Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BHR
Title	:	DENGUE VIRUS RNA HELICASE
Authors	:	Xu, T.; Sampath, A.; Chao, A.; Wen, D.; Nanao, M.; Chene, P.; Vasudevan, S.G.; Lescar, J.
Deposited on	:	2005-01-17
Resolution	:	2.80 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:

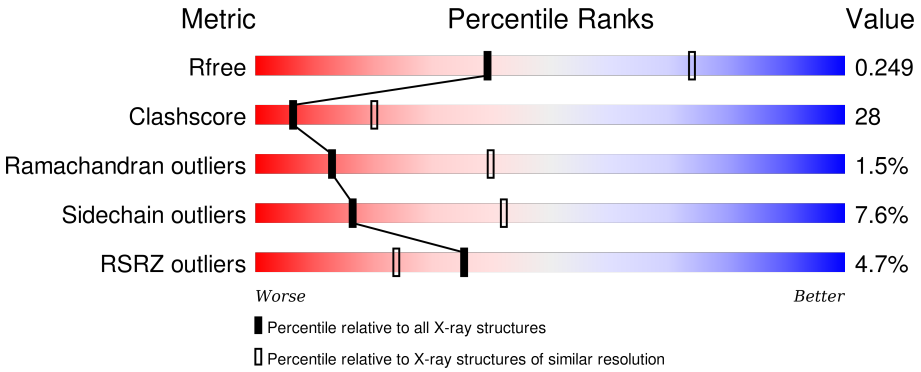
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	451	6%, 53%, 38%, 5%
1	B	451	3%, 51%, 42%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7139 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.

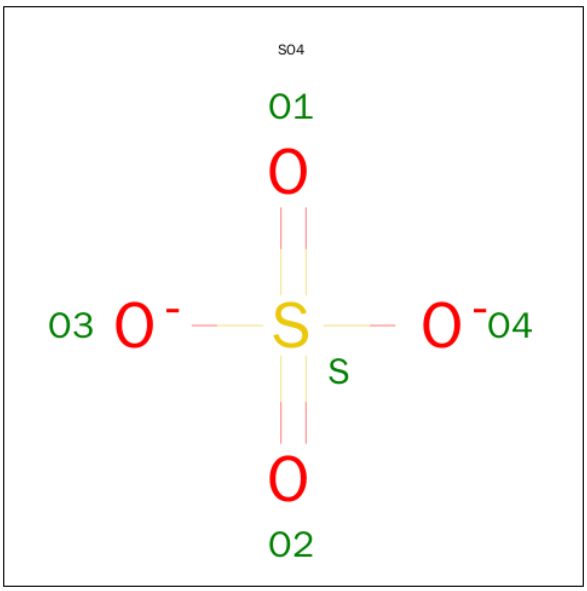
- Molecule 1 is a protein called RNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3462	2184	624	634	20			
1	B	439	Total	C	N	O	S	0	0	0
			3526	2221	633	652	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	ALA	-	EXPRESSION TAG	UNP Q91H74
A	169	MET	-	EXPRESSION TAG	UNP Q91H74
A	170	ALA	-	EXPRESSION TAG	UNP Q91H74
B	168	ALA	-	EXPRESSION TAG	UNP Q91H74
B	169	MET	-	EXPRESSION TAG	UNP Q91H74
B	170	ALA	-	EXPRESSION TAG	UNP Q91H74

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

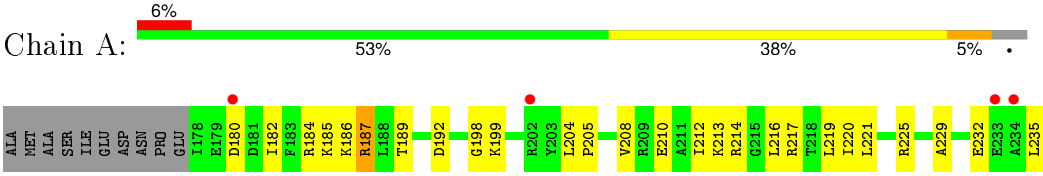
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	74	Total O 74 74	0	0

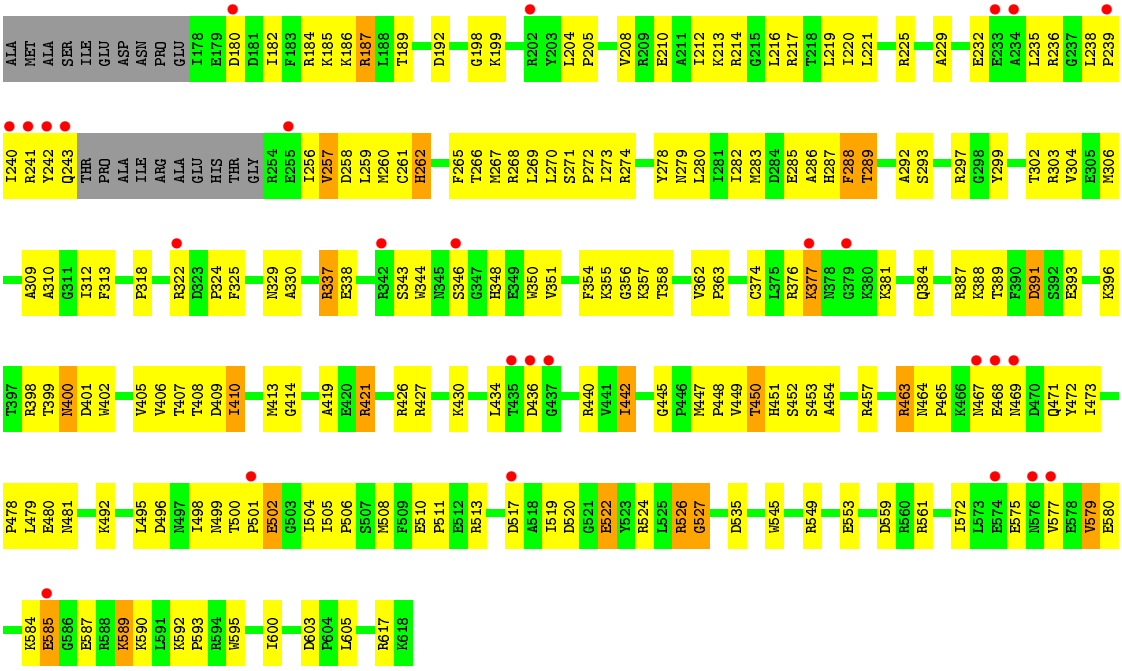
3 Residue-property plots (i)

