP P10408
B	3	HIS	-	EXPRESSION TAG	UNP P10408
B	4	HIS	-	EXPRESSION TAG	UNP P10408
B	5	HIS	-	EXPRESSION TAG	UNP P10408
B	368	ALA	GLU	ENGINEERED	UNP P10408

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

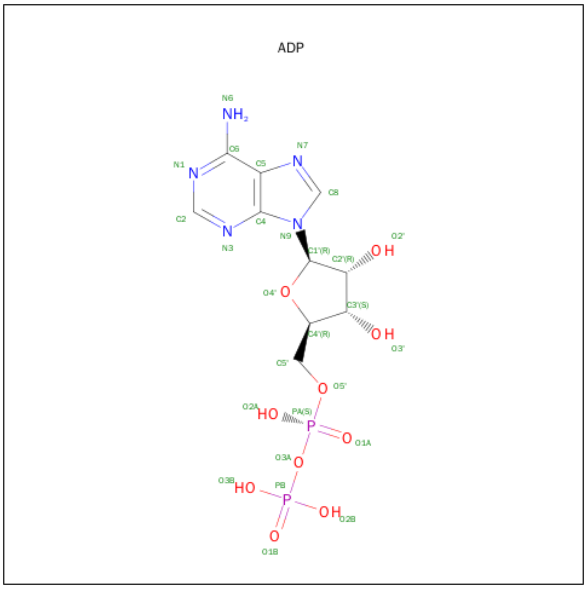
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 7 3	0	0
3	B	1	Total C N 10 7 3	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

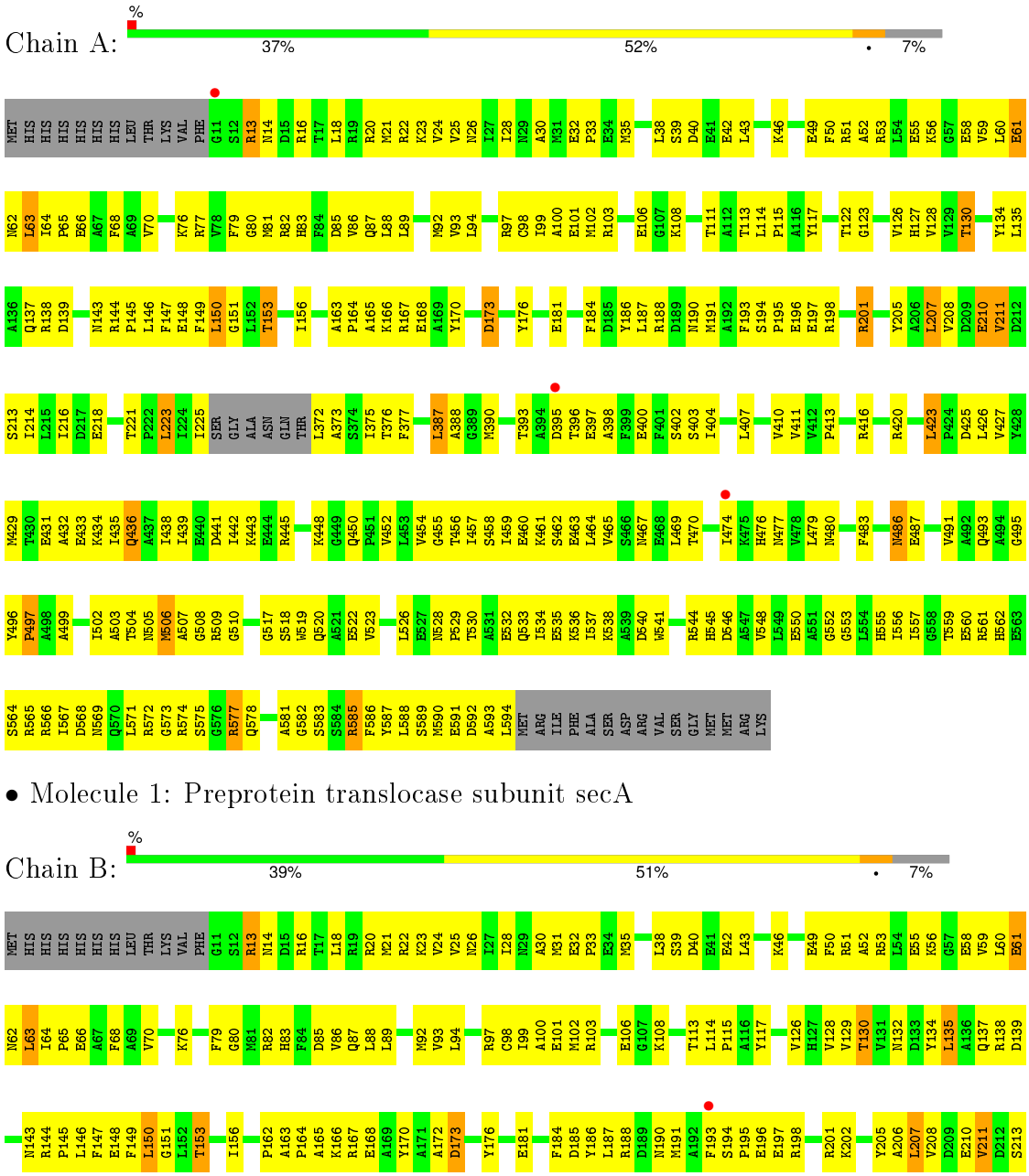
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total	O	0	0
			89	89		
5	B	82	Total	O	0	0
			82	82		

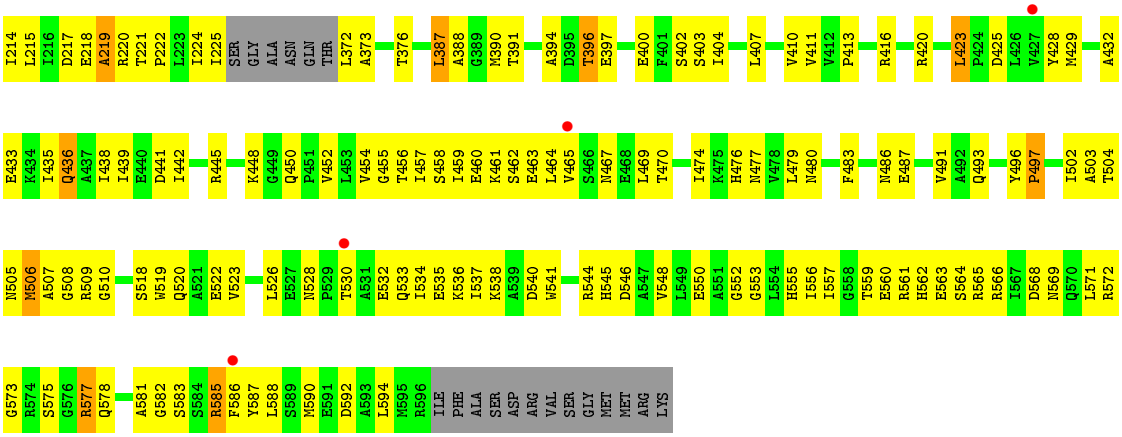
3 Residue-property plots (i)

