Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:28 PM GMT

PDB ID	:	1KFI
Title	:	Crystal Structure of the Exocytosis-Sensitive Phosphoprotein, pp63/Parafusin (phosphoglucomutase) from Paramecium
Authors	:	Mueller, S.; Diederichs, K.; Breed, J.; Kissmehl, R.; Hauser, K.; Plattner, H.; Welte, W.
Deposited on	:	2001-11-21
Resolution	:	2.40 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:

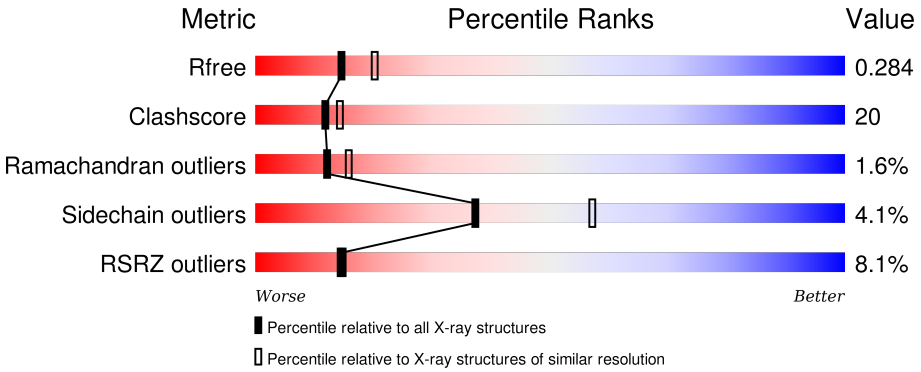
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	572	4% 70% 27%
1	B	572	12% 62% 34%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9207 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.

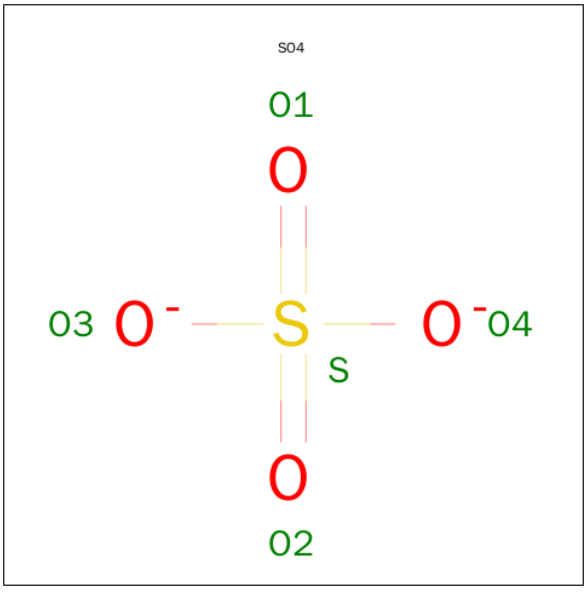
- Molecule 1 is a protein called phosphoglucomutase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4490	2858	769	850	13			
1	B	570	Total	C	N	O	S	0	0	0
			4490	2858	769	850	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

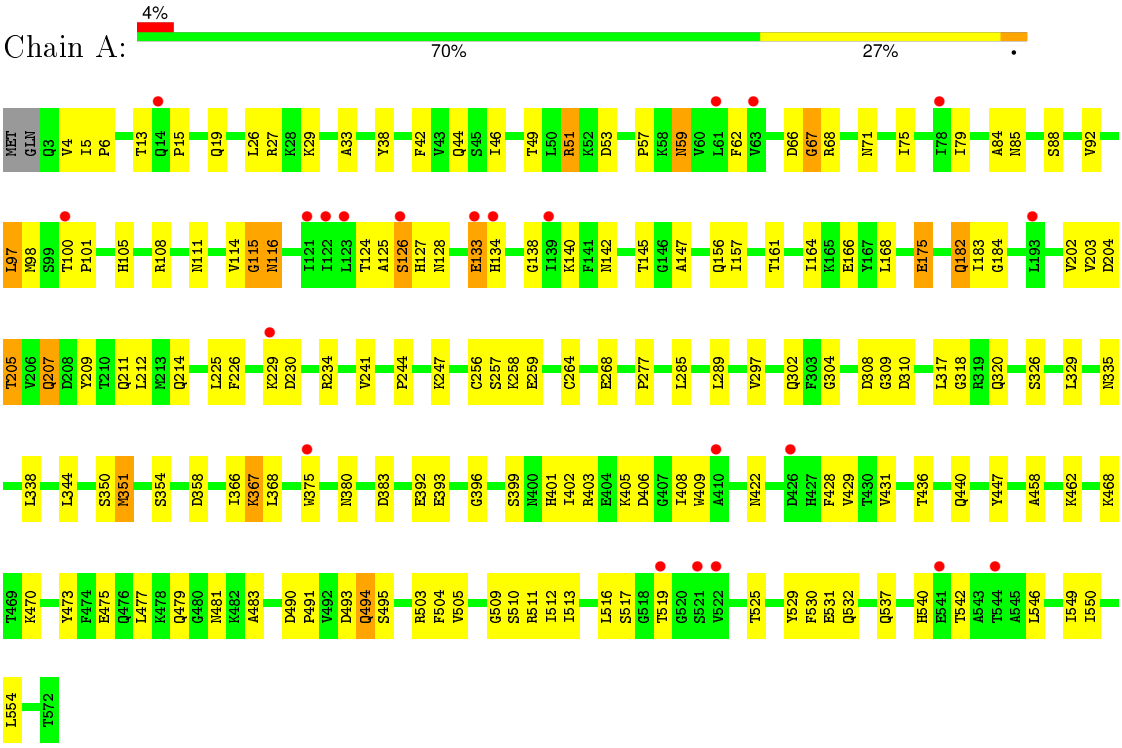
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	126	Total O 126 126	0	0
4	B	79	Total O 79 79	0	0

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.