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: RNA HELICASE

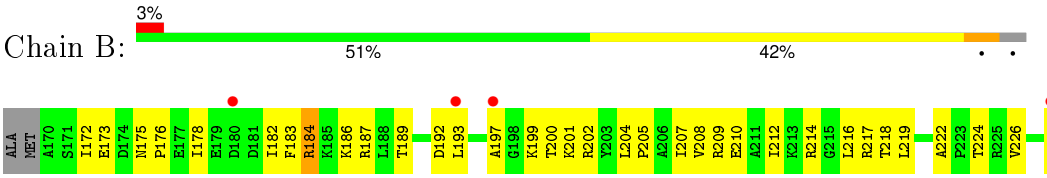
Chain A:

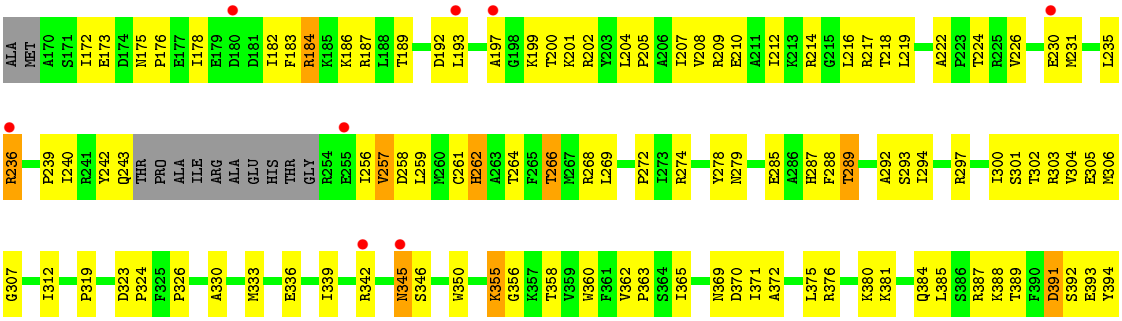


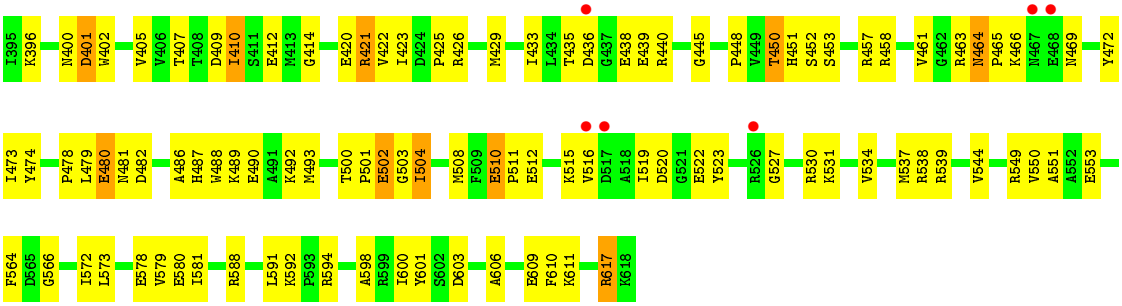


- Molecule 1: RNA HELICASE

Chain B:






I395 K396 N400 D401 W402 V405 V406 T407 T408 D409 I410 S411 E412 N413 G414 E420 R421 V422 I423 D424 P425 R426 M429 I433 I434 T435 D436 G437 E438 E439 R440 G445 P448 V449 T450 H451 S452 S453 R457 R458 V461 G462 R463 N464 P465 K466 N467 E468 N469 Y472
I473 Y474 P478 L479 E480 N481 D482 A486 H487 W488 K489 E490 A491 K492 M493 T500 P501 E502 G503 I504 M508 F509 E510 P511 E512 K515 V516 D517 A518 I519 D520 G521 E522 Y523 R526 G527 R530 K531 V534 M537 R538 R539 V544 R549 V550 A551 A552 E553
F564 D565 G566 I572 L573 E578 V579 E580 I581 R588 L591 K592 P593 R594 A598 R599 I600 Y601 S602 D603 A606 E609 F610 K611 R617 K618

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.72Å 165.97Å 54.71Å 90.00° 101.88° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.80) 99.0 (19.83-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.45 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.252 0.205 , 0.249	Depositor DCC
R_{free} test set	1198 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 65.2	EDS
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 23185 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7139	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: SO4

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	0.38	0/3536	0.65	0/4775
1	B	0.39	0/3601	0.67	1/4864 (0.0%)
All	All	0.39	0/7137	0.66	1/9639 (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	B	401	ASP	N-CA-C	-5.14	97.11	111.00

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	3462	0	3460	192	0
1	B	3526	0	3514	204	0
2	A	10	0	0	0	0
3	A	67	0	0	14	0
3	B	74	0	0	19	0
All	All	7139	0	6974	387	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 28.

