Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:44 AM GMT

PDB ID : 2J50
Title : STRUCTURE OF AURORA-2 IN COMPLEX WITH PHA-739358
Authors : Cameron, A.D.; Izzo, G.; Storici, P.; Rusconi, L.; Fancelli, D.; Varasi, M.; Berta, D.; Bindi, S.; Forte, B.; Severino, D.; Tonani, R.; Vianello, P.
Deposited on : 2006-09-08
Resolution : 3.00 Å(reported)

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

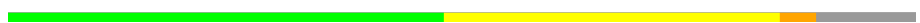|		
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.211
Clashscore		25
Ramachandran outliers		2.0%
Sidechain outliers		5.9%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
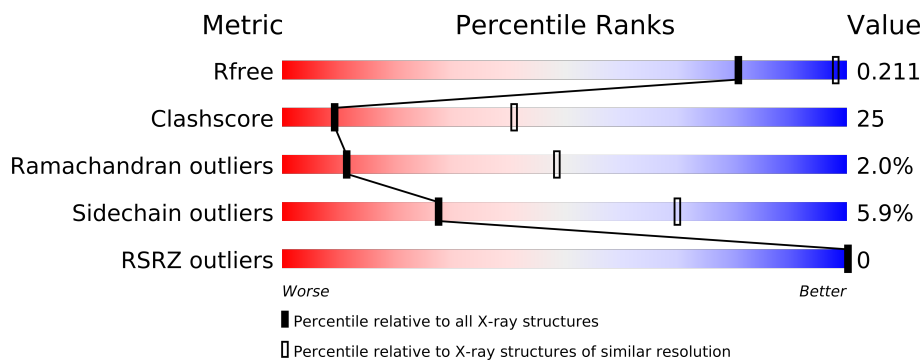
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol	Chain	Length	Quality of chain
1	A	280	
1	B	280	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4164 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SERINE/THREONINE-PROTEINKINASE 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	1
			2042	1318	352	367	5			
1	B	250	Total	C	N	O	S	0	0	1
			2042	1318	352	367	5			

- Molecule 2 is N-[(3E)-5-[(2R)-2-METHOXY-2-PHENYLACETYL]PYRROLO[3,4-C]PYRAZOL-3(5H)-YLIDENE]-4-(4-METHYLPIPERAZIN-1-YL)BENZAMIDE (three-letter code: 627) (formula: $C_{26}H_{26}N_6O_3$).
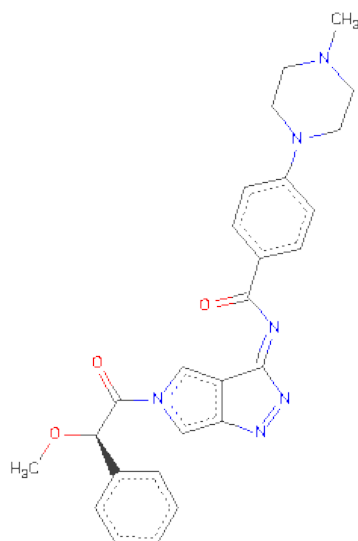
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	26	6	3		
2	B	1	Total	C	N	O	0	0
			35	26	6	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
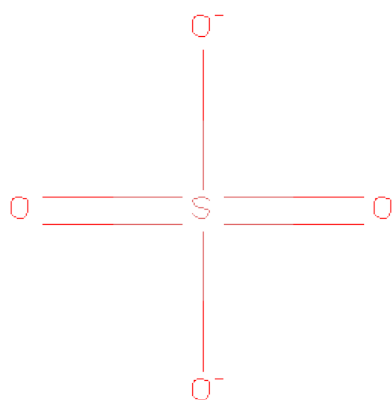
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
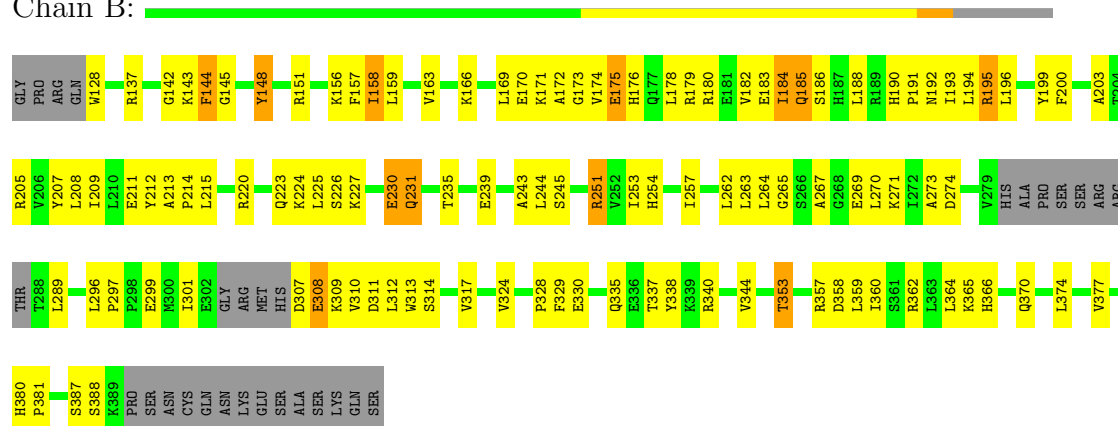
- Molecule 1: SERINE/THREONINE-PROTEINKINASE 6