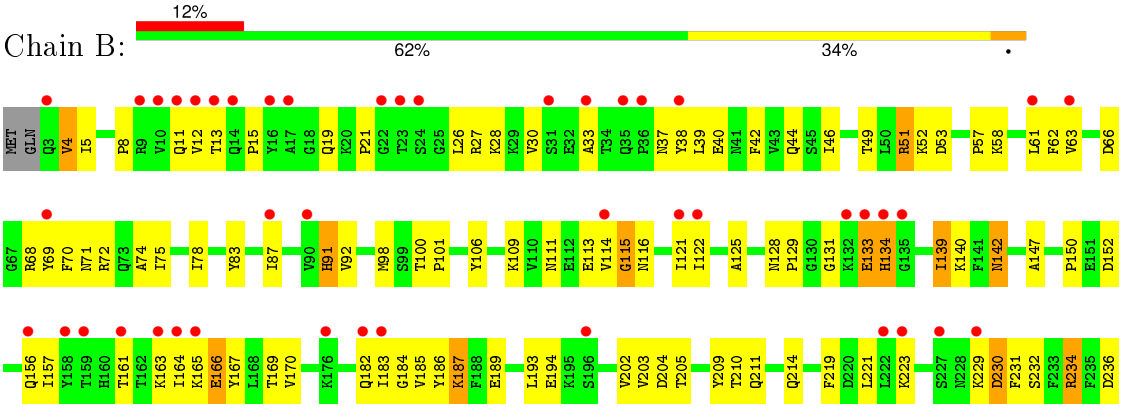
- Molecule 1: phosphoglucomutase 1

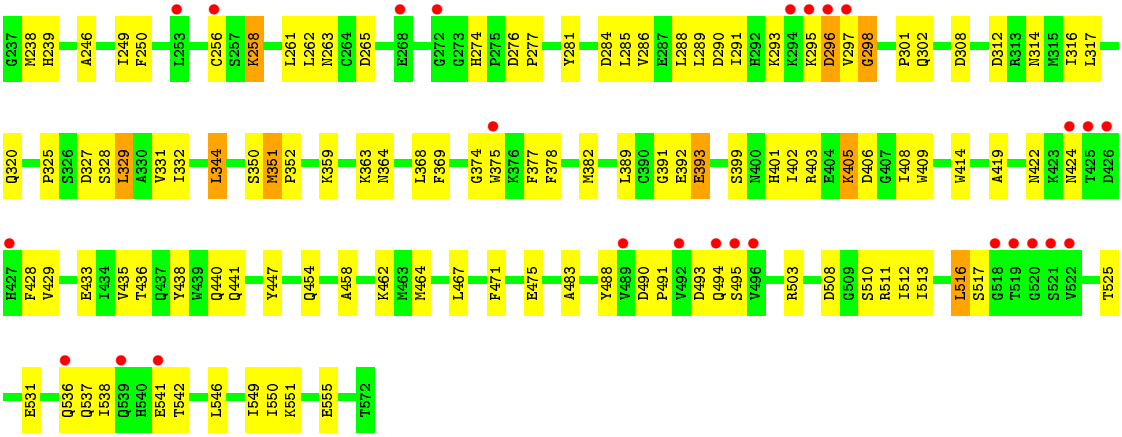
Chain A:



- Molecule 1: phosphoglucomutase 1

Chain B:




G237 M238 H239 A246 I249 F250 L253 C256 S257 K258 L261 L262 N263 C264 D265 E268 G272 G273 H274 P275 D276 P277 Y281 D284 L285 V286 E287 L288 L289 D290 I291 H292 K293 K294 K295 D296 V297 G298 P301 Q302 D308 D312 N313 N314 M315 I316 L317
Q320 P325 S326 D327 S328 L329 A330 V331 I332 L344 S350 M351 P352 K359 K363 N364 L368 F369 G374 W375 K376 F377 F378 M382 L389 C390 G391 E392 E393 S399 N400 H401 I402 R403 E404 K405 D406 G407 I408 W409 W414 A419 N422 K423 N424 T425 D426
H427 F428 V429 E433 I434 V435 T436 Q437 Y438 W439 Q440 Q441 Y447 Q454 A458 K462 M463 M464 L467 F471 E475 A483 Y488 V489 D490 P491 V492 D493 Q494 S495 V496 R503 D508 G509 S510 R511 I512 I513 L516 S517 G518 T519 G520 S521 V522 T525
E531 Q536 Q537 I538 Q539 H540 E541 T542 L546 I549 I550 K551 E555 T572

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.35Å 133.61Å 150.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 27.96 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.40) 93.8 (27.96-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.89 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.286 0.233 , 0.284	Depositor DCC
R_{free} test set	971 reflections (1.96%)	DCC
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 49705 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9207	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: ZN, 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	0.37	0/4592	0.62	0/6207
1	B	0.36	0/4592	0.61	1/6207 (0.0%)
All	All	0.37	0/9184	0.61	1/12414 (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	541	GLU	N-CA-C	-5.34	96.59	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	4490	0	4386	160	0
1	B	4490	0	4386	205	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	126	0	0	4	0
4	B	79	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9207	0	8772	358	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 20.