All (387) 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:439:GLU:HG3	3:B:2038:HOH:O	1.40	1.20
1:B:372:ALA:HB1	1:B:376:ARG:HH12	1.15	1.10
1:B:385:LEU:HB2	1:B:407:THR:HG22	1.35	1.07
1:A:337:ARG:HH11	1:A:337:ARG:HB2	1.23	1.01
1:B:581:ILE:HD11	1:B:611:LYS:HG2	1.46	0.98
1:B:306:MET:SD	3:B:2055:HOH:O	2.23	0.96
1:A:217:ARG:H	1:A:279:ASN:HD22	1.15	0.94
1:B:385:LEU:HB2	1:B:407:THR:CG2	2.01	0.91
1:A:285:GLU:HG2	1:A:287:HIS:HE1	1.35	0.90
1:A:495:LEU:HD22	1:A:506:PRO:HB2	1.55	0.89
1:B:539:ARG:HD3	3:B:2058:HOH:O	1.73	0.88
1:A:285:GLU:HG2	1:A:287:HIS:CE1	2.10	0.86
1:B:279:ASN:HA	3:B:2023:HOH:O	1.76	0.85
1:A:362:VAL:HG22	1:A:363:PRO:HD2	1.59	0.85
1:A:272:PRO:HG2	1:A:273:ILE:HD12	1.59	0.85
1:A:303:ARG:HH12	1:A:501:PRO:HD2	1.42	0.83
1:A:377:LYS:HA	1:A:377:LYS:HE3	1.59	0.83
1:B:464:ASN:ND2	1:B:466:LYS:H	1.75	0.83
1:B:617:ARG:NH1	1:B:617:ARG:HB3	1.94	0.83
1:A:348:HIS:O	1:A:351:VAL:HG12	1.79	0.83
1:B:385:LEU:HD12	1:B:407:THR:HG21	1.59	0.83
1:A:242:TYR:HD2	1:A:259:LEU:HD22	1.44	0.82
1:A:479:LEU:HD22	1:A:481:ASN:HB2	1.62	0.81
1:B:510:GLU:HB3	1:B:511:PRO:HD3	1.61	0.81
1:B:372:ALA:HB1	1:B:376:ARG:NH1	1.95	0.80
1:A:266:THR:HA	1:A:269:LEU:HD12	1.64	0.80
1:A:450:THR:HG22	1:A:453:SER:H	1.44	0.80
1:B:385:LEU:CB	1:B:407:THR:HG22	2.11	0.79
1:A:388:LYS:HD3	1:A:605:LEU:HD12	1.64	0.79
1:A:355:LYS:HG3	1:A:356:GLY:H	1.47	0.78
1:B:617:ARG:HH11	1:B:617:ARG:HB3	1.48	0.78
1:A:204:LEU:HB3	1:A:205:PRO:HD3	1.66	0.78
1:B:492:LYS:NZ	1:B:520:ASP:HA	1.98	0.77
1:B:492:LYS:HZ1	1:B:520:ASP:HA	1.48	0.77
1:A:199:LYS:NZ	1:A:285:GLU:HG3	2.00	0.77
1:A:393:GLU:HA	1:A:396:LYS:HZ3	1.49	0.77
1:A:519:ILE:N	1:A:519:ILE:HD12	2.00	0.77
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ASP:OD2	3:B:2030:HOH:O	2.03	0.76
1:B:217:ARG:H	1:B:279:ASN:HD22	1.31	0.75
1:A:324:PRO:HG2	1:A:325:PHE:CD1	2.22	0.74
1:A:396:LYS:HE3	1:B:519:ILE:HG12	1.69	0.74
1:B:204:LEU:HB3	1:B:205:PRO:HD3	1.67	0.74
1:A:389:THR:HG23	1:A:393:GLU:HG3	1.70	0.74
1:B:199:LYS:HD3	3:B:2007:HOH:O	1.88	0.73
1:A:376:ARG:HH22	1:A:384:GLN:HE21	1.37	0.73
1:A:337:ARG:HB2	1:A:337:ARG:NH1	2.00	0.72
1:A:324:PRO:HD3	3:A:2042:HOH:O	1.87	0.72
1:A:584:LYS:HG3	1:A:585:GLU:OE1	1.90	0.72
1:A:355:LYS:HG3	1:A:356:GLY:N	2.05	0.72
1:B:519:ILE:O	1:B:522:GLU:HB3	1.91	0.71
1:B:579:VAL:HG13	1:B:591:LEU:HB3	1.73	0.71
1:A:393:GLU:HA	1:A:396:LYS:NZ	2.05	0.71
1:B:487:HIS:HD2	3:B:2022:HOH:O	1.74	0.71
1:A:440:ARG:HD3	3:A:2037:HOH:O	1.92	0.70
1:B:342:ARG:HB2	1:B:370:ASP:OD2	1.92	0.70
1:B:539:ARG:NH1	3:B:2059:HOH:O	2.24	0.70
1:B:537:MET:CE	1:B:544:VAL:HG22	2.21	0.70
1:A:572:ILE:O	1:A:579:VAL:HG12	1.92	0.70
1:B:176:PRO:HG3	1:B:202:ARG:NH2	2.06	0.69
1:B:200:THR:HG23	1:B:201:LYS:HG3	1.73	0.69
1:A:289:THR:OG1	3:A:2014:HOH:O	2.10	0.69
1:A:337:ARG:HG3	1:A:338:GLU:N	2.08	0.68
1:B:572:ILE:O	1:B:579:VAL:HG12	1.92	0.68
1:B:184:ARG:HB3	1:B:187:ARG:HD3	1.75	0.68
1:A:396:LYS:CE	1:B:519:ILE:HG12	2.24	0.68
1:B:479:LEU:O	1:B:481:ASN:N	2.27	0.68
1:A:467:ASN:ND2	1:A:469:ASN:H	1.92	0.68
1:A:242:TYR:O	1:A:243:GLN:HG3	1.93	0.67
1:B:451:HIS:CD2	1:B:480:GLU:HB2	2.29	0.67
1:A:198:GLY:HA2	3:A:2002:HOH:O	1.94	0.67
1:A:617:ARG:HH11	1:A:617:ARG:HG2	1.60	0.66
1:A:337:ARG:HG3	1:A:338:GLU:H	1.60	0.66
1:B:272:PRO:HG3	1:B:531:LYS:HE3	1.76	0.66
1:B:262:HIS:O	1:B:266:THR:HG22	1.96	0.66
1:A:182:ILE:HD12	1:A:189:THR:HG21	1.78	0.66
1:A:500:THR:OG1	1:A:504:ILE:HG13	1.96	0.65
1:A:240:ILE:HG23	1:A:257:VAL:HG22	1.79	0.65
1:A:192:ASP:HB2	1:A:318:PRO:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLU:HB3	1:A:511:PRO:HD3	1.79	0.65
1:A:362:VAL:CG2	1:A:363:PRO:HD2	2.26	0.64
1:B:433:ILE:HG22	3:B:2038:HOH:O	1.97	0.64
1:A:451:HIS:HD2	1:A:480:GLU:HG3	1.63	0.64
1:B:362:VAL:HG22	1:B:363:PRO:HD2	1.79	0.64
1:A:587:GLU:HB3	1:A:589:LYS:HD3	1.80	0.64
1:B:527:GLY:O	1:B:531:LYS:HG2	1.96	0.64
1:B:451:HIS:HD2	1:B:480:GLU:HB2	1.61	0.63
1:B:202:ARG:HH11	1:B:202:ARG:HG2	1.63	0.63
1:B:289:THR:HB	3:B:2022:HOH:O	1.98	0.63
1:A:393:GLU:CG	1:A:396:LYS:HZ3	2.11	0.63
1:A:442:ILE:HD11	3:A:2039:HOH:O	1.98	0.63
1:A:354:PHE:HB2	1:A:421:ARG:NH2	2.14	0.63
1:B:330:ALA:HB2	1:B:465:PRO:HA	1.81	0.62
1:B:175:ASN:OD1	1:B:209:ARG:NH1	2.32	0.62
1:B:537:MET:HE3	1:B:544:VAL:HG22	1.80	0.62
1:B:617:ARG:CB	1:B:617:ARG:HH11	2.13	0.62
1:A:344:TRP:H	1:A:344:TRP:HE3	1.48	0.62