Chain A:
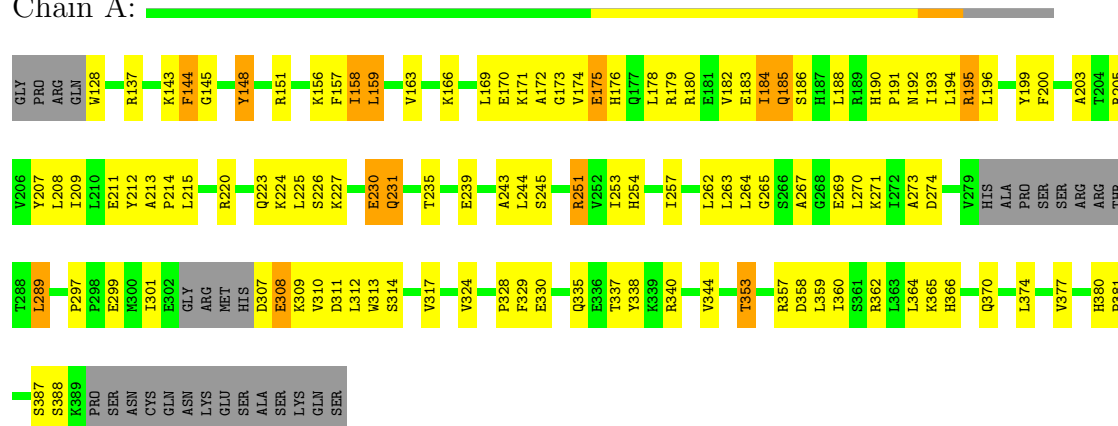
- Molecule 1: SERINE/THREONINE-PROTEINKINASE 6