All (358) 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:124:THR:HG22	1:A:126:SER:H	1.12	1.10
1:B:375:TRP:CZ3	1:B:405:LYS:HB2	1.96	1.01
1:A:375:TRP:NE1	1:A:405:LYS:HE3	1.81	0.95
1:A:422:ASN:HD21	1:A:429:VAL:H	1.17	0.91
1:B:91:HIS:HD2	1:B:106:TYR:OH	1.55	0.89
1:A:422:ASN:HD21	1:A:429:VAL:N	1.76	0.83
1:A:59:ASN:ND2	1:A:88:SER:H	1.78	0.81
1:B:422:ASN:HD21	1:B:429:VAL:N	1.78	0.81
1:B:351:MET:CE	1:B:513:ILE:HG12	2.10	0.81
1:A:422:ASN:ND2	1:A:429:VAL:H	1.79	0.81
1:B:19:GLN:HE21	1:B:161:THR:HB	1.46	0.80
1:B:8:PRO:HA	1:B:170:VAL:HG12	1.64	0.78
1:B:169:THR:HG22	1:B:170:VAL:H	1.48	0.78
1:B:133:GLU:HG2	1:B:134:HIS:H	1.49	0.77
1:A:124:THR:HG22	1:A:126:SER:N	1.95	0.77
1:A:396:GLY:HA3	1:A:405:LYS:HE2	1.67	0.77
1:B:302:GLN:HG2	1:B:428:PHE:CE1	2.19	0.76
1:A:285:LEU:CD1	1:A:317:LEU:HD12	2.15	0.76
1:A:302:GLN:HG2	1:A:428:PHE:CE2	2.20	0.76
1:A:399:SER:HB3	1:A:401:HIS:HD2	1.51	0.75
1:B:285:LEU:HD12	1:B:317:LEU:HD12	1.67	0.75
1:B:232:SER:HB2	1:B:302:GLN:H	1.50	0.75
1:A:44:GLN:HE22	1:A:85:ASN:HD21	1.34	0.75
1:B:297:VAL:HG23	1:B:298:GLY:H	1.52	0.75
1:B:422:ASN:HD21	1:B:429:VAL:H	1.34	0.74
1:B:312:ASP:OD1	1:B:375:TRP:HH2	1.70	0.74
1:B:68:ARG:NH1	1:B:125:ALA:H	1.86	0.73
1:A:66:ASP:OD1	1:A:124:THR:HG23	1.87	0.73
1:B:351:MET:HE1	1:B:513:ILE:HG12	1.70	0.73
1:B:236:ASP:HB2	1:B:285:LEU:HD23	1.70	0.73
1:B:62:PHE:CZ	1:B:98:MET:HG2	2.23	0.73
1:B:182:GLN:O	1:B:202:VAL:HG11	1.89	0.73
1:A:140:LYS:HE2	1:A:142:ASN:HD21	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PHE:HZ	1:B:98:MET:HG2	1.54	0.72
1:B:33:ALA:HA	1:B:38:TYR:CD2	2.25	0.71
1:A:19:GLN:HE21	1:A:161:THR:HB	1.55	0.71
1:A:182:GLN:O	1:A:202:VAL:HG11	1.93	0.69
1:B:295:LYS:NZ	1:B:296:ASP:H	1.91	0.69
1:A:542:THR:HG23	4:A:805:HOH:O	1.93	0.69
1:B:258:LYS:H	1:B:258:LYS:HE2	1.58	0.68
1:B:19:GLN:NE2	1:B:161:THR:HB	2.10	0.67
1:A:436:THR:O	1:A:440:GLN:HG3	1.93	0.67
1:B:133:GLU:CD	1:B:133:GLU:H	1.98	0.67
1:B:375:TRP:CH2	1:B:405:LYS:HB2	2.29	0.67
1:B:39:LEU:HD21	1:B:74:ALA:HA	1.76	0.66
1:B:183:ILE:HA	1:B:202:VAL:HG13	1.77	0.66
1:B:314:ASN:HD22	1:B:316:ILE:HD13	1.59	0.66
1:B:351:MET:HE3	1:B:513:ILE:HG12	1.77	0.66
1:B:350:SER:HB2	1:B:392:GLU:HG2	1.76	0.66
1:B:83:TYR:CE1	1:B:170:VAL:HG11	2.31	0.66
1:A:97:LEU:O	1:A:205:THR:HB	1.96	0.65
1:A:318:GLY:HA3	1:A:431:VAL:CG2	2.27	0.65
1:B:15:PRO:HG3	1:B:164:ILE:O	1.97	0.65
1:B:66:ASP:OD2	1:B:68:ARG:NH1	2.30	0.64
1:A:71:ASN:O	1:A:75:ILE:HG13	1.97	0.64
1:A:351:MET:HE2	1:A:351:MET:O	1.98	0.64
1:A:358:ASP:HA	1:A:368:LEU:HD22	1.80	0.64
1:A:68:ARG:CZ	1:A:125:ALA:HB3	2.28	0.64
1:A:105:HIS:CD2	1:A:212:LEU:HD22	2.34	0.63
1:A:29:LYS:NZ	1:A:134:HIS:HA	2.14	0.63
1:A:289:LEU:HD22	1:A:317:LEU:HB2	1.79	0.63
1:B:436:THR:O	1:B:440:GLN:HG3	2.00	0.62
1:A:15:PRO:HG3	1:A:164:ILE:O	2.00	0.62
1:B:285:LEU:CD1	1:B:317:LEU:HD12	2.29	0.62
1:A:375:TRP:HE1	1:A:405:LYS:HE3	1.61	0.61
1:B:351:MET:HE2	1:B:511:ARG:HH21	1.65	0.61
1:A:318:GLY:HA3	1:A:431:VAL:HG22	1.81	0.61
1:B:406:ASP:HB3	1:B:409:TRP:HB3	1.83	0.61
1:A:62:PHE:CZ	1:A:98:MET:HG2	2.36	0.60
1:A:351:MET:HE3	1:A:513:ILE:HG12	1.82	0.60
1:A:51:ARG:HH21	1:B:51:ARG:HH21	1.47	0.60
1:A:59:ASN:ND2	1:A:59:ASN:H	2.00	0.60
1:B:285:LEU:HD13	1:B:289:LEU:HD13	1.84	0.60
1:B:422:ASN:ND2	1:B:429:VAL:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:O	1:B:161:THR:HG23	2.01	0.60
1:B:286:VAL:HG13	1:B:291:ILE:CG1	2.32	0.60
1:B:406:ASP:OD2	1:B:409:TRP:HB2	2.02	0.60
1:B:83:TYR:CD1	1:B:170:VAL:HG11	2.36	0.59
1:A:358:ASP:CG	1:A:368:LEU:HD21	2.22	0.59
1:B:314:ASN:ND2	1:B:316:ILE:HD13	2.18	0.59
1:A:207:GLN:HE21	1:A:207:GLN:HA	1.68	0.59
1:A:75:ILE:O	1:A:79:ILE:HG13	2.02	0.59
1:B:91:HIS:CD2	1:B:106:TYR:OH	2.46	0.59
1:B:312:ASP:OD1	1:B:375:TRP:CH2	2.53	0.58
1:A:100:THR:HB	1:A:101:PRO:HD3	1.85	0.58
1:B:12:VAL:HA	1:B:166:GLU:HB3	1.85	0.58
1:A:124:THR:HG21	1:A:310:ASP:HB3	1.85	0.58
1:A:68:ARG:HD3	4:A:733:HOH:O	2.03	0.58
1:A:380:ASN:HD21	1:B:52:LYS:CE	2.15	0.58
1:B:511:ARG:NH1	1:B:531:GLU:OE1	2.36	0.58
1:A:375:TRP:CZ2	1:A:405:LYS:HB3	2.39	0.58