1:A:225:ARG:HH21	1:A:391:ASP:CB	2.12	0.62
1:A:350:TRP:CH2	1:A:473:ILE:HG21	2.36	0.61
1:A:451:HIS:HB3	3:A:2042:HOH:O	2.01	0.61
1:B:426:ARG:NH1	1:B:478:PRO:HD3	2.16	0.61
1:B:450:THR:HG23	3:B:2045:HOH:O	2.01	0.61
1:A:526:ARG:HD3	3:A:2052:HOH:O	2.01	0.61
1:A:199:LYS:HZ1	1:A:285:GLU:HG3	1.66	0.60
1:B:224:THR:HB	3:B:2030:HOH:O	2.02	0.60
1:A:302:THR:O	1:A:306:MET:HG3	2.01	0.60
1:B:448:PRO:CB	1:B:479:LEU:HD13	2.33	0.59
1:B:592:LYS:O	1:B:592:LYS:HG3	2.02	0.59
1:B:303:ARG:NH1	1:B:501:PRO:HD2	2.18	0.59
1:B:193:LEU:HB2	3:B:2007:HOH:O	2.02	0.59
1:B:214:ARG:HG3	1:B:214:ARG:NH1	2.16	0.59
1:A:402:TRP:CE3	1:A:405:VAL:HG23	2.38	0.59
1:B:176:PRO:HG3	1:B:202:ARG:CZ	2.34	0.58
1:A:388:LYS:CD	1:A:605:LEU:HD12	2.32	0.58
1:B:516:VAL:O	1:B:516:VAL:HG13	2.03	0.58
1:B:405:VAL:HG12	1:B:407:THR:HG23	1.85	0.58
1:B:285:GLU:OE2	1:B:285:GLU:HA	2.02	0.58
1:A:324:PRO:HG2	1:A:325:PHE:CE1	2.39	0.58
1:B:184:ARG:O	1:B:187:ARG:HB2	2.04	0.58
1:B:362:VAL:CG2	1:B:363:PRO:HD2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ILE:HD12	1:B:410:ILE:N	2.17	0.58
1:B:489:LYS:O	1:B:493:MET:HG3	2.04	0.57
1:A:393:GLU:HG2	1:A:396:LYS:HZ3	1.68	0.57
1:A:239:PRO:O	1:A:257:VAL:HG13	2.04	0.57
1:A:387:ARG:HH12	1:A:409:ASP:HB2	1.69	0.57
1:B:183:PHE:HB3	1:B:216:LEU:HD11	1.87	0.57
1:A:545:TRP:O	1:A:549:ARG:HG2	2.03	0.57
1:A:519:ILE:H	1:A:519:ILE:HD12	1.67	0.57
1:B:302:THR:O	1:B:306:MET:HG3	2.04	0.57
1:B:464:ASN:HD21	1:B:466:LYS:HG2	1.70	0.57
1:A:605:LEU:O	1:A:605:LEU:HD13	2.05	0.56
1:A:451:HIS:CE1	1:A:478:PRO:HB2	2.39	0.56
1:A:463:ARG:HG2	1:A:463:ARG:HH11	1.71	0.56
1:B:360:TRP:CZ2	1:B:371:ILE:HD13	2.40	0.56
1:A:242:TYR:CD2	1:A:259:LEU:HD22	2.34	0.56
1:A:504:ILE:C	1:A:504:ILE:HD12	2.26	0.56
1:B:189:THR:HA	3:B:2005:HOH:O	2.05	0.56
1:B:464:ASN:HD22	1:B:465:PRO:N	2.04	0.56
1:B:520:ASP:C	1:B:522:GLU:H	2.09	0.56
1:B:178:ILE:HG12	1:B:207:ILE:HG12	1.87	0.56
1:B:389:THR:HG23	1:B:393:GLU:HG2	1.88	0.55
1:A:280:LEU:HA	1:A:310:ALA:O	2.06	0.55
1:A:400:ASN:HB2	1:B:504:ILE:HD13	1.88	0.55
1:B:489:LYS:HE3	1:B:523:TYR:OH	2.06	0.55
1:A:559:ASP:OD1	1:A:561:ARG:NH2	2.39	0.55
1:A:396:LYS:NZ	1:B:519:ILE:HG21	2.21	0.55
1:B:219:LEU:HB2	1:B:278:TYR:CD2	2.41	0.55
1:B:345:ASN:C	1:B:345:ASN:HD22	2.09	0.55
1:A:288:PHE:O	1:A:297:ARG:NH2	2.40	0.54
1:A:526:ARG:CD	3:A:2052:HOH:O	2.54	0.54
1:B:553:GLU:OE2	1:B:553:GLU:HA	2.07	0.54
1:B:365:ILE:HG22	1:B:369:ASN:HD21	1.73	0.54
1:A:214:ARG:HB2	1:A:216:LEU:HG	1.89	0.54
1:B:210:GLU:CD	1:B:214:ARG:HH12	2.11	0.54
1:A:330:ALA:HB2	1:A:465:PRO:HA	1.89	0.54
1:B:186:LYS:HA	1:B:304:VAL:O	2.08	0.54
1:B:303:ARG:HH12	1:B:501:PRO:HD2	1.71	0.54
1:B:478:PRO:O	1:B:479:LEU:HD12	2.07	0.54
1:B:481:ASN:O	3:B:2050:HOH:O	2.18	0.54
1:A:303:ARG:NH1	1:A:500:THR:HB	2.23	0.53
1:B:236:ARG:HD3	1:B:236:ARG:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:THR:HG21	1:A:292:ALA:O	2.08	0.53
1:A:617:ARG:NH1	1:A:617:ARG:HG2	2.23	0.53
1:A:471:GLN:NE2	1:A:473:ILE:HD11	2.23	0.53
1:B:388:LYS:NZ	1:B:609:GLU:OE2	2.36	0.53
1:A:297:ARG:HG2	1:A:313:PHE:CE1	2.44	0.53
1:B:339:ILE:HD11	1:B:473:ILE:HG22	1.91	0.53
1:B:288:PHE:O	1:B:297:ARG:NH2	2.34	0.53
1:B:355:LYS:HG2	1:B:356:GLY:N	2.22	0.53
1:B:264:THR:O	1:B:268:ARG:HG3	2.09	0.53
1:A:393:GLU:CA	1:A:396:LYS:HZ3	2.19	0.53
1:B:200:THR:HG23	1:B:201:LYS:N	2.24	0.53
1:B:537:MET:HE1	1:B:544:VAL:HG22	1.88	0.53
1:A:427:ARG:NH1	1:A:448:PRO:HD3	2.24	0.53
1:A:471:GLN:NE2	3:A:2046:HOH:O	2.42	0.52
1:A:199:LYS:HZ1	1:A:285:GLU:CG	2.23	0.52
1:B:410:ILE:HD12	1:B:410:ILE:H	1.75	0.52
1:A:450:THR:HG23	1:A:452:SER:H	1.75	0.52
1:B:530:ARG:O	1:B:534:VAL:HG23	2.08	0.52
1:A:502:GLU:HG2	1:A:504:ILE:HG23	1.90	0.52
1:B:387:ARG:HG2	1:B:410:ILE:HG23	1.91	0.52
1:A:354:PHE:HB2	1:A:421:ARG:CZ	2.39	0.52
1:A:213:LYS:HB3	1:A:213:LYS:NZ	2.23	0.52
1:A:265:PHE:CE2	1:A:269:LEU:HD11	2.45	0.52
1:A:242:TYR:C	1:A:243:GLN:HG3	2.31	0.51
1:A:212:ILE:HD13	1:A:239:PRO:HD2	1.92	0.51
1:B:285:GLU:OE2	1:B:287:HIS:HE1	1.93	0.51
1:B:422:VAL:HG23	1:B:461:VAL:HG13	1.92	0.51
1:A:396:LYS:HZ2	1:B:519:ILE:HG21	1.75	0.51
1:A:393:GLU:CD	1:A:396:LYS:HE2	2.30	0.51
1:A:219:LEU:HD21	1:A:221:LEU:HD21	1.91	0.51
1:B:266:THR:HA	1:B:269:LEU:HD12	1.93	0.51
1:A:242:TYR:N	1:A:242:TYR:CD1	2.78	0.51
1:B:355:LYS:HE3	1:B:420:GLU:HG2	1.93	0.51
1:A:501:PRO:HD3	3:A:2017:HOH:O	2.10	0.51