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 subunit secA



- Molecule 1: Preprotein translocase subunit secA


I214 L215 T216 D217 E218 A219 R220 T221 P222 L223 I224 I225 SER GLY ALA ASN GLN THR L372 A373 T376 L387 A388 G389 M390 T391 A394 D395 T396 E397 E400 F401 S402 S403 I404 L407 V410 V411 V412 P413 R416 R420 L423 P424 D425 L426 V427 Y428 M429 A432
E433 K434 I435 Q436 A437 I438 I439 E440 D441 I442 R445 K448 G449 Q450 P451 V452 L453 V454 G455 T456 I457 S458 I459 E460 K461 S462 E463 L464 V465 S466 N467 E468 L469 T470 I474 K475 H476 N477 V478 L479 N480 F483 N486 E487 V491 A492 Q493 Y496 P497 I502 A503 T504
N505 M506 A507 G508 R509 G510 S518 W519 Q520 A521 E522 V523 L526 E527 N528 P529 T530 A531 E532 Q533 I534 E535 K536 I537 K538 A539 D540 W541 R544 H545 D546 A547 V548 L549 E550 A551 G552 G553 L554 H555 I556 I557 G558 T559 E560 R561 H562 E563 S564 R565 R566 I567 D568 N569 Q570 L571 R572
G573 R574 S575 G576 R577 Q578 A581 G582 S583 S584 R585 F586 Y587 L588 S589 M590 E591 D592 A593 L594 M595 R596 ILE PHE ALA SER ASP ARG VAL SER GLY MET MET ARG LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.82Å 71.36Å 119.54Å 90.00° 128.82° 90.00°	Depositor
Resolution (Å)	46.58 – 3.00 46.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.58-3.00) 84.1 (46.57-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.305 0.243 , 0.297	Depositor DCC
R_{free} test set	2317 reflections (9.86%)	DCC
Wilson B-factor (Å^2)	83.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 23500 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7106	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: MG, SPD, 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	0.40	0/3472	0.63	1/4689 (0.0%)
1	B	0.39	0/3491	0.63	0/4713
All	All	0.39	0/6963	0.63	1/9402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	486	ASN	CB-CA-C	-5.01	100.38	110.40

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	3420	0	3431	283	0
1	B	3439	0	3453	275	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	19	4	0
3	B	10	0	19	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	89	0	0	19	0
5	B	82	0	0	22	0
All	All	7106	0	6946	550	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 40.