1:A:145:THR:HG23	1:B:53:ASP:HB2	1.86	0.58
1:B:27:ARG:NH1	1:B:128:ASN:ND2	2.52	0.58
1:B:74:ALA:O	1:B:78:ILE:HG13	2.03	0.58
1:A:126:SER:HB2	3:A:601:SO4:O1	2.04	0.57
1:A:209:TYR:OH	1:A:408:ILE:HB	2.05	0.57
1:A:59:ASN:HD21	1:A:88:SER:H	1.53	0.57
1:B:21:PRO:HG3	1:B:42:PHE:CZ	2.40	0.57
1:B:314:ASN:HD22	1:B:316:ILE:CD1	2.18	0.57
1:B:229:LYS:HG3	1:B:230:ASP:OD1	2.05	0.57
1:B:26:LEU:HD23	1:B:139:ILE:HD13	1.87	0.56
1:B:13:THR:HG22	1:B:166:GLU:CA	2.36	0.56
1:B:111:ASN:HA	1:B:115:GLY:HA2	1.87	0.56
1:A:75:ILE:HD13	1:A:92:VAL:HG21	1.86	0.56
1:B:351:MET:CE	1:B:511:ARG:HH21	2.19	0.56
1:B:140:LYS:NZ	1:B:142:ASN:HD21	2.03	0.56
1:B:142:ASN:N	1:B:142:ASN:HD22	2.02	0.56
1:B:256:CYS:SG	1:B:261:LEU:HD21	2.46	0.56
1:A:509:GLY:O	1:A:511:ARG:HG3	2.06	0.56
1:A:257:SER:OG	1:A:259:GLU:HG2	2.05	0.55
1:A:59:ASN:H	1:A:59:ASN:HD22	1.55	0.55
1:A:351:MET:CE	1:A:513:ILE:HD13	2.37	0.55
1:B:185:VAL:HG12	1:B:187:LYS:HD2	1.87	0.55
1:A:108:ARG:NH1	1:A:403:ARG:NH1	2.55	0.55
1:A:399:SER:HB3	1:A:401:HIS:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:HG3	1:A:230:ASP:OD1	2.07	0.55
1:B:152:ASP:O	1:B:156:GLN:HG2	2.07	0.55
1:B:114:VAL:O	1:B:116:ASN:N	2.40	0.55
1:B:258:LYS:CE	1:B:258:LYS:H	2.19	0.55
1:B:290:ASP:O	1:B:320:GLN:HG2	2.06	0.55
1:B:375:TRP:N	1:B:375:TRP:CD1	2.73	0.55
1:A:68:ARG:NH2	1:A:125:ALA:HB3	2.22	0.54
1:B:297:VAL:HG23	1:B:298:GLY:N	2.21	0.54
1:B:219:PHE:O	1:B:223:LYS:HB2	2.07	0.54
1:A:66:ASP:OD2	1:A:68:ARG:HD2	2.07	0.54
1:B:75:ILE:HD13	1:B:92:VAL:HG21	1.89	0.54
1:B:183:ILE:HG22	1:B:184:GLY:N	2.23	0.53
1:B:374:GLY:O	1:B:377:PHE:HD1	1.91	0.53
1:B:246:ALA:O	1:B:250:PHE:HB2	2.08	0.53
1:B:13:THR:HG22	1:B:166:GLU:N	2.23	0.53
1:A:380:ASN:HD21	1:B:52:LYS:HE2	1.72	0.53
1:A:493:ASP:OD2	1:A:495:SER:HB2	2.08	0.53
1:A:51:ARG:HH21	1:B:51:ARG:NH2	2.05	0.53
1:B:26:LEU:HD11	1:B:28:LYS:HE2	1.89	0.53
1:A:62:PHE:HZ	1:A:98:MET:HG2	1.73	0.53
1:A:473:TYR:CZ	1:A:477:LEU:HD21	2.44	0.53
1:B:21:PRO:HG3	1:B:42:PHE:HZ	1.75	0.52
1:A:517:SER:HB3	1:A:525:THR:HB	1.91	0.52
1:B:359:LYS:O	1:B:363:LYS:HG2	2.09	0.52
1:B:68:ARG:CZ	1:B:125:ALA:HB3	2.40	0.52
1:A:133:GLU:CD	1:A:133:GLU:H	2.12	0.52
1:B:42:PHE:CE2	1:B:139:ILE:HB	2.46	0.51
1:B:203:VAL:HG22	1:B:204:ASP:N	2.26	0.51
1:A:13:THR:HG22	1:A:166:GLU:HA	1.92	0.51
1:B:51:ARG:N	1:B:51:ARG:HD2	2.25	0.51
1:A:326:SER:HB3	1:A:354:SER:OG	2.11	0.51
1:B:239:HIS:NE2	1:B:263:ASN:ND2	2.59	0.51
1:A:447:TYR:HA	1:A:530:PHE:O	2.11	0.51
1:B:58:LYS:HE3	4:B:751:HOH:O	2.11	0.51
1:A:124:THR:CG2	1:A:126:SER:H	2.02	0.51
1:A:396:GLY:CA	1:A:405:LYS:HE2	2.38	0.51
1:B:286:VAL:HG13	1:B:291:ILE:HG13	1.92	0.51
1:B:13:THR:HG22	1:B:166:GLU:HA	1.91	0.51
1:B:42:PHE:HE2	1:B:139:ILE:HB	1.76	0.50
1:B:546:LEU:O	1:B:549:ILE:HG22	2.11	0.50
1:A:396:GLY:HA3	1:A:405:LYS:CE	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:HD11	1:B:317:LEU:HD13	1.92	0.50
1:B:66:ASP:CG	1:B:68:ARG:NH1	2.65	0.50
1:A:114:VAL:O	1:A:116:ASN:N	2.42	0.50
1:A:289:LEU:HD22	1:A:317:LEU:CB	2.41	0.50
1:B:165:LYS:O	1:B:166:GLU:HB3	2.12	0.50
1:A:350:SER:HB3	1:A:392:GLU:HG2	1.92	0.50
1:A:277:PRO:CD	1:A:308:ASP:HB3	2.42	0.50
1:A:66:ASP:OD2	1:A:66:ASP:O	2.29	0.50
1:B:295:LYS:HZ2	1:B:296:ASP:H	1.58	0.50
1:B:193:LEU:O	1:B:194:GLU:HB2	2.11	0.50
1:A:211:GLN:HA	1:A:214:GLN:HE21	1.76	0.50
1:A:511:ARG:O	1:A:549:ILE:HD11	2.12	0.49
1:A:183:ILE:HA	1:A:202:VAL:HG13	1.95	0.49
1:A:126:SER:O	1:A:128:ASN:N	2.45	0.49
1:B:513:ILE:HD12	1:B:513:ILE:N	2.27	0.49
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.77	0.49
1:B:517:SER:HB3	1:B:525:THR:HB	1.94	0.49
1:B:39:LEU:CD2	1:B:74:ALA:HA	2.41	0.49
1:B:265:ASP:HB2	4:B:772:HOH:O	2.12	0.49
1:B:139:ILE:H	1:B:139:ILE:HD12	1.77	0.49
1:A:108:ARG:HH12	1:A:403:ARG:HH12	1.61	0.49
1:A:27:ARG:NH1	1:A:27:ARG:HB3	2.28	0.49
1:B:238:MET:HE1	1:B:276:ASP:N	2.28	0.48
1:A:44:GLN:HE22	1:A:85:ASN:ND2	2.07	0.48
1:B:517:SER:CB	1:B:525:THR:HB	2.43	0.48
1:B:100:THR:HB	1:B:101:PRO:HD3	1.96	0.48
1:A:483:ALA:HA	1:A:503:ARG:O	2.13	0.48
1:A:258:LYS:HE2	1:A:258:LYS:H	1.78	0.48
1:A:335:ASN:HD22	1:A:338:LEU:HD12	1.78	0.48