1:A:225:ARG:HH21	1:A:391:ASP:HB2	1.76	0.51
1:B:448:PRO:HB3	1:B:479:LEU:HD13	1.92	0.50
1:A:303:ARG:HH12	1:A:501:PRO:CD	2.20	0.50
1:B:426:ARG:HH11	1:B:478:PRO:HD3	1.74	0.50
1:B:172:ILE:HG23	1:B:173:GLU:N	2.26	0.50
1:A:285:GLU:CD	1:A:414:GLY:H	2.15	0.50
1:A:217:ARG:H	1:A:279:ASN:ND2	1.97	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ILE:N	1:A:519:ILE:CD1	2.71	0.50
1:A:398:ARG:NH2	3:A:2031:HOH:O	2.44	0.50
1:A:402:TRP:CZ3	1:A:405:VAL:HG23	2.47	0.50
1:A:273:ILE:HD12	1:A:273:ILE:N	2.27	0.49
1:B:464:ASN:OD1	1:B:466:LYS:HB2	2.12	0.49
1:A:453:SER:O	1:A:457:ARG:HG3	2.12	0.49
1:B:421:ARG:HG2	1:B:422:VAL:N	2.27	0.49
1:B:486:ALA:O	1:B:490:GLU:HG3	2.12	0.49
1:A:210:GLU:O	1:A:214:ARG:HG3	2.12	0.49
1:B:339:ILE:HD13	1:B:423:ILE:HG23	1.93	0.49
1:B:426:ARG:HH21	1:B:472:TYR:HE2	1.61	0.49
1:B:600:ILE:HG13	1:B:610:PHE:HB2	1.94	0.49
1:A:399:THR:HG21	1:B:520:ASP:HB3	1.95	0.49
1:B:450:THR:HG22	1:B:452:SER:N	2.27	0.49
1:B:301:SER:O	1:B:304:VAL:HG22	2.13	0.49
1:B:488:TRP:CZ2	1:B:515:LYS:HD3	2.48	0.49
1:A:329:ASN:HB2	1:A:463:ARG:O	2.13	0.49
1:A:500:THR:HA	3:A:2017:HOH:O	2.11	0.49
1:B:464:ASN:C	1:B:464:ASN:HD22	2.15	0.49
1:B:182:ILE:CG2	1:B:312:ILE:HD11	2.43	0.49
1:A:357:LYS:HB2	1:A:419:ALA:HA	1.95	0.48
1:A:526:ARG:CZ	1:A:527:GLY:H	2.27	0.48
1:B:222:ALA:O	1:B:261:CYS:HA	2.13	0.48
1:B:303:ARG:HD2	3:B:2055:HOH:O	2.12	0.48
1:B:205:PRO:O	1:B:209:ARG:HG3	2.14	0.48
1:B:300:ILE:O	1:B:304:VAL:HG13	2.14	0.48
1:B:294:ILE:HG21	1:B:508:MET:HE1	1.95	0.48
1:B:226:VAL:HG11	1:B:394:TYR:CD2	2.49	0.48
1:A:473:ILE:N	1:A:473:ILE:HD12	2.29	0.48
1:B:464:ASN:HD21	1:B:466:LYS:CG	2.27	0.47
1:B:208:VAL:O	1:B:212:ILE:HG13	2.14	0.47
1:B:450:THR:HG22	1:B:453:SER:H	1.79	0.47
1:B:381:LYS:HD3	1:B:401:ASP:O	2.15	0.47
1:B:266:THR:HG21	1:B:292:ALA:O	2.15	0.47
1:A:426:ARG:HH21	1:A:472:TYR:HE2	1.62	0.47
1:B:500:THR:OG1	1:B:502:GLU:HG2	2.15	0.47
1:A:199:LYS:NZ	1:A:285:GLU:CG	2.74	0.47
1:A:463:ARG:CG	1:A:463:ARG:HH11	2.26	0.47
1:A:180:ASP:OD1	1:A:214:ARG:NH1	2.48	0.47
1:A:492:LYS:NZ	1:A:520:ASP:HA	2.30	0.47
1:B:231:MET:O	1:B:235:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:GLU:C	1:A:577:VAL:H	2.17	0.47
1:A:243:GLN:NE2	1:A:268:ARG:NH1	2.63	0.47
1:B:235:LEU:HD23	1:B:240:ILE:HD13	1.97	0.47
1:B:464:ASN:ND2	1:B:464:ASN:C	2.68	0.46
1:A:283:MET:HG2	1:A:286:ALA:HB2	1.97	0.46
1:B:376:ARG:HH22	1:B:384:GLN:HE21	1.63	0.46
1:A:387:ARG:HG2	1:A:410:ILE:HG23	1.97	0.46
1:B:600:ILE:HG13	1:B:610:PHE:CG	2.50	0.46
1:A:271:SER:HB2	1:A:272:PRO:HD2	1.98	0.46
1:A:273:ILE:HD12	1:A:273:ILE:H	1.80	0.46
1:B:193:LEU:HB3	1:B:197:ALA:HB3	1.97	0.46
1:A:464:ASN:HD21	1:A:467:ASN:HB2	1.81	0.46
1:B:262:HIS:HD2	1:B:293:SER:OG	1.99	0.46
1:A:350:TRP:CZ3	1:A:473:ILE:HG21	2.50	0.46
1:A:185:LYS:O	1:A:186:LYS:HB3	2.14	0.46
1:A:553:GLU:HA	1:A:553:GLU:OE2	2.16	0.46
1:B:435:THR:HA	1:B:439:GLU:HA	1.98	0.46
1:A:496:ASP:OD1	1:A:520:ASP:O	2.34	0.46
1:A:384:GLN:HA	1:A:406:VAL:O	2.15	0.46
1:A:467:ASN:HD22	1:A:468:GLU:H	1.63	0.46
1:B:450:THR:HG22	1:B:452:SER:H	1.81	0.46
1:B:385:LEU:HD12	1:B:407:THR:CG2	2.39	0.46
1:A:500:THR:HG21	1:A:504:ILE:HD11	1.98	0.46
1:B:458:ARG:HD2	1:B:472:TYR:CD2	2.51	0.46
1:B:375:LEU:O	1:B:380:LYS:HB2	2.16	0.46
1:B:350:TRP:O	1:B:421:ARG:NH2	2.44	0.46
1:B:226:VAL:HG23	3:B:2030:HOH:O	2.16	0.45
1:B:409:ASP:O	1:B:412:GLU:HB2	2.15	0.45
1:A:400:ASN:HB2	1:B:504:ILE:CD1	2.47	0.45
1:B:199:LYS:HG3	1:B:200:THR:N	2.31	0.45
1:B:453:SER:O	1:B:457:ARG:HG3	2.16	0.45
1:A:343:SER:HB2	1:A:374:CYS:HB2	1.97	0.45
1:B:502:GLU:CD	1:B:502:GLU:H	2.19	0.45
1:A:240:ILE:HB	1:A:242:TYR:CZ	2.52	0.45
1:B:492:LYS:HZ2	1:B:520:ASP:HA	1.81	0.45
1:A:580:GLU:HG2	1:A:590:LYS:HG2	1.96	0.45
1:A:451:HIS:ND1	1:A:478:PRO:HB2	2.32	0.45
1:B:363:PRO:O	1:B:429:MET:HG2	2.17	0.45
1:A:377:LYS:HA	1:A:377:LYS:CE	2.40	0.45
1:B:218:THR:O	1:B:257:VAL:HA	2.17	0.45
1:B:400:ASN:HD22	1:B:400:ASN:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASP:CG	1:A:517:ASP:O	2.55	0.45
1:B:433:ILE:HD12	1:B:489:LYS:HD2	1.99	0.44
1:A:463:ARG:HB2	3:A:2045:HOH:O	2.16	0.44
1:B:504:ILE:O	1:B:504:ILE:HG13	2.18	0.44
1:A:396:LYS:HG2	1:B:519:ILE:HG23	1.99	0.44
1:A:502:GLU:H	1:A:502:GLU:CD	2.17	0.44
1:A:396:LYS:HE3	1:B:519:ILE:HG23	1.98	0.44
1:A:463:ARG:CG	1:A:463:ARG:NH1	2.80	0.44
1:A:304:VAL:HA	1:A:309:ALA:O	2.18	0.44