All (550) 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:A:506:MET:H	1:A:506:MET:HE2	1.12	1.13
1:B:506:MET:H	1:B:506:MET:HE2	1.12	1.06
1:A:221:THR:HG22	1:A:376:THR:HG22	1.05	1.03
1:B:556:ILE:HD13	1:B:571:LEU:HG	1.45	0.98
1:A:504:THR:HG22	1:A:505:ASN:H	1.28	0.98
1:A:556:ILE:HD13	1:A:571:LEU:HG	1.45	0.94
1:B:99:ILE:HD11	1:B:407:LEU:HD13	1.48	0.94
1:A:64:ILE:HG13	1:A:65:PRO:CD	1.96	0.94
1:A:457:ILE:HG23	1:A:560:GLU:HG3	1.49	0.93
1:A:99:ILE:HD11	1:A:407:LEU:HD13	1.49	0.93
1:A:64:ILE:HG13	1:A:65:PRO:HD3	1.51	0.93
1:B:561:ARG:HH22	1:B:572:ARG:HH22	1.14	0.93
1:B:64:ILE:HG13	1:B:65:PRO:CD	1.98	0.92
1:B:504:THR:HG22	1:B:505:ASN:H	1.31	0.92
1:B:64:ILE:HG13	1:B:65:PRO:HD3	1.52	0.91
1:B:562:HIS:HD2	1:B:564:SER:H	1.17	0.91
1:A:221:THR:CG2	1:A:376:THR:HG22	1.98	0.89
1:A:436:GLN:HG3	5:A:951:HOH:O	1.72	0.87
1:A:221:THR:HG22	1:A:376:THR:CG2	2.00	0.85
1:B:506:MET:HE2	1:B:506:MET:N	1.91	0.85
1:B:63:LEU:HD23	1:B:63:LEU:H	1.41	0.84
1:A:506:MET:HE2	1:A:506:MET:N	1.92	0.83
1:B:60:LEU:HD12	1:B:61:GLU:N	1.94	0.83
1:A:445:ARG:HA	1:A:448:LYS:HD3	1.60	0.83
1:A:63:LEU:HD23	1:A:63:LEU:H	1.44	0.82
1:B:225:ILE:HG22	1:B:372:LEU:HD22	1.61	0.81
1:B:445:ARG:HA	1:B:448:LYS:HD3	1.60	0.81
1:B:14:ASN:HD21	1:B:411:VAL:H	1.30	0.80
1:A:454:VAL:HG22	1:A:557:ILE:HD11	1.64	0.80
1:A:60:LEU:HD12	1:A:61:GLU:N	1.96	0.79
1:A:14:ASN:HD21	1:A:411:VAL:H	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:PRO:HD3	5:A:990:HOH:O	1.84	0.77
1:B:568:ASP:HB3	5:B:964:HOH:O	1.83	0.77
1:B:94:LEU:HD13	1:B:207:LEU:HD21	1.66	0.77
1:B:425:ASP:HB3	1:B:588:LEU:HD13	1.67	0.76
1:B:553:GLY:HA3	1:B:581:ALA:O	1.85	0.76
1:B:454:VAL:HG22	1:B:557:ILE:HD11	1.65	0.76
1:B:491:VAL:HG21	1:B:508:GLY:HA3	1.68	0.75
1:A:491:VAL:HG21	1:A:508:GLY:HA3	1.67	0.75
1:A:425:ASP:HB3	1:A:588:LEU:HD13	1.68	0.75
1:B:562:HIS:CD2	1:B:564:SER:H	2.02	0.75
1:A:53:ARG:HA	1:A:56:LYS:HE2	1.69	0.75
1:B:459:ILE:O	1:B:463:GLU:HG2	1.86	0.75
1:A:459:ILE:O	1:A:463:GLU:HG2	1.87	0.75
1:A:562:HIS:HD2	1:A:564:SER:H	1.30	0.74
1:A:577:ARG:NH1	1:A:578:GLN:HB2	2.03	0.74
1:A:553:GLY:HA3	1:A:581:ALA:O	1.86	0.74
1:B:53:ARG:HA	1:B:56:LYS:HE2	1.67	0.74
1:B:201:ARG:HD2	5:B:961:HOH:O	1.87	0.74
1:B:217:ASP:O	1:B:220:ARG:HG2	1.87	0.74
1:B:561:ARG:HH22	1:B:572:ARG:NH2	1.84	0.74
1:B:577:ARG:NH1	1:B:578:GLN:HB2	2.03	0.74
1:A:66:GLU:O	1:A:70:VAL:HG23	1.87	0.74
1:A:76:LYS:O	1:A:80:GLY:HA2	1.88	0.73
1:A:94:LEU:HD13	1:A:207:LEU:HD21	1.69	0.73
1:A:504:THR:HG22	1:A:505:ASN:N	2.04	0.73
1:B:457:ILE:HG23	1:B:560:GLU:HG3	1.68	0.73
1:A:18:LEU:HD21	1:A:413:PRO:HD3	1.69	0.72
1:A:561:ARG:HH22	1:A:572:ARG:HH22	1.36	0.72
1:B:66:GLU:O	1:B:70:VAL:HG23	1.89	0.72
1:B:526:LEU:HD23	1:B:528:ASN:H	1.54	0.72
1:B:18:LEU:HD21	1:B:413:PRO:HD3	1.70	0.72
5:A:979:HOH:O	1:B:222:PRO:HB3	1.88	0.72
1:A:115:PRO:HG2	1:A:207:LEU:HD11	1.72	0.72
1:B:25:VAL:HG21	1:B:89:LEU:HD13	1.72	0.72
1:B:115:PRO:HG2	1:B:207:LEU:HD11	1.72	0.72
1:B:76:LYS:O	1:B:80:GLY:HA2	1.90	0.71
1:A:562:HIS:CD2	1:A:564:SER:H	2.08	0.71
1:B:50:PHE:CD2	1:B:63:LEU:HD12	2.26	0.70
1:A:526:LEU:HD23	1:A:528:ASN:H	1.55	0.70
1:B:504:THR:HG22	1:B:505:ASN:N	2.05	0.70
1:A:544:ARG:O	1:A:548:VAL:HG23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG21	1:A:89:LEU:HD13	1.73	0.69
1:B:68:PHE:CD2	1:B:114:LEU:HD13	2.27	0.69
1:A:210:GLU:HG3	5:A:981:HOH:O	1.91	0.69
1:A:455:GLY:O	1:A:559:THR:HG23	1.93	0.68
1:B:455:GLY:O	1:B:559:THR:HG23	1.93	0.68
1:A:225:ILE:HG12	1:A:372:LEU:HG	1.73	0.68
1:A:50:PHE:CD2	1:A:63:LEU:HD12	2.28	0.68
1:B:79:PHE:CE1	1:B:146:LEU:HB2	2.29	0.68
1:B:144:ARG:HG2	1:B:148:GLU:HG3	1.76	0.67
1:A:469:LEU:HD23	1:A:474:ILE:HB	1.76	0.67
1:B:544:ARG:O	1:B:548:VAL:HG23	1.94	0.67
1:B:538:LYS:O	1:B:538:LYS:HD3	1.95	0.67
1:A:213:SER:O	1:A:218:GLU:HG2	1.95	0.67
1:A:538:LYS:HD3	1:A:538:LYS:O	1.95	0.67
1:A:123:GLY:HA2	5:A:957:HOH:O	1.95	0.66
1:A:79:PHE:CE1	1:A:146:LEU:HB2	2.29	0.66
1:A:60:LEU:HB2	5:A:909:HOH:O	1.96	0.66
1:A:68:PHE:CD2	1:A:114:LEU:HD13	2.30	0.66
1:B:469:LEU:HD23	1:B:474:ILE:HB	1.76	0.66
1:B:503:ALA:HB1	1:B:507:ALA:HB3	1.77	0.66
1:B:396:THR:HB	1:B:397:GLU:OE1	1.95	0.66
1:A:503:ALA:HB1	1:A:507:ALA:HB3	1.78	0.65
1:B:467:ASN:HA	1:B:470:THR:HG22	1.78	0.65
1:B:506:MET:HB3	1:B:509:ARG:HD2	1.79	0.65
1:B:39:SER:OG	1:B:42:GLU:HG3	1.96	0.65
1:A:504:THR:H	1:A:507:ALA:HB2	1.61	0.64
1:B:43:LEU:O	1:B:46:LYS:HB2	1.97	0.64
1:A:39:SER:OG	1:A:42:GLU:HG3	1.97	0.64
1:A:467:ASN:HA	1:A:470:THR:HG22	1.79	0.64
1:A:506:MET:HB3	1:A:509:ARG:HD2	1.79	0.64
1:A:454:VAL:HG22	1:A:557:ILE:CD1	2.28	0.64
1:A:377:PHE:HA	1:B:191:MET:CE	2.27	0.63
1:B:60:LEU:HD11	5:B:968:HOH:O	1.97	0.63
1:B:87:GLN:NE2	4:B:902:ADP:N7	2.47	0.63
1:A:23:LYS:HA	1:A:26:ASN:HD22	1.64	0.63
1:B:504:THR:H	1:B:507:ALA:HB2	1.62	0.63
1:A:373:ALA:HB2	5:B:966:HOH:O	1.98	0.63
1:A:441:ASP:O	1:A:445:ARG:HG3	1.98	0.62
1:B:454:VAL:HG22	1:B:557:ILE:CD1	2.29	0.62
1:A:114:LEU:HB2	1:A:115:PRO:CD	2.29	0.62
1:B:441:ASP:O	1:B:445:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:H	1:A:196:GLU:CD	2.02	0.62
1:B:214:ILE:O	1:B:218:GLU:HB2	1.99	0.62
1:B:153:THR:N	1:B:173:ASP:OD2	2.28	0.62
1:B:561:ARG:NH2	1:B:572:ARG:HH22	1.93	0.62
1:A:94:LEU:HD21	1:A:390:MET:HB3	1.82	0.62
1:A:144:ARG:HG2	1:A:148:GLU:HG3	1.81	0.62
1:A:165:ALA:O	1:A:168:GLU:HB2	1.99	0.62
1:A:43:LEU:O	1:A:46:LYS:HB2	1.99	0.62
1:B:165:ALA:O	1:B:168:GLU:HB2	1.99	0.62
1:A:487:GLU:O	1:A:491:VAL:HG23	1.99	0.62
1:B:60:LEU:HD12	1:B:61:GLU:H	1.65	0.62
1:B:108:LYS:HE2	5:B:914:HOH:O	2.00	0.62
1:B:526:LEU:HD22	1:B:528:ASN:O	2.00	0.62
1:A:395:ASP:HA	1:A:398:ALA:HB2	1.83	0.61
1:B:94:LEU:HD21	1:B:390:MET:HB3	1.82	0.61
1:A:434:LYS:HE3	1:A:589:SER:HB2	1.81	0.61
1:B:130:THR:HG21	1:B:135:LEU:HB3	1.81	0.61
1:B:114:LEU:HB2	1:B:115:PRO:CD	2.31	0.61
1:A:130:THR:HG21	1:A:135:LEU:HB3	1.81	0.61
1:A:457:ILE:HD13	5:A:948:HOH:O	2.01	0.60
1:A:49:GLU:O	1:A:53:ARG:HG3	2.01	0.60
1:B:23:LYS:HA	1:B:26:ASN:HD22	1.66	0.60
1:A:153:THR:N	1:A:173:ASP:OD2	2.29	0.60
1:B:196:GLU:H	1:B:196:GLU:CD	2.04	0.60
1:A:61:GLU:HG2	1:A:64:ILE:HD13	1.83	0.60