1:B:183:ILE:CG2	1:B:184:GLY:N	2.75	0.48
1:A:27:ARG:HB3	1:A:27:ARG:HH11	1.78	0.48
1:A:513:ILE:HB	1:A:529:TYR:HB2	1.96	0.48
1:A:108:ARG:HH12	1:A:403:ARG:NH1	2.11	0.48
1:B:4:VAL:HA	1:B:189:GLU:O	2.14	0.48
1:B:351:MET:HB3	1:B:352:PRO:HD3	1.96	0.48
1:B:150:PRO:HG3	4:B:775:HOH:O	2.13	0.48
1:A:289:LEU:HD21	1:A:304:GLY:N	2.29	0.47
1:B:131:GLY:HA3	1:B:133:GLU:OE2	2.14	0.47
1:B:186:TYR:HE1	1:B:202:VAL:HG12	1.79	0.47
1:A:458:ALA:O	1:A:462:LYS:HG3	2.14	0.47
1:B:139:ILE:HD12	1:B:139:ILE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ALA:O	1:B:462:LYS:HG3	2.14	0.47
1:B:464:MET:HA	1:B:467:LEU:HD12	1.97	0.47
1:B:234:ARG:CD	1:B:288:LEU:HD13	2.45	0.47
1:B:399:SER:HB3	1:B:401:HIS:ND1	2.30	0.47
1:B:378:PHE:O	1:B:382:MET:HG3	2.14	0.47
1:A:203:VAL:HG22	1:A:204:ASP:N	2.29	0.47
1:A:318:GLY:HA3	1:A:431:VAL:HG21	1.95	0.47
1:A:351:MET:HE2	1:A:511:ARG:NH2	2.30	0.47
1:A:403:ARG:CG	1:A:403:ARG:HH11	2.28	0.47
1:B:551:LYS:O	1:B:555:GLU:HG3	2.15	0.47
1:B:351:MET:HE3	1:B:513:ILE:CG1	2.43	0.47
1:A:19:GLN:NE2	1:A:161:THR:HB	2.27	0.47
1:A:277:PRO:HD2	1:A:308:ASP:HB3	1.97	0.47
1:B:471:PHE:O	1:B:475:GLU:HG3	2.14	0.47
1:A:285:LEU:HD13	1:A:317:LEU:HD12	1.92	0.47
1:A:205:THR:HG23	4:A:812:HOH:O	2.15	0.46
1:A:546:LEU:O	1:A:549:ILE:HG22	2.15	0.46
1:B:239:HIS:H	1:B:263:ASN:HB3	1.80	0.46
1:B:232:SER:HB2	1:B:302:GLN:N	2.27	0.46
1:A:510:SER:C	1:A:511:ARG:HG3	2.35	0.46
1:B:147:ALA:HB2	1:B:403:ARG:HB3	1.97	0.46
1:B:295:LYS:HZ2	1:B:295:LYS:HB3	1.81	0.46
1:A:351:MET:HE1	1:A:513:ILE:HD13	1.96	0.46
1:B:185:VAL:CG1	1:B:187:LYS:HD2	2.45	0.46
1:B:209:TYR:OH	1:B:408:ILE:HB	2.15	0.46
1:B:351:MET:O	1:B:511:ARG:NH2	2.48	0.46
1:A:519:THR:HG22	1:A:519:THR:O	2.15	0.46
1:A:383:ASP:OD2	1:A:403:ARG:NH1	2.48	0.46
1:A:111:ASN:HB3	1:B:57:PRO:HB3	1.98	0.46
1:A:84:ALA:HB1	1:A:168:LEU:HB3	1.97	0.46
1:A:66:ASP:O	1:A:71:ASN:ND2	2.49	0.46
1:A:67:GLY:O	1:A:268:GLU:HA	2.16	0.46
1:A:124:THR:HG21	1:A:310:ASP:CB	2.46	0.45
1:A:59:ASN:HD22	1:A:59:ASN:N	2.14	0.45
1:B:510:SER:C	1:B:511:ARG:HG3	2.36	0.45
1:B:327:ASP:O	1:B:331:VAL:HG23	2.16	0.45
1:B:109:LYS:O	1:B:113:GLU:HG3	2.16	0.45
1:B:210:THR:HG23	1:B:249:ILE:HG12	1.97	0.45
1:A:258:LYS:CE	1:A:258:LYS:H	2.29	0.45
1:A:247:LYS:HE3	1:A:264:CYS:O	2.17	0.45
1:B:288:LEU:O	1:B:301:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:VAL:HG13	1:B:433:GLU:OE2	2.17	0.45
1:A:511:ARG:CZ	1:A:513:ILE:HD11	2.47	0.45
1:B:122:ILE:HB	1:B:140:LYS:HG2	1.98	0.45
1:A:42:PHE:O	1:A:46:ILE:HG13	2.15	0.45
1:A:126:SER:C	1:A:128:ASN:H	2.20	0.45
1:B:234:ARG:HD3	1:B:288:LEU:HD13	1.98	0.45
1:A:157:ILE:O	1:A:161:THR:HG23	2.17	0.45
1:A:532:GLN:HB3	1:A:546:LEU:HD23	1.99	0.45
1:A:101:PRO:HG3	1:A:405:LYS:O	2.17	0.45
1:A:302:GLN:HG3	4:A:775:HOH:O	2.17	0.45
1:B:71:ASN:O	1:B:75:ILE:HG13	2.16	0.45
1:B:33:ALA:O	1:B:38:TYR:HB3	2.17	0.45
1:A:530:PHE:CE1	1:A:550:ILE:HA	2.51	0.45
1:B:393:GLU:HG3	1:B:447:TYR:OH	2.17	0.45
1:B:375:TRP:N	1:B:375:TRP:HD1	2.15	0.44
1:B:236:ASP:OD1	1:B:238:MET:N	2.44	0.44
1:B:92:VAL:O	1:B:202:VAL:HA	2.17	0.44
1:A:59:ASN:ND2	1:A:88:SER:N	2.58	0.44
1:B:202:VAL:O	1:B:202:VAL:HG13	2.17	0.44
1:B:290:ASP:OD1	1:B:293:LYS:HA	2.17	0.44
1:A:125:ALA:O	1:A:126:SER:O	2.35	0.44
1:B:285:LEU:HD12	1:B:317:LEU:CD1	2.43	0.44
1:B:11:GLN:O	1:B:166:GLU:HA	2.18	0.44
1:A:490:ASP:HA	1:A:491:PRO:HD3	1.87	0.44
1:A:504:PHE:HB2	1:A:512:ILE:HB	1.99	0.44
1:B:312:ASP:OD1	1:B:312:ASP:C	2.56	0.44
1:A:111:ASN:HA	1:A:115:GLY:HA2	1.99	0.44
1:A:490:ASP:O	1:A:494:GLN:HA	2.17	0.44
1:A:537:GLN:HB3	1:A:540:HIS:NE2	2.32	0.44
1:B:69:TYR:O	1:B:70:PHE:HB3	2.17	0.44
1:B:68:ARG:NH2	1:B:128:ASN:O	2.51	0.44
1:A:59:ASN:HD21	1:A:88:SER:N	2.14	0.44
1:B:368:LEU:HD13	1:B:369:PHE:N	2.33	0.44
1:B:375:TRP:CD2	1:B:405:LYS:HD3	2.53	0.43
1:B:295:LYS:HZ3	1:B:296:ASP:H	1.64	0.43
1:B:37:ASN:HA	1:B:40:GLU:OE2	2.18	0.43
1:A:26:LEU:O	1:A:138:GLY:HA2	2.17	0.43
1:B:66:ASP:OD1	1:B:68:ARG:HG2	2.18	0.43
1:A:297:VAL:HG12	1:A:320:GLN:NE2	2.33	0.43
1:A:241:VAL:HG12	1:A:309:GLY:O	2.18	0.43