1:B:202:ARG:NH1	1:B:202:ARG:HG2	2.31	0.44
1:B:512:GLU:O	1:B:515:LYS:HG3	2.17	0.44
1:B:402:TRP:CZ3	1:B:405:VAL:HG23	2.53	0.44
1:A:299:TYR:CZ	1:A:303:ARG:HD3	2.53	0.44
1:B:345:ASN:HD22	1:B:346:SER:N	2.15	0.44
1:B:297:ARG:NH1	1:B:512:GLU:OE1	2.51	0.43
1:B:305:GLU:C	1:B:307:GLY:H	2.20	0.43
1:B:402:TRP:CE3	1:B:405:VAL:HG23	2.53	0.43
1:A:526:ARG:NE	1:A:527:GLY:H	2.15	0.43
1:A:505:ILE:HD11	1:A:524:ARG:HD2	2.00	0.43
1:B:478:PRO:C	1:B:479:LEU:HD12	2.39	0.43
1:B:566:GLY:HA2	1:B:594:ARG:HA	2.01	0.43
1:B:323:ASP:HA	1:B:324:PRO:HD3	1.82	0.43
1:B:388:LYS:HZ2	1:B:606:ALA:HA	1.84	0.43
1:B:438:GLU:O	1:B:440:ARG:NH1	2.51	0.43
1:A:350:TRP:O	1:A:421:ARG:NH2	2.50	0.43
1:B:488:TRP:CE2	1:B:515:LYS:HD3	2.53	0.43
1:A:508:MET:HB3	1:A:513:ARG:HG2	2.00	0.43
1:B:451:HIS:CE1	1:B:478:PRO:HG2	2.53	0.43
1:A:387:ARG:HH11	1:A:387:ARG:HG3	1.84	0.43
1:A:235:LEU:HD22	1:A:238:LEU:HD12	1.99	0.43
1:A:306:MET:CE	1:A:504:ILE:HG12	2.48	0.43
1:A:241:ARG:HD3	1:A:258:ASP:OD1	2.19	0.43
1:A:389:THR:HG22	1:A:393:GLU:HB2	2.01	0.43
1:A:519:ILE:HD13	1:A:522:GLU:HG2	2.00	0.43
1:A:358:THR:HA	1:A:421:ARG:O	2.18	0.43
1:B:183:PHE:HB3	1:B:216:LEU:CD1	2.47	0.43
1:A:219:LEU:HB2	1:A:278:TYR:CE2	2.53	0.43
1:A:344:TRP:N	1:A:344:TRP:CE3	2.85	0.42
1:B:450:THR:CG2	1:B:452:SER:H	2.32	0.42
1:B:239:PRO:O	1:B:257:VAL:HG13	2.19	0.42
1:A:553:GLU:HG2	1:A:595:TRP:HH2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:TYR:HD2	1:B:259:LEU:HD22	1.84	0.42
1:A:451:HIS:CD2	1:A:480:GLU:HG3	2.48	0.42
1:B:425:PRO:HG2	3:B:2046:HOH:O	2.19	0.42
1:B:178:ILE:HD12	1:B:178:ILE:N	2.35	0.42
1:A:288:PHE:O	1:A:293:SER:HB2	2.20	0.42
1:B:336:GLU:HA	1:B:474:TYR:O	2.18	0.42
1:B:551:ALA:C	1:B:553:GLU:H	2.22	0.42
1:A:213:LYS:NZ	1:A:213:LYS:CB	2.83	0.42
1:B:598:ALA:HA	1:B:601:TYR:CE2	2.54	0.42
1:B:303:ARG:NH1	1:B:502:GLU:OE1	2.53	0.42
1:B:501:PRO:C	1:B:503:GLY:H	2.22	0.42
1:A:426:ARG:NH1	1:A:478:PRO:HD3	2.35	0.42
1:A:492:LYS:HZ1	1:A:520:ASP:HA	1.85	0.42
1:B:451:HIS:CD2	1:B:480:GLU:H	2.38	0.42
1:B:178:ILE:HG12	1:B:207:ILE:CG1	2.50	0.42
1:B:218:THR:HG22	1:B:219:LEU:N	2.35	0.41
1:A:288:PHE:CG	1:A:413:MET:HG2	2.54	0.41
1:B:550:VAL:O	1:B:553:GLU:HB3	2.19	0.41
1:A:229:ALA:O	1:A:232:GLU:HB3	2.20	0.41
1:B:264:THR:HA	1:B:538:ARG:HH21	1.85	0.41
1:A:430:LYS:HE2	1:A:447:MET:SD	2.61	0.41
1:A:261:CYS:O	1:A:262:HIS:C	2.58	0.41
1:A:495:LEU:HD23	1:A:498:ILE:HD12	2.02	0.41
1:A:259:LEU:HD23	1:A:259:LEU:C	2.41	0.41
1:A:471:GLN:HE21	1:A:473:ILE:HD11	1.85	0.41
1:B:389:THR:HG23	1:B:393:GLU:CG	2.50	0.41
1:B:218:THR:HB	1:B:257:VAL:HB	2.02	0.41
1:B:422:VAL:HG23	1:B:461:VAL:CG1	2.50	0.41
1:B:580:GLU:OE1	1:B:588:ARG:NH1	2.47	0.41
1:A:299:TYR:O	1:A:303:ARG:HG2	2.20	0.41
1:A:387:ARG:HG2	1:A:410:ILE:CG2	2.51	0.41
1:A:213:LYS:HZ3	1:A:213:LYS:HB3	1.83	0.41
1:A:592:LYS:HA	1:A:593:PRO:HD2	1.86	0.41
1:B:600:ILE:HA	1:B:600:ILE:HD12	1.88	0.41
1:B:519:ILE:HG22	1:B:520:ASP:O	2.21	0.41
1:B:306:MET:HE1	1:B:504:ILE:HG21	2.02	0.41
1:A:182:ILE:HG22	1:A:312:ILE:HD11	2.01	0.41
1:B:502:GLU:HG2	1:B:504:ILE:HG23	2.02	0.41
1:B:242:TYR:C	1:B:243:GLN:HG3	2.41	0.41
1:A:272:PRO:HG2	1:A:273:ILE:CD1	2.41	0.41
1:A:184:ARG:O	1:A:187:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:CG2	1:A:220:ILE:HD11	2.50	0.41
1:B:482:ASP:OD2	1:B:482:ASP:C	2.59	0.41
1:A:454:ALA:HB1	3:A:2033:HOH:O	2.20	0.41
1:B:464:ASN:HD22	1:B:465:PRO:CD	2.34	0.41
1:A:426:ARG:C	1:A:449:VAL:HG13	2.41	0.41
1:B:358:THR:HG23	1:B:421:ARG:HD3	2.02	0.41
1:A:407:THR:OG1	1:A:408:THR:N	2.54	0.41
1:A:381:LYS:HD3	1:A:401:ASP:O	2.21	0.41
1:B:217:ARG:H	1:B:279:ASN:ND2	2.07	0.40
1:B:520:ASP:O	1:B:522:GLU:N	2.53	0.40
1:A:282:ILE:HD12	1:A:282:ILE:N	2.35	0.40
1:B:573:LEU:HD23	1:B:578:GLU:HA	2.03	0.40
1:B:214:ARG:CG	1:B:214:ARG:NH1	2.80	0.40
1:A:221:LEU:HA	1:A:260:MET:O	2.21	0.40
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.85	0.40
1:B:175:ASN:O	1:B:176:PRO:C	2.58	0.40
1:A:504:ILE:HD12	1:A:504:ILE:O	2.20	0.40
1:B:289:THR:CB	3:B:2022:HOH:O	2.65	0.40
1:A:225:ARG:HH21	1:A:391:ASP:HB3	1.84	0.40
1:B:530:ARG:HB2	1:B:530:ARG:HE	1.73	0.40
1:A:256:ILE:O	1:A:256:ILE:HG13	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	427/451 (95%)	384 (90%)	37 (9%)	6 (1%)	14	42
1	B	435/451 (96%)	396 (91%)	32 (7%)	7 (2%)	12	38
All	All	862/902 (96%)	780 (90%)	69 (8%)	13 (2%)	13	40