1:A:526:LEU:HD22	1:A:528:ASN:O	2.01	0.60
1:B:102:MET:O	1:B:108:LYS:HE3	2.01	0.60
1:B:487:GLU:O	1:B:491:VAL:HG23	2.02	0.59
1:B:139:ASP:O	1:B:143:ASN:HB2	2.03	0.59
1:A:493:GLN:NE2	1:A:518:SER:H	1.99	0.59
1:B:454:VAL:HG22	1:B:557:ILE:CG1	2.32	0.59
1:A:434:LYS:CE	1:A:589:SER:HB2	2.33	0.59
1:B:493:GLN:NE2	1:B:518:SER:H	2.01	0.59
1:B:387:LEU:HG	5:B:970:HOH:O	2.01	0.59
1:A:454:VAL:HG22	1:A:557:ILE:CG1	2.33	0.59
1:B:113:THR:HG22	1:B:143:ASN:HD21	1.67	0.59
1:A:493:GLN:HE22	1:A:518:SER:H	1.51	0.59
1:B:506:MET:H	1:B:506:MET:CE	2.02	0.59
1:B:509:ARG:HG2	5:B:976:HOH:O	2.02	0.58
1:A:83:HIS:ND1	1:A:114:LEU:HD21	2.18	0.58
1:B:194:SER:HB2	1:B:196:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:HG2	1:B:64:ILE:HD13	1.85	0.58
1:A:138:ARG:NH2	1:A:510:GLY:O	2.35	0.58
1:A:457:ILE:CG2	1:A:560:GLU:HG3	2.29	0.58
1:A:506:MET:CE	1:A:506:MET:H	2.00	0.58
1:A:18:LEU:O	1:A:22:ARG:HB2	2.04	0.58
1:B:503:ALA:HB1	1:B:507:ALA:CB	2.34	0.57
1:B:114:LEU:HB2	1:B:115:PRO:HD3	1.87	0.57
1:A:102:MET:O	1:A:108:LYS:HE3	2.04	0.57
1:A:376:THR:O	1:B:191:MET:HE3	2.04	0.57
1:B:224:ILE:HB	1:B:373:ALA:HB3	1.87	0.57
1:B:519:TRP:O	1:B:522:GLU:HB2	2.05	0.57
1:A:114:LEU:HB2	1:A:115:PRO:HD3	1.87	0.57
1:B:49:GLU:O	1:B:53:ARG:HG3	2.05	0.57
1:A:60:LEU:HD12	1:A:61:GLU:HB2	1.86	0.57
1:B:18:LEU:O	1:B:22:ARG:HB2	2.04	0.57
1:A:113:THR:HG22	1:A:143:ASN:HD21	1.68	0.57
1:B:211:VAL:HG22	1:B:390:MET:N	2.20	0.56
1:A:503:ALA:HB1	1:A:507:ALA:CB	2.34	0.56
1:A:568:ASP:HB2	1:A:586:PHE:CZ	2.40	0.56
1:B:59:VAL:HB	1:B:62:ASN:HB2	1.87	0.56
1:B:63:LEU:N	1:B:63:LEU:HD23	2.18	0.56
1:B:432:ALA:O	1:B:436:GLN:HB2	2.05	0.56
1:B:16:ARG:O	1:B:20:ARG:HB2	2.05	0.56
1:A:194:SER:HB2	1:A:196:GLU:OE2	2.05	0.56
1:A:432:ALA:O	1:A:436:GLN:HB2	2.05	0.56
1:A:585:ARG:HG3	1:A:585:ARG:HH11	1.71	0.56
1:B:60:LEU:HD12	1:B:61:GLU:HB2	1.88	0.56
1:A:211:VAL:HG22	1:A:390:MET:N	2.20	0.56
1:B:496:TYR:HE2	1:B:544:ARG:HH11	1.53	0.55
1:B:83:HIS:ND1	1:B:114:LEU:HD21	2.21	0.55
1:B:493:GLN:HE22	1:B:518:SER:H	1.53	0.55
1:A:59:VAL:HB	1:A:62:ASN:HB2	1.87	0.55
1:A:60:LEU:HD12	1:A:61:GLU:H	1.67	0.55
1:A:16:ARG:O	1:A:20:ARG:HB2	2.06	0.55
1:A:496:TYR:HE2	1:A:544:ARG:HH11	1.54	0.54
1:A:377:PHE:HA	1:B:191:MET:HE1	1.89	0.54
1:B:568:ASP:HB2	1:B:586:PHE:CZ	2.41	0.54
1:A:191:MET:SD	1:B:186:TYR:CE2	3.01	0.54
1:A:137:GLN:HG3	1:A:156:ILE:HG21	1.90	0.54
1:A:504:THR:CG2	1:A:505:ASN:H	2.09	0.54
1:B:469:LEU:HD23	1:B:469:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HG13	1:A:205:TYR:HD2	1.73	0.54
1:A:519:TRP:O	1:A:522:GLU:HB2	2.08	0.54
1:B:585:ARG:HH11	1:B:585:ARG:HG3	1.71	0.54
1:A:469:LEU:O	1:A:469:LEU:HD23	2.07	0.54
1:A:493:GLN:NE2	1:A:518:SER:HB3	2.23	0.54
1:B:218:GLU:O	1:B:220:ARG:N	2.32	0.54
1:B:397:GLU:OE1	1:B:566:ARG:HD3	2.07	0.54
1:B:206:ALA:HB3	5:B:970:HOH:O	2.07	0.54
1:B:565:ARG:NH1	1:B:572:ARG:HH12	2.05	0.54
1:B:460:GLU:O	1:B:464:LEU:HG	2.08	0.54
1:B:32:GLU:N	1:B:33:PRO:HD2	2.23	0.53
1:B:552:GLY:O	1:B:582:GLY:HA2	2.08	0.53
1:A:541:TRP:HA	1:A:544:ARG:NH2	2.23	0.53
1:B:420:ARG:HH12	1:B:573:GLY:HA2	1.72	0.53
1:A:565:ARG:NH1	1:A:572:ARG:HH12	2.06	0.53
1:B:590:MET:C	1:B:592:ASP:H	2.11	0.53
1:A:64:ILE:HG13	1:A:65:PRO:HD2	1.83	0.53
1:A:460:GLU:O	1:A:464:LEU:HG	2.07	0.53
1:B:450:GLN:HG3	1:B:553:GLY:O	2.08	0.53
1:B:541:TRP:HA	1:B:544:ARG:NH2	2.23	0.53
1:A:420:ARG:HH12	1:A:573:GLY:HA2	1.73	0.53
1:B:64:ILE:HG13	1:B:65:PRO:HD2	1.86	0.53
1:A:63:LEU:N	1:A:63:LEU:HD23	2.20	0.53
1:A:225:ILE:CG2	1:A:372:LEU:HD12	2.39	0.53
1:A:463:GLU:HG3	3:A:905:SPD:N6	2.24	0.53
1:A:450:GLN:HG3	1:A:553:GLY:O	2.08	0.53
1:A:191:MET:SD	1:B:186:TYR:HE2	2.32	0.53
1:A:456:THR:HG21	1:A:462:SER:HA	1.90	0.53
1:A:438:ILE:HG22	1:A:587:TYR:CD2	2.44	0.53
1:B:438:ILE:HG22	1:B:587:TYR:CD2	2.43	0.53
1:B:530:THR:HB	1:B:533:GLN:HE22	1.74	0.53
1:B:456:THR:HG21	1:B:462:SER:HA	1.91	0.53
1:B:572:ARG:HD3	5:B:919:HOH:O	2.08	0.52
1:A:108:LYS:HD2	5:A:966:HOH:O	2.08	0.52
1:B:126:VAL:HG13	1:B:205:TYR:HD2	1.74	0.52
1:B:479:LEU:CD1	1:B:491:VAL:HG22	2.39	0.52
1:B:172:ALA:O	1:B:201:ARG:NH2	2.41	0.52
1:A:127:HIS:CD2	5:A:973:HOH:O	2.61	0.52
1:A:377:PHE:HA	1:B:191:MET:HE3	1.90	0.52
1:B:101:GLU:HG2	5:B:982:HOH:O	2.09	0.52
1:B:117:TYR:CE1	1:B:150:LEU:HD13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:HG22	1:A:452:VAL:HG21	1.90	0.52
1:A:21:MET:O	1:A:25:VAL:HG23	2.10	0.52
1:B:144:ARG:O	1:B:147:PHE:N	2.42	0.52
1:A:400:GLU:CG	1:A:404:ILE:HD11	2.40	0.52
1:A:463:GLU:HG3	3:A:905:SPD:HN6	1.74	0.52
1:B:173:ASP:HA	5:B:971:HOH:O	2.10	0.52
1:A:530:THR:HB	1:A:533:GLN:HE22	1.74	0.52
1:B:217:ASP:OD1	1:B:566:ARG:NH2	2.39	0.52
1:A:32:GLU:N	1:A:33:PRO:HD2	2.24	0.52
1:B:442:ILE:HG22	1:B:452:VAL:HG21	1.91	0.52
1:B:166:LYS:NZ	1:B:181:GLU:OE1	2.42	0.52
1:B:504:THR:CG2	1:B:505:ASN:H	2.12	0.51
1:B:400:GLU:CG	1:B:404:ILE:HD11	2.40	0.51
1:B:137:GLN:HG3	1:B:156:ILE:HG21	1.91	0.51
1:A:589:SER:HB3	1:A:592:ASP:OD2	2.10	0.51
1:A:400:GLU:O	1:A:404:ILE:HG13	2.10	0.51
1:B:391:THR:CG2	1:B:394:ALA:HB2	2.39	0.51
1:A:499:ALA:HA	5:A:937:HOH:O	2.10	0.51
1:A:593:ALA:O	1:A:594:LEU:HD23	2.10	0.51
1:B:461:LYS:O	1:B:465:VAL:HG23	2.10	0.51
1:A:534:ILE:HG13	1:A:535:GLU:N	2.26	0.51
1:A:166:LYS:NZ	1:A:181:GLU:OE1	2.43	0.51
1:B:93:VAL:O	1:B:98:CYS:HB2	2.11	0.51
1:A:103:ARG:O	1:A:106:GLU:HB2	2.11	0.51
1:A:81:MET:HA	5:A:983:HOH:O	2.10	0.51
1:A:83:HIS:CE1	1:A:114:LEU:HD21	2.46	0.50
1:B:493:GLN:NE2	1:B:518:SER:HB3	2.26	0.50
1:B:103:ARG:HD3	5:B:977:HOH:O	2.11	0.50
1:A:479:LEU:CD1	1:A:491:VAL:HG22	2.41	0.50
1:B:60:LEU:CD1	1:B:61:GLU:N	2.72	0.50
1:A:588:LEU:HD12	1:A:588:LEU:N	2.26	0.50
1:A:400:GLU:HG2	1:A:404:ILE:HD11	1.94	0.50
1:A:461:LYS:O	1:A:465:VAL:HG23	2.10	0.50
1:A:93:VAL:O	1:A:98:CYS:HB2	2.11	0.50
1:A:520:GLN:N	1:A:520:GLN:OE1	2.45	0.50
1:B:53:ARG:HB3	1:B:58:GLU:OE2	2.10	0.50
1:A:552:GLY:O	1:A:582:GLY:HA2	2.10	0.50
1:B:400:GLU:O	1:B:404:ILE:HG13	2.11	0.50
1:B:149:PHE:C	1:B:151:GLY:H	2.15	0.50
1:A:577:ARG:HH11	1:A:578:GLN:HB2	1.75	0.50