1:B:351:MET:CE	1:B:511:ARG:NH2	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:HD21	1:B:52:LYS:HE3	1.83	0.43
1:B:284:ASP:HB2	4:B:731:HOH:O	2.17	0.43
1:B:302:GLN:HG3	4:B:750:HOH:O	2.18	0.43
1:A:13:THR:HG22	1:A:166:GLU:CA	2.48	0.43
1:B:42:PHE:O	1:B:46:ILE:HG13	2.19	0.43
1:B:488:TYR:OH	1:B:491:PRO:HD3	2.18	0.43
1:B:66:ASP:OD1	1:B:68:ARG:NH1	2.51	0.43
1:B:27:ARG:NH1	1:B:128:ASN:HD21	2.17	0.43
1:B:49:THR:HG23	1:B:156:GLN:HB2	2.01	0.43
1:B:546:LEU:O	1:B:550:ILE:HG13	2.19	0.43
1:B:5:ILE:N	1:B:189:GLU:O	2.50	0.43
1:A:49:THR:HG23	1:A:156:GLN:HB2	1.99	0.43
1:B:328:SER:O	1:B:332:ILE:HG13	2.19	0.43
1:B:239:HIS:N	1:B:263:ASN:HB3	2.34	0.43
1:B:375:TRP:NE1	1:B:392:GLU:OE1	2.52	0.42
1:B:276:ASP:HB3	1:B:281:TYR:CD2	2.54	0.42
1:A:5:ILE:HA	1:A:6:PRO:HD3	1.84	0.42
1:B:129:PRO:HG3	1:B:274:HIS:HA	2.01	0.42
1:B:221:LEU:HG	1:B:419:ALA:HB1	2.01	0.42
1:B:510:SER:O	1:B:511:ARG:HG3	2.19	0.42
1:A:184:GLY:N	1:A:202:VAL:HG13	2.34	0.42
1:B:100:THR:N	1:B:101:PRO:CD	2.83	0.42
1:A:406:ASP:HB3	1:A:409:TRP:HB3	2.02	0.42
1:A:351:MET:O	1:A:511:ARG:NH2	2.46	0.42
1:A:422:ASN:ND2	1:A:428:PHE:HA	2.35	0.42
1:B:39:LEU:HD21	1:B:74:ALA:CA	2.47	0.42
1:A:344:LEU:HD23	1:A:366:ILE:HG21	2.02	0.42
1:B:344:LEU:HB2	4:B:738:HOH:O	2.19	0.42
1:B:295:LYS:NZ	1:B:295:LYS:HB3	2.35	0.42
1:B:147:ALA:HB2	1:B:403:ARG:CB	2.50	0.42
1:B:493:ASP:O	1:B:495:SER:N	2.53	0.42
1:A:468:LYS:C	1:A:470:LYS:H	2.23	0.42
1:A:351:MET:HE2	1:A:511:ARG:HH21	1.85	0.42
1:B:163:LYS:HG2	1:B:163:LYS:O	2.19	0.42
1:A:33:ALA:HA	1:A:38:TYR:CD2	2.55	0.42
1:A:59:ASN:ND2	1:A:59:ASN:N	2.60	0.42
1:A:124:THR:CG2	1:A:310:ASP:HB3	2.48	0.41
1:B:512:ILE:C	1:B:513:ILE:HD12	2.41	0.41
1:A:29:LYS:HZ3	1:A:134:HIS:HA	1.82	0.41
1:A:147:ALA:HB2	1:A:403:ARG:HB3	2.02	0.41
1:B:61:LEU:HD22	1:B:87:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HZ1	1:A:134:HIS:HA	1.82	0.41
1:A:367:LYS:HD2	1:A:367:LYS:HA	1.87	0.41
1:B:211:GLN:HA	1:B:214:GLN:NE2	2.35	0.41
1:B:63:VAL:HA	1:B:121:ILE:O	2.20	0.41
1:B:133:GLU:HB2	1:B:134:HIS:CE1	2.55	0.41
1:B:30:VAL:O	1:B:33:ALA:N	2.54	0.41
1:A:207:GLN:HE21	1:A:207:GLN:CA	2.33	0.41
1:B:508:ASP:C	1:B:508:ASP:OD1	2.58	0.41
1:A:175:GLU:H	1:A:175:GLU:HG2	1.45	0.41
1:B:536:GLN:O	1:B:538:ILE:N	2.53	0.41
1:A:401:HIS:HE1	1:A:406:ASP:OD2	2.04	0.41
1:A:511:ARG:NH1	1:A:531:GLU:OE2	2.50	0.41
1:B:26:LEU:HD11	1:B:28:LYS:CE	2.50	0.41
1:A:53:ASP:O	1:A:57:PRO:HD3	2.20	0.41
1:B:364:ASN:N	1:B:364:ASN:HD22	2.18	0.41
1:B:375:TRP:HZ2	4:B:702:HOH:O	2.03	0.41
1:B:167:TYR:CE1	1:B:169:THR:OG1	2.73	0.41
1:B:277:PRO:CD	1:B:308:ASP:HB3	2.50	0.41
1:B:516:LEU:HD12	1:B:516:LEU:HA	1.85	0.41
1:A:226:PHE:HE2	1:A:256:CYS:HB3	1.86	0.41
1:A:475:GLU:HA	1:A:481:ASN:HB2	2.02	0.41
1:B:435:VAL:O	1:B:438:TYR:HB3	2.20	0.41
1:B:231:PHE:HD1	1:B:428:PHE:HZ	1.69	0.41
1:B:49:THR:HG23	1:B:156:GLN:CB	2.50	0.41
1:A:473:TYR:CE1	1:A:477:LEU:HD21	2.56	0.41
1:B:277:PRO:HD3	1:B:308:ASP:CA	2.51	0.41
1:B:329:LEU:HG	1:B:391:GLY:HA3	2.03	0.41
1:A:66:ASP:O	1:A:68:ARG:N	2.48	0.40
1:B:490:ASP:HA	1:B:491:PRO:HD3	1.90	0.40
1:B:44:GLN:HG2	1:B:167:TYR:CB	2.51	0.40
1:B:203:VAL:CG2	1:B:204:ASP:N	2.84	0.40
1:B:72:ARG:O	1:B:75:ILE:HB	2.22	0.40
1:B:331:VAL:HG11	1:B:414:TRP:CH2	2.57	0.40
1:A:241:VAL:O	1:A:244:PRO:HD2	2.22	0.40
1:B:211:GLN:HA	1:B:214:GLN:HE21	1.86	0.40
1:A:380:ASN:HA	1:A:380:ASN:HD22	1.69	0.40
1:A:550:ILE:O	1:A:554:LEU:HG	2.22	0.40
1:B:483:ALA:HA	1:B:503:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/572 (99%)	531 (94%)	28 (5%)	9 (2%)	12	16
1	B	568/572 (99%)	515 (91%)	44 (8%)	9 (2%)	12	16
All	All	1136/1144 (99%)	1046 (92%)	72 (6%)	18 (2%)	12	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	127	HIS
1	B	494	GLN
1	A	115	GLY
1	A	133	GLU
1	B	115	GLY
1	B	424	ASN
1	A	479	GLN
1	B	166	GLU
1	A	4	VAL
1	A	67	GLY
1	B	4	VAL
1	B	133	GLU
1	B	537	GLN
1	A	402	ILE
1	A	494	GLN
1	B	402	ILE
1	B	298	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	479/481 (100%)	463 (97%)	16 (3%)	45	66
1	B	479/481 (100%)	456 (95%)	23 (5%)	31	49
All	All	958/962 (100%)	919 (96%)	39 (4%)	37	57