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	480	GLU
1	A	527	GLY
1	B	192	ASP
1	B	445	GLY
1	A	445	GLY
1	A	391	ASP
1	A	522	GLU
1	B	502	GLU
1	A	346	SER
1	B	355	LYS
1	A	262	HIS
1	B	326	PRO
1	B	414	GLY

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	366/384 (95%)	339 (93%)	27 (7%)	17	43
1	B	374/384 (97%)	345 (92%)	29 (8%)	16	41
All	All	740/768 (96%)	684 (92%)	56 (8%)	16	42

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	236	ARG
1	A	257	VAL
1	A	267	MET
1	A	270	LEU
1	A	288	PHE
1	A	289	THR
1	A	322	ARG
1	A	337	ARG
1	A	377	LYS

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Mol	Chain	Res	Type
1	A	400	ASN
1	A	410	ILE
1	A	421	ARG
1	A	434	LEU
1	A	436	ASP
1	A	442	ILE
1	A	450	THR
1	A	463	ARG
1	A	499	ASN
1	A	502	GLU
1	A	526	ARG
1	A	535	ASP
1	A	579	VAL
1	A	585	GLU
1	A	589	LYS
1	A	600	ILE
1	A	603	ASP
1	B	184	ARG
1	B	230	GLU
1	B	236	ARG
1	B	256	ILE
1	B	257	VAL
1	B	258	ASP
1	B	262	HIS
1	B	266	THR
1	B	274	ARG
1	B	289	THR
1	B	319	PRO
1	B	333	MET
1	B	345	ASN
1	B	391	ASP
1	B	392	SER
1	B	396	LYS
1	B	410	ILE
1	B	421	ARG
1	B	436	ASP
1	B	450	THR
1	B	463	ARG
1	B	464	ASN
1	B	469	ASN
1	B	504	ILE
1	B	510	GLU