1:A:22:ARG:NH1	5:A:968:HOH:O	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:C	1:A:372:LEU:HD23	2.31	0.50
1:B:134:TYR:HD2	1:B:135:LEU:HD22	1.77	0.50
1:B:219:ALA:HA	5:B:975:HOH:O	2.11	0.50
1:A:555:HIS:HA	1:A:583:SER:O	2.12	0.49
1:B:89:LEU:O	1:B:93:VAL:HG23	2.11	0.49
1:A:541:TRP:HA	1:A:544:ARG:CZ	2.42	0.49
1:A:211:VAL:CG2	1:A:390:MET:N	2.76	0.49
1:A:149:PHE:C	1:A:151:GLY:H	2.15	0.49
1:B:534:ILE:HG13	1:B:535:GLU:N	2.26	0.49
1:B:213:SER:O	1:B:218:GLU:HG2	2.11	0.49
1:A:457:ILE:HG21	5:A:948:HOH:O	2.11	0.49
1:A:561:ARG:HH11	1:A:561:ARG:HG2	1.76	0.49
1:A:76:LYS:HE2	1:A:82:ARG:HB2	1.94	0.49
1:B:113:THR:HG22	1:B:143:ASN:ND2	2.28	0.49
1:A:465:VAL:O	1:A:469:LEU:HB2	2.13	0.49
1:A:541:TRP:CA	1:A:544:ARG:HH21	2.26	0.49
1:B:35:MET:HA	1:B:38:LEU:HD13	1.94	0.49
1:B:555:HIS:HA	1:B:583:SER:O	2.13	0.49
1:B:21:MET:HB2	1:B:92:MET:SD	2.53	0.49
1:A:117:TYR:CE1	1:A:150:LEU:HD13	2.47	0.49
1:A:21:MET:HB2	1:A:92:MET:SD	2.53	0.49
1:B:526:LEU:CD2	1:B:528:ASN:H	2.23	0.49
1:B:76:LYS:HE2	1:B:82:ARG:HB2	1.95	0.49
1:B:429:MET:HB2	1:B:433:GLU:OE2	2.13	0.49
1:B:21:MET:O	1:B:25:VAL:HG23	2.12	0.49
1:A:469:LEU:HD13	1:A:502:ILE:HD11	1.95	0.49
1:B:60:LEU:CD1	1:B:61:GLU:H	2.25	0.49
1:B:530:THR:HG22	1:B:532:GLU:H	1.78	0.49
1:A:530:THR:HG22	1:A:532:GLU:H	1.78	0.49
1:A:454:VAL:CG2	1:A:557:ILE:HD11	2.38	0.48
1:B:577:ARG:HH11	1:B:578:GLN:HB2	1.75	0.48
1:A:541:TRP:HA	1:A:544:ARG:NE	2.28	0.48
1:B:400:GLU:HG2	1:B:404:ILE:HD11	1.94	0.48
1:A:163:ALA:HB3	1:A:164:PRO:HD3	1.95	0.48
1:A:461:LYS:HA	1:A:464:LEU:HD12	1.94	0.48
1:A:97:ARG:O	1:A:97:ARG:HG2	2.13	0.48
1:A:457:ILE:HG13	1:A:458:SER:N	2.28	0.48
1:B:22:ARG:O	1:B:25:VAL:HB	2.13	0.48
1:B:541:TRP:HA	1:B:544:ARG:CZ	2.43	0.48
1:A:128:VAL:HG11	1:A:176:TYR:CE2	2.48	0.48
1:B:402:SER:HA	1:B:407:LEU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:O	1:A:147:PHE:N	2.46	0.48
1:A:35:MET:HA	1:A:38:LEU:HD13	1.94	0.48
1:A:493:GLN:HE22	1:A:518:SER:N	2.10	0.48
1:B:24:VAL:O	1:B:28:ILE:HG13	2.14	0.48
1:A:496:TYR:CD1	1:A:497:PRO:HD2	2.48	0.48
1:B:541:TRP:HA	1:B:544:ARG:NE	2.29	0.48
1:B:461:LYS:HA	1:B:464:LEU:HD12	1.95	0.48
1:B:201:ARG:HB3	5:B:961:HOH:O	2.13	0.48
1:A:163:ALA:CB	1:A:167:ARG:HH12	2.27	0.48
1:B:225:ILE:HG22	1:B:372:LEU:CD2	2.37	0.47
1:B:465:VAL:O	1:B:469:LEU:HB2	2.13	0.47
1:A:541:TRP:CA	1:A:544:ARG:NH2	2.78	0.47
1:B:541:TRP:CA	1:B:544:ARG:HH21	2.26	0.47
1:A:134:TYR:HD2	1:A:135:LEU:HD22	1.76	0.47
1:B:128:VAL:HG11	1:B:176:TYR:CE2	2.48	0.47
1:B:93:VAL:HG11	1:B:410:VAL:HB	1.96	0.47
1:B:428:TYR:O	1:B:590:MET:N	2.47	0.47
1:A:167:ARG:HH21	1:A:197:GLU:HA	1.79	0.47
1:B:51:ARG:HD3	5:B:910:HOH:O	2.14	0.47
1:B:562:HIS:CD2	1:B:563:GLU:N	2.82	0.47
1:B:214:ILE:HA	1:B:218:GLU:HG3	1.96	0.47
1:A:89:LEU:O	1:A:93:VAL:HG23	2.13	0.47
1:B:493:GLN:HE22	1:B:518:SER:N	2.12	0.47
1:B:30:ALA:O	1:B:33:PRO:HD2	2.15	0.47
1:B:520:GLN:OE1	1:B:520:GLN:N	2.47	0.47
1:A:429:MET:HB2	1:A:433:GLU:OE2	2.15	0.47
1:B:144:ARG:HB3	1:B:145:PRO:HD3	1.95	0.47
1:B:195:PRO:HD3	5:B:920:HOH:O	2.15	0.47
1:A:113:THR:HG22	1:A:143:ASN:ND2	2.29	0.47
1:A:126:VAL:HG13	1:A:205:TYR:CD2	2.49	0.47
1:A:397:GLU:OE2	1:A:566:ARG:HD3	2.15	0.47
1:B:496:TYR:CD1	1:B:497:PRO:HD2	2.49	0.47
1:B:186:TYR:O	1:B:190:ASN:ND2	2.48	0.47
1:A:163:ALA:N	1:A:164:PRO:CD	2.77	0.47
1:B:97:ARG:HG2	1:B:97:ARG:O	2.15	0.47
1:B:163:ALA:HB3	1:B:164:PRO:HD3	1.97	0.47
1:A:479:LEU:HB2	1:A:507:ALA:HB1	1.96	0.47
1:A:60:LEU:CD1	1:A:61:GLU:H	2.27	0.47
1:B:541:TRP:CA	1:B:544:ARG:NH2	2.78	0.47
1:A:30:ALA:O	1:A:33:PRO:HD2	2.15	0.47
1:A:221:THR:HB	1:A:375:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:SER:HA	1:A:407:LEU:H	1.79	0.46
1:A:564:SER:HB3	5:A:972:HOH:O	2.15	0.46
1:B:457:ILE:HG13	1:B:458:SER:N	2.30	0.46
1:A:526:LEU:CD2	1:A:528:ASN:H	2.24	0.46
1:B:137:GLN:HG3	1:B:156:ILE:HD13	1.97	0.46
1:B:103:ARG:O	1:B:106:GLU:HB2	2.15	0.46
1:B:219:ALA:CA	5:B:975:HOH:O	2.63	0.46
1:B:163:ALA:N	1:B:164:PRO:CD	2.78	0.46
1:B:454:VAL:CG2	1:B:557:ILE:HD11	2.39	0.46
1:B:522:GLU:OE1	1:B:537:ILE:HD12	2.15	0.46
1:A:442:ILE:HG13	1:A:443:LYS:N	2.30	0.46
1:B:167:ARG:HH21	1:B:197:GLU:HA	1.79	0.46
1:B:423:LEU:HB2	1:B:585:ARG:HG2	1.97	0.46
1:A:530:THR:HB	1:A:533:GLN:NE2	2.31	0.46
1:A:128:VAL:HG11	1:A:176:TYR:HE2	1.81	0.46
1:A:51:ARG:O	1:A:55:GLU:HB2	2.16	0.46
1:B:588:LEU:N	1:B:588:LEU:HD12	2.30	0.46
1:A:108:LYS:HB3	1:A:390:MET:SD	2.55	0.46
1:B:126:VAL:HG13	1:B:205:TYR:CD2	2.50	0.46
1:B:138:ARG:NH2	1:B:510:GLY:O	2.40	0.46
1:B:573:GLY:C	1:B:575:SER:N	2.69	0.46
1:A:211:VAL:HG22	1:A:390:MET:H	1.80	0.46
1:A:122:THR:HG21	5:A:946:HOH:O	2.15	0.46
1:B:211:VAL:CG2	1:B:390:MET:N	2.79	0.46
1:A:589:SER:O	1:A:592:ASP:HB2	2.15	0.46
1:B:128:VAL:HG11	1:B:176:TYR:HE2	1.80	0.46
1:B:520:GLN:HA	1:B:523:VAL:HG22	1.97	0.46
1:A:566:ARG:O	1:A:569:ASN:HB2	2.15	0.46
1:B:565:ARG:HH12	1:B:572:ARG:HH12	1.64	0.46
1:B:566:ARG:O	1:B:569:ASN:HB2	2.15	0.46
1:A:493:GLN:HE22	1:A:518:SER:CA	2.29	0.46
1:A:585:ARG:CG	1:A:585:ARG:HH11	2.28	0.46
1:B:585:ARG:HH11	1:B:585:ARG:CG	2.29	0.46
1:A:573:GLY:C	1:A:575:SER:N	2.68	0.46
1:A:85:ASP:HA	1:A:88:LEU:HD12	1.98	0.45
1:A:522:GLU:OE1	1:A:537:ILE:HD12	2.16	0.45
1:A:573:GLY:C	1:A:575:SER:H	2.19	0.45
1:A:536:LYS:O	1:A:540:ASP:HB2	2.16	0.45
1:B:467:ASN:O	1:B:470:THR:HG22	2.16	0.45
1:A:431:GLU:HG2	1:A:591:GLU:OE1	2.16	0.45
1:B:573:GLY:C	1:B:575:SER:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:THR:HB	1:B:533:GLN:NE2	2.31	0.45
1:B:166:LYS:O	1:B:170:TYR:HD2	2.00	0.45
1:A:186:TYR:O	1:A:190:ASN:ND2	2.48	0.45
1:B:208:VAL:CG1	1:B:214:ILE:HD12	2.46	0.45
1:A:85:ASP:N	1:A:85:ASP:OD1	2.50	0.45
1:B:194:SER:HA	5:B:920:HOH:O	2.15	0.45
1:B:416:ARG:HG3	1:B:416:ARG:HH11	1.82	0.45
1:A:24:VAL:O	1:A:28:ILE:HG13	2.17	0.45
1:A:550:GLU:HB3	5:A:964:HOH:O	2.16	0.45
1:B:487:GLU:HB2	5:B:980:HOH:O	2.16	0.45
1:B:479:LEU:HB2	1:B:507:ALA:HB1	1.97	0.45
1:B:108:LYS:HB3	1:B:390:MET:SD	2.57	0.45
1:A:578:GLN:HG3	5:A:949:HOH:O	2.16	0.45
1:A:93:VAL:HG11	1:A:410:VAL:HB	1.98	0.45
1:A:423:LEU:HB2	1:A:585:ARG:HG2	1.98	0.45
1:A:463:GLU:OE2	3:A:905:SPD:H81	2.17	0.45