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	59	ASN
1	A	97	LEU
1	A	116	ASN
1	A	175	GLU
1	A	182	GLN
1	A	205	THR
1	A	207	GLN
1	A	225	LEU
1	A	234	ARG
1	A	329	LEU
1	A	351	MET
1	A	367	LYS
1	A	393	GLU
1	A	505	VAL
1	A	516	LEU
1	B	51	ARG
1	B	91	HIS
1	B	134	HIS
1	B	139	ILE
1	B	142	ASN
1	B	187	LYS
1	B	205	THR
1	B	230	ASP
1	B	234	ARG
1	B	258	LYS
1	B	262	LEU
1	B	296	ASP
1	B	325	PRO
1	B	329	LEU
1	B	344	LEU
1	B	351	MET
1	B	389	LEU

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Mol	Chain	Res	Type
1	B	393	GLU
1	B	405	LYS
1	B	441	GLN
1	B	454	GLN
1	B	516	LEU
1	B	542	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	19	GLN
1	A	37	ASN
1	A	41	ASN
1	A	59	ASN
1	A	73	GLN
1	A	85	ASN
1	A	105	HIS
1	A	116	ASN
1	A	128	ASN
1	A	142	ASN
1	A	207	GLN
1	A	214	GLN
1	A	239	HIS
1	A	263	ASN
1	A	320	GLN
1	A	335	ASN
1	A	337	ASN
1	A	364	ASN
1	A	380	ASN
1	A	401	HIS
1	A	422	ASN
1	A	441	GLN
1	A	461	ASN
1	A	472	GLN
1	A	476	GLN
1	A	479	GLN
1	A	500	GLN
1	A	561	GLN
1	A	566	ASN
1	B	14	GLN
1	B	19	GLN