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Mol	Chain	Res	Type
1	B	549	ARG
1	B	564	PHE
1	B	603	ASP
1	B	617	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	287	HIS
1	A	327	GLN
1	A	329	ASN
1	A	384	GLN
1	A	400	ASN
1	A	451	HIS
1	A	456	GLN
1	A	467	ASN
1	A	471	GLN
1	A	499	ASN
1	A	569	ASN
1	A	576	ASN
1	B	262	HIS
1	B	279	ASN
1	B	329	ASN
1	B	345	ASN
1	B	384	GLN
1	B	400	ASN
1	B	451	HIS
1	B	456	GLN
1	B	464	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 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	SO4	A	4396	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	A	4397	-	4,4,4	0.20	0	6,6,6	0.11	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
2	SO4	A	4396	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4397	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	431/451 (95%)	0.16	27 (6%)	23	14	20, 43, 75, 99	1 (0%)
1	B	439/451 (97%)	-0.00	14 (3%)	51	39	18, 37, 65, 86	1 (0%)
All	All	870/902 (96%)	0.08	41 (4%)	35	24	18, 40, 70, 99	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	PRO	7.0
1	B	517	ASP	4.8
1	A	576	ASN	4.4
1	A	346	SER	4.3
1	A	233	GLU	4.1
1	A	517	ASP	4.0
1	A	435	THR	3.7
1	A	243	GLN	3.5
1	A	241	ARG	3.4
1	A	180	ASP	3.4
1	B	236	ARG	3.3
1	A	239	PRO	2.9
1	A	242	TYR	2.9
1	A	255	GLU	2.9
1	A	585	GLU	2.9
1	B	193	LEU	2.9
1	B	526	ARG	2.8
1	A	322	ARG	2.7
1	B	516	VAL	2.7
1	A	342	ARG	2.7
1	A	436	ASP	2.7
1	A	574	GLU	2.6
1	A	202	ARG	2.5
1	A	468	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	240	ILE	2.5
1	A	577	VAL	2.5
1	A	379	GLY	2.4
1	B	345	ASN	2.4
1	B	255	GLU	2.4
1	A	437	GLY	2.4
1	B	342	ARG	2.4
1	B	467	ASN	2.3
1	A	469	ASN	2.2
1	A	377	LYS	2.2
1	B	468	GLU	2.2
1	B	230	GLU	2.1
1	A	467	ASN	2.1
1	B	197	ALA	2.1
1	B	180	ASP	2.0
1	B	436	ASP	2.0
1	A	234	ALA	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^{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
2	SO4	A	4396	5/5	0.95	0.15	-0.66	75,75,76,77	0
2	SO4	A	4397	5/5	0.97	0.14	-0.67	54,54,54,56	0

6.5 Other polymers (i)

There are no such residues in this entry.