1:A:476:HIS:HD2	1:A:502:ILE:HD12	1.82	0.45
1:A:53:ARG:HB3	1:A:58:GLU:OE2	2.15	0.45
1:B:51:ARG:O	1:B:55:GLU:HB2	2.17	0.45
1:B:60:LEU:CG	1:B:61:GLU:H	2.30	0.44
1:A:108:LYS:HG3	4:A:901:ADP:O3B	2.16	0.44
1:A:565:ARG:HH12	1:A:572:ARG:HH12	1.65	0.44
1:A:427:VAL:HG11	1:A:590:MET:HE3	2.00	0.44
1:A:60:LEU:CD1	1:A:61:GLU:N	2.74	0.44
1:A:520:GLN:HA	1:A:523:VAL:HG22	1.98	0.44
1:B:387:LEU:HD22	1:B:388:ALA:N	2.32	0.44
1:A:60:LEU:CG	1:A:61:GLU:H	2.31	0.44
1:A:225:ILE:HG23	1:A:372:LEU:HD12	2.00	0.44
1:B:469:LEU:HD13	1:B:502:ILE:HD11	1.99	0.44
1:A:137:GLN:HG3	1:A:156:ILE:HD13	1.98	0.44
1:A:21:MET:HA	1:A:24:VAL:HG23	2.00	0.44
1:A:138:ARG:NH1	1:A:139:ASP:OD1	2.49	0.44
1:B:425:ASP:HB3	1:B:588:LEU:CD1	2.42	0.44
1:A:425:ASP:HB3	1:A:588:LEU:CD1	2.45	0.44
1:B:13:ARG:C	1:B:13:ARG:HD3	2.38	0.44
1:B:184:PHE:O	1:B:188:ARG:HG3	2.17	0.44
1:A:223:LEU:CD2	1:A:372:LEU:HD21	2.48	0.44
1:B:224:ILE:O	1:B:372:LEU:HA	2.17	0.43
1:B:211:VAL:HG22	1:B:390:MET:H	1.83	0.43
1:B:53:ARG:HA	1:B:56:LYS:CE	2.44	0.43
1:B:400:GLU:HA	1:B:403:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LYS:HG3	5:B:984:HOH:O	2.18	0.43
1:A:400:GLU:HA	1:A:403:SER:OG	2.19	0.43
1:A:184:PHE:O	1:A:188:ARG:HG3	2.18	0.43
1:A:427:VAL:HG11	1:A:590:MET:CE	2.49	0.43
1:B:536:LYS:O	1:B:540:ASP:HB2	2.17	0.43
1:A:416:ARG:HG3	1:A:416:ARG:HH11	1.83	0.43
1:A:93:VAL:HB	1:A:100:ALA:HB2	2.00	0.43
1:B:590:MET:O	1:B:594:LEU:HG	2.18	0.43
1:B:546:ASP:O	1:B:550:GLU:HG3	2.18	0.43
1:A:166:LYS:O	1:A:170:TYR:HD2	2.01	0.43
1:A:483:PHE:HB3	1:A:486:ASN:HD22	1.83	0.43
1:B:522:GLU:OE1	1:B:537:ILE:HG23	2.19	0.43
1:A:557:ILE:HG13	1:A:557:ILE:O	2.19	0.43
1:B:397:GLU:N	1:B:397:GLU:OE1	2.43	0.43
1:B:163:ALA:CB	1:B:167:ARG:HH12	2.31	0.43
1:A:375:ILE:HG22	1:B:188:ARG:HG2	2.01	0.43
1:A:467:ASN:O	1:A:470:THR:HG22	2.18	0.43
1:A:163:ALA:HB1	1:A:167:ARG:HH12	1.84	0.43
1:B:138:ARG:NH1	1:B:139:ASP:OD1	2.45	0.43
1:B:493:GLN:HE22	1:B:518:SER:CA	2.32	0.43
1:A:22:ARG:O	1:A:25:VAL:HB	2.19	0.42
1:B:117:TYR:HE1	1:B:150:LEU:HB3	1.84	0.42
1:A:63:LEU:CD2	1:A:63:LEU:H	2.25	0.42
1:B:129:VAL:HG12	1:B:214:ILE:HD13	2.01	0.42
1:A:493:GLN:NE2	1:A:518:SER:O	2.51	0.42
1:B:557:ILE:O	1:B:557:ILE:HG13	2.19	0.42
1:B:218:GLU:C	1:B:220:ARG:H	2.20	0.42
1:B:18:LEU:HD21	1:B:413:PRO:CD	2.46	0.42
1:B:493:GLN:NE2	1:B:518:SER:O	2.51	0.42
1:A:565:ARG:N	5:A:972:HOH:O	2.52	0.42
1:A:25:VAL:HG11	1:A:85:ASP:HB2	2.02	0.42
1:A:517:GLY:O	1:A:541:TRP:NE1	2.51	0.42
1:B:476:HIS:HD2	1:B:502:ILE:HD12	1.84	0.42
1:A:387:LEU:HD22	1:A:388:ALA:N	2.35	0.42
1:A:208:VAL:CG1	1:A:214:ILE:HD12	2.49	0.42
1:B:68:PHE:CE2	1:B:114:LEU:HD13	2.54	0.42
1:B:25:VAL:HG11	1:B:85:ASP:HB2	2.01	0.42
1:A:423:LEU:HD22	1:A:423:LEU:H	1.84	0.42
1:A:393:THR:HB	1:A:566:ARG:HG2	2.02	0.42
1:A:13:ARG:C	1:A:13:ARG:HD3	2.39	0.42
1:A:460:GLU:OE1	3:A:905:SPD:H32	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ARG:NH1	1:B:568:ASP:OD2	2.53	0.42
1:A:144:ARG:HB3	1:A:145:PRO:HD3	2.01	0.42
1:B:132:ASN:ND2	1:B:135:LEU:HD23	2.34	0.42
1:B:83:HIS:CE1	1:B:114:LEU:HD21	2.54	0.42
1:B:52:ALA:O	1:B:56:LYS:HG3	2.20	0.42
1:A:225:ILE:HG21	1:A:372:LEU:HD12	2.01	0.42
1:A:519:TRP:HB2	1:A:537:ILE:HG22	2.02	0.42
1:A:426:LEU:HD12	1:A:587:TYR:HE1	1.85	0.42
1:A:546:ASP:O	1:A:550:GLU:HG3	2.19	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.85	0.42
1:A:505:ASN:HB3	1:A:506:MET:HE2	2.01	0.42
1:B:94:LEU:HD22	1:B:207:LEU:HD21	2.01	0.42
1:A:223:LEU:HD21	1:A:372:LEU:HD21	2.02	0.42
1:A:108:LYS:HB3	1:A:390:MET:CE	2.49	0.41
1:B:469:LEU:CD2	1:B:474:ILE:HB	2.48	0.41
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.78	0.41
1:A:18:LEU:HD21	1:A:413:PRO:CD	2.44	0.41
1:B:85:ASP:OD1	1:B:85:ASP:N	2.54	0.41
1:B:470:THR:HB	1:B:476:HIS:HE1	1.85	0.41
1:A:117:TYR:HE1	1:A:150:LEU:HB3	1.85	0.41
1:A:461:LYS:HG3	1:A:560:GLU:OE2	2.21	0.41
1:B:21:MET:HA	1:B:24:VAL:HG23	2.01	0.41
1:B:85:ASP:HA	1:B:88:LEU:HD12	2.02	0.41
1:A:493:GLN:C	1:A:495:GLY:H	2.24	0.41
1:B:166:LYS:NZ	1:B:185:ASP:OD2	2.49	0.41
1:A:170:TYR:O	1:A:201:ARG:NH2	2.52	0.41
1:B:416:ARG:HD3	5:B:957:HOH:O	2.20	0.41
1:A:87:GLN:O	1:A:111:THR:HG23	2.20	0.41
1:B:435:ILE:O	1:B:439:ILE:HG23	2.20	0.41
1:A:60:LEU:C	1:A:62:ASN:H	2.24	0.41
1:B:60:LEU:C	1:B:62:ASN:H	2.24	0.41
1:B:93:VAL:HB	1:B:100:ALA:HB2	2.03	0.41
1:A:225:ILE:HG23	1:A:372:LEU:HB2	2.03	0.41
1:A:43:LEU:HD22	1:A:77:ARG:NH1	2.36	0.41
1:B:519:TRP:HB2	1:B:537:ILE:HG22	2.02	0.41
1:B:483:PHE:HB3	1:B:486:ASN:HD22	1.85	0.41
1:B:214:ILE:HG22	1:B:215:LEU:HD23	2.02	0.41
1:A:541:TRP:N	1:A:544:ARG:HH21	2.18	0.41
1:A:585:ARG:CG	1:A:585:ARG:NH1	2.82	0.41
1:B:423:LEU:HD22	1:B:423:LEU:H	1.84	0.41
1:B:592:ASP:C	1:B:594:LEU:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HA	1:A:387:LEU:O	2.21	0.41
1:A:195:PRO:HA	1:A:198:ARG:HD2	2.02	0.41
1:A:435:ILE:O	1:A:439:ILE:HG23	2.21	0.41
1:A:504:THR:N	1:A:507:ALA:HB2	2.33	0.41
1:B:457:ILE:CG2	1:B:560:GLU:HG3	2.44	0.41
1:B:82:ARG:HD2	5:B:938:HOH:O	2.21	0.41
1:B:541:TRP:N	1:B:544:ARG:HH21	2.19	0.41
1:B:195:PRO:HA	1:B:198:ARG:HD2	2.03	0.41
1:A:216:ILE:HG21	1:A:566:ARG:HH12	1.86	0.41
1:B:163:ALA:HB1	1:B:167:ARG:HH12	1.86	0.41
1:A:470:THR:HB	1:A:476:HIS:HE1	1.86	0.40
1:B:108:LYS:HB3	1:B:390:MET:CE	2.51	0.40
1:A:52:ALA:O	1:A:56:LYS:HG3	2.21	0.40
1:B:31:MET:CE	1:B:66:GLU:HG3	2.51	0.40
1:B:25:VAL:CG1	1:B:85:ASP:HB2	2.51	0.40
1:B:146:LEU:O	1:B:146:LEU:HD23	2.21	0.40
1:A:469:LEU:CD2	1:A:474:ILE:HB	2.48	0.40
1:B:467:ASN:CA	1:B:470:THR:HG22	2.48	0.40
1:A:60:LEU:O	1:A:63:LEU:HD23	2.22	0.40
1:B:470:THR:HB	1:B:476:HIS:CE1	2.57	0.40
1:A:567:ILE:C	1:A:569:ASN:H	2.25	0.40
1:A:187:LEU:HD22	1:B:187:LEU:HD22	2.04	0.40
1:A:555:HIS:HE2	1:A:557:ILE:CG2	2.35	0.40
1:B:43:LEU:O	1:B:46:LYS:CB	2.67	0.40
1:A:467:ASN:CA	1:A:470:THR:HG22	2.49	0.40
1:A:101:GLU:HB3	1:A:411:VAL:HA	2.03	0.40
1:A:574:ARG:NH1	5:A:906:HOH:O	2.53	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	434/471 (92%)	380 (88%)	49 (11%)	5 (1%)	16	56
1	B	436/471 (93%)	382 (88%)	47 (11%)	7 (2%)	12	48
All	All	870/942 (92%)	762 (88%)	96 (11%)	12 (1%)	14	51