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Mol	Chain	Res	Type
1	B	37	ASN
1	B	44	GLN
1	B	48	ASN
1	B	85	ASN
1	B	91	HIS
1	B	142	ASN
1	B	179	ASN
1	B	207	GLN
1	B	214	GLN
1	B	263	ASN
1	B	314	ASN
1	B	320	GLN
1	B	335	ASN
1	B	337	ASN
1	B	364	ASN
1	B	380	ASN
1	B	422	ASN
1	B	461	ASN
1	B	472	GLN
1	B	479	GLN
1	B	481	ASN
1	B	561	GLN
1	B	566	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	SO4	A	601	2	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	A	603	-	4,4,4	0.19	0	6,6,6	0.09	0
3	SO4	B	602	2	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	B	604	-	4,4,4	0.23	0	6,6,6	0.10	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
3	SO4	A	601	2	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	2	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SO4	1	0

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	570/572 (99%)	0.27	22 (3%) 43 44	11, 29, 52, 85	0
1	B	570/572 (99%)	0.59	70 (12%) 5 5	10, 31, 54, 86	0
All	All	1140/1144 (99%)	0.43	92 (8%) 15 14	10, 30, 53, 86	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	VAL	8.0
1	A	522	VAL	7.6
1	B	521	SER	6.4
1	B	520	GLY	5.8
1	B	134	HIS	4.7
1	B	295	LYS	4.5
1	B	296	ASP	4.4
1	B	227	SER	4.4
1	B	426	ASP	4.2
1	A	121	ILE	4.0
1	B	519	THR	4.0
1	B	518	GLY	3.9
1	B	424	ASN	3.9
1	B	133	GLU	3.8
1	B	12	VAL	3.8
1	B	375	TRP	3.7
1	B	132	LYS	3.7
1	B	14	GLN	3.6
1	B	294	LYS	3.6
1	A	521	SER	3.6
1	A	544	THR	3.5
1	B	229	LYS	3.5
1	B	13	THR	3.5
1	B	496	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	23	THR	3.4
1	B	427	HIS	3.4
1	B	161	THR	3.4
1	A	63	VAL	3.3
1	B	495	SER	3.3
1	B	22	GLY	3.2
1	B	425	THR	3.2
1	B	16	TYR	3.2
1	B	33	ALA	3.1
1	B	3	GLN	3.1
1	A	375	TRP	3.1
1	A	139	ILE	3.0
1	B	114	VAL	3.0
1	B	196	SER	3.0
1	B	297	VAL	2.9
1	B	541	GLU	2.9
1	B	121	ILE	2.9
1	B	36	PRO	2.9
1	B	489	VAL	2.9
1	B	164	ILE	2.9
1	B	90	VAL	2.8
1	B	183	ILE	2.8
1	A	134	HIS	2.8
1	A	14	GLN	2.7
1	A	123	LEU	2.7
1	B	165	LYS	2.7
1	B	11	GLN	2.6
1	A	133	GLU	2.6
1	A	541	GLU	2.6
1	B	268	GLU	2.6
1	A	126	SER	2.5
1	B	17	ALA	2.5
1	A	193	LEU	2.5
1	A	426	ASP	2.5
1	B	35	GLN	2.5
1	B	256	CYS	2.4
1	B	494	GLN	2.4
1	B	492	VAL	2.4
1	A	519	THR	2.4
1	B	38	TYR	2.4
1	B	536	GLN	2.4
1	B	159	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	410	ALA	2.3
1	A	61	LEU	2.3
1	B	63	VAL	2.3
1	B	158	TYR	2.3
1	B	24	SER	2.3
1	B	253	LEU	2.3
1	B	182	GLN	2.3
1	B	61	LEU	2.2
1	B	135	GLY	2.2
1	B	87	ILE	2.2
1	A	100	THR	2.2
1	B	31	SER	2.1
1	A	122	ILE	2.1
1	B	122	ILE	2.1
1	B	272	GLY	2.1
1	B	176	LYS	2.1
1	B	163	LYS	2.1
1	B	156	GLN	2.1
1	A	229	LYS	2.1
1	B	539	GLN	2.0
1	B	223	LYS	2.0
1	B	10	VAL	2.0
1	B	69	TYR	2.0
1	B	222	LEU	2.0
1	A	78	ILE	2.0
1	B	9	ARG	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
3	SO4	B	602	5/5	0.93	0.23	0.32	71,73,77,80	0
3	SO4	A	603	5/5	0.97	0.13	-0.70	38,39,41,42	0
3	SO4	B	604	5/5	0.98	0.07	-1.09	47,47,52,54	0
3	SO4	A	601	5/5	0.98	0.12	-1.86	38,41,50,52	0
2	ZN	B	700	1/1	0.99	0.09	-2.09	33,33,33,33	0
2	ZN	A	700	1/1	0.99	0.11	-2.11	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.