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	THR
1	A	396	THR
1	B	219	ALA
1	A	150	LEU
1	B	221	THR
1	B	545	HIS
1	A	61	GLU
1	A	545	HIS
1	B	61	GLU
1	B	150	LEU
1	B	497	PRO
1	A	497	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/388 (92%)	338 (94%)	21 (6%)	25	63
1	B	361/388 (93%)	339 (94%)	22 (6%)	23	61
All	All	720/776 (93%)	677 (94%)	43 (6%)	24	62

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	40	ASP
1	A	63	LEU
1	A	86	VAL

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Mol	Chain	Res	Type
1	A	130	THR
1	A	153	THR
1	A	173	ASP
1	A	193	PHE
1	A	201	ARG
1	A	207	LEU
1	A	210	GLU
1	A	211	VAL
1	A	223	LEU
1	A	387	LEU
1	A	423	LEU
1	A	436	GLN
1	A	477	ASN
1	A	480	ASN
1	A	506	MET
1	A	577	ARG
1	A	585	ARG
1	B	13	ARG
1	B	40	ASP
1	B	63	LEU
1	B	86	VAL
1	B	130	THR
1	B	135	LEU
1	B	153	THR
1	B	162	PRO
1	B	173	ASP
1	B	193	PHE
1	B	207	LEU
1	B	210	GLU
1	B	211	VAL
1	B	376	THR
1	B	387	LEU
1	B	423	LEU
1	B	436	GLN
1	B	477	ASN
1	B	480	ASN
1	B	506	MET
1	B	577	ARG
1	B	585	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	26	ASN
1	A	127	HIS
1	A	143	ASN
1	A	415	ASN
1	A	486	ASN
1	A	493	GLN
1	A	528	ASN
1	A	562	HIS
1	B	14	ASN
1	B	26	ASN
1	B	127	HIS
1	B	143	ASN
1	B	415	ASN
1	B	486	ASN
1	B	493	GLN
1	B	528	ASN
1	B	533	GLN
1	B	562	HIS

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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	ADP	A	901	2	22,29,29	1.86	7 (31%)	27,45,45	2.98	4 (14%)
3	SPD	A	905	-	9,9,9	0.73	0	8,8,8	0.62	0
4	ADP	B	902	-	22,29,29	1.74	7 (31%)	27,45,45	2.75	4 (14%)
3	SPD	B	906	-	9,9,9	0.73	0	8,8,8	0.57	0

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
4	ADP	A	901	2	-	0/12/32/32	0/3/3/3
3	SPD	A	905	-	-	0/7/7/7	0/0/0/0
4	ADP	B	902	-	-	0/12/32/32	0/3/3/3
3	SPD	B	906	-	-	0/7/7/7	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	ADP	PA-O2A	-2.34	1.45	1.54
4	A	901	ADP	PA-O2A	-2.28	1.45	1.54
4	B	902	ADP	C5-C4	2.01	1.45	1.40
4	B	902	ADP	C2-N1	2.10	1.37	1.33
4	A	901	ADP	C5-C4	2.11	1.45	1.40
4	B	902	ADP	PB-O2B	2.25	1.62	1.54
4	A	901	ADP	PB-O2B	2.29	1.62	1.54
4	B	902	ADP	C2-N3	2.39	1.36	1.32
4	A	901	ADP	C4-N3	2.46	1.39	1.35
4	A	901	ADP	C2-N3	2.69	1.37	1.32
4	A	901	ADP	C2-N1	2.76	1.39	1.33
4	B	902	ADP	C4-N3	2.95	1.40	1.35
4	B	902	ADP	O4'-C1'	4.58	1.47	1.41
4	A	901	ADP	O4'-C1'	4.84	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	ADP	N3-C2-N1	-14.18	118.03	128.89
4	B	902	ADP	N3-C2-N1	-12.64	119.22	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	902	ADP	C4-C5-N7	-4.18	105.63	109.48
4	A	901	ADP	C4-C5-N7	-3.37	106.38	109.48
4	A	901	ADP	C2-N1-C6	2.01	122.36	118.77
4	B	902	ADP	C2-N1-C6	2.02	122.38	118.77
4	A	901	ADP	C2'-C3'-C4'	2.93	108.64	102.61
4	B	902	ADP	C2'-C3'-C4'	3.25	109.28	102.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ADP	1	0
3	A	905	SPD	4	0
4	B	902	ADP	1	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^{th} 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	438/471 (92%)	0.04	3 (0%)	89	70	46, 78, 128, 152	0
1	B	440/471 (93%)	0.04	5 (1%)	82	58	48, 78, 129, 152	0
All	All	878/942 (93%)	0.04	8 (0%)	85	64	46, 78, 129, 152	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	530	THR	3.4
1	B	465	VAL	3.3
1	A	474	ILE	2.8
1	A	11	GLY	2.2
1	B	427	VAL	2.2
1	A	395	ASP	2.1
1	B	193	PHE	2.1
1	B	586	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
4	ADP	B	902	27/27	0.93	0.22	0.17	64,70,71,72	0
4	ADP	A	901	27/27	0.96	0.21	-0.19	57,63,68,72	0
2	MG	B	904	1/1	0.98	0.36	-	41,41,41,41	0
3	SPD	B	906	10/10	0.67	0.46	-	74,80,82,82	0
2	MG	A	903	1/1	0.97	0.23	-	23,23,23,23	0
3	SPD	A	905	10/10	0.69	0.50	-	76,78,80,81	0

6.5 Other polymers (i)

There are no such residues in this entry.