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.69Å 86.78Å 86.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.53 – 3.00 28.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (28.53-3.00) 99.8 (28.53-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.00Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.221 , 0.268 0.219 , 0.211	Depositor DCC
R_{free} test set	616 reflections (5.48%)	DCC
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.1	EDS
Estimated twinning fraction	0.469 for -h,l,k	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 11861 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 627, 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	0.43	0/2091	0.64	0/2827
1	B	0.43	0/2091	0.64	0/2827
All	All	0.43	0/4182	0.64	0/5654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2042	0	2041	100	3
1	B	2042	0	2041	102	3
2	A	35	0	26	3	0
2	B	35	0	26	3	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
All	All	4164	0	4134	206	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (206) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:158:ILE:HD13	1:B:158:ILE:H	1.29	0.95
1:A:158:ILE:H	1:A:158:ILE:HD13	1.29	0.95
1:B:158:ILE:N	1:B:158:ILE:HD13	1.92	0.84
1:A:158:ILE:N	1:A:158:ILE:HD13	1.92	0.83
1:B:230:GLU:OE1	1:B:353:THR:HG21	1.81	0.81
1:A:230:GLU:OE1	1:A:353:THR:HG21	1.81	0.79
1:A:254:HIS:HB3	1:A:311:ASP:OD2	1.82	0.79
1:B:254:HIS:HB3	1:B:311:ASP:OD2	1.82	0.79
1:B:190:HIS:HE1	1:B:192:ASN:HD22	1.34	0.76
1:A:190:HIS:HE1	1:A:192:ASN:HD22	1.34	0.75
1:A:353:THR:O	1:A:357:ARG:HG3	1.92	0.70
1:B:353:THR:O	1:B:357:ARG:HG3	1.92	0.69
1:B:253:ILE:HG22	1:B:254:HIS:H	1.60	0.67
1:A:253:ILE:HG22	1:A:254:HIS:H	1.60	0.67
1:B:143:LYS:HB2	1:B:144:PHE:CE1	2.30	0.67
1:B:365:LYS:HG2	1:B:370:GLN:HB2	1.76	0.67
1:A:365:LYS:HG2	1:A:370:GLN:HB2	1.77	0.67
1:A:166:LYS:O	1:A:170:GLU:HG2	1.95	0.67
1:B:166:LYS:O	1:B:170:GLU:HG2	1.95	0.67
1:A:143:LYS:HB2	1:A:144:PHE:CE1	2.30	0.66
1:B:143:LYS:HG2	3:B:1391:SO4:O2	1.98	0.64
1:A:262:LEU:HD22	1:A:270:LEU:HD21	1.80	0.63
1:A:143:LYS:HG2	3:A:1391:SO4:O2	1.98	0.63
1:B:170:GLU:HA	1:B:175:GLU:CG	2.29	0.62
1:B:262:LEU:HD22	1:B:270:LEU:HD21	1.80	0.62
1:A:170:GLU:HA	1:A:175:GLU:CG	2.29	0.61
1:A:235:THR:O	1:A:239:GLU:HG3	2.01	0.60
1:B:235:THR:O	1:B:239:GLU:HG3	2.01	0.60
1:A:215:LEU:HB2	1:A:264:LEU:HB2	1.83	0.60
1:B:215:LEU:HB2	1:B:264:LEU:HB2	1.83	0.59
1:A:299:GLU:N	1:A:299:GLU:OE1	2.32	0.59
1:B:299:GLU:OE1	1:B:299:GLU:N	2.32	0.59
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.69	0.58
1:B:231:GLN:HE21	1:B:231:GLN:H	1.50	0.57
1:A:231:GLN:HE21	1:A:231:GLN:H	1.50	0.57
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.69	0.57
1:B:312:LEU:HD21	1:B:374:LEU:HD23	1.87	0.57
1:A:158:ILE:CD1	1:A:158:ILE:H	1.99	0.57
1:A:185:GLN:HA	1:A:188:LEU:HD12	1.87	0.57
1:A:312:LEU:HD21	1:A:374:LEU:HD23	1.87	0.57
1:B:253:ILE:HG22	1:B:254:HIS:N	2.20	0.56
1:B:173:GLY:HA2	1:B:175:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:GLY:HA2	1:A:175:GLU:OE1	2.05	0.56
1:B:185:GLN:HA	1:B:188:LEU:HD12	1.87	0.56
1:B:213:ALA:O	2:B:1390:627:H9	2.05	0.56
1:A:253:ILE:HG22	1:A:254:HIS:N	2.20	0.56
1:B:307:ASP:O	1:B:309:LYS:N	2.37	0.56
1:A:267:ALA:N	1:A:269:GLU:OE1	2.39	0.56
1:B:158:ILE:N	1:B:158:ILE:CD1	2.63	0.56
1:B:179:ARG:O	1:B:182:VAL:HG12	2.06	0.56
1:A:254:HIS:CD2	1:A:257:ILE:HG12	2.42	0.55
1:B:254:HIS:CD2	1:B:257:ILE:HG12	2.42	0.55
1:B:267:ALA:N	1:B:269:GLU:OE1	2.39	0.55
1:B:231:GLN:NE2	1:B:231:GLN:H	2.05	0.55
1:A:179:ARG:O	1:A:182:VAL:HG12	2.06	0.55
1:B:170:GLU:HA	1:B:175:GLU:HG3	1.88	0.55
1:A:213:ALA:O	2:A:1390:627:H9	2.05	0.55
1:A:170:GLU:HA	1:A:175:GLU:HG3	1.88	0.55
1:A:231:GLN:NE2	1:A:231:GLN:H	2.05	0.55
1:B:190:HIS:CG	1:B:191:PRO:HD2	2.42	0.55
1:A:158:ILE:CD1	1:A:158:ILE:N	2.63	0.55
1:B:231:GLN:N	1:B:231:GLN:NE2	2.55	0.55
1:A:231:GLN:N	1:A:231:GLN:NE2	2.55	0.54
1:A:307:ASP:O	1:A:309:LYS:N	2.37	0.54
1:A:190:HIS:CG	1:A:191:PRO:HD2	2.42	0.54
1:B:170:GLU:HA	1:B:175:GLU:HG2	1.90	0.54
1:B:195:ARG:HH11	1:B:195:ARG:HB2	1.73	0.53
1:A:170:GLU:HA	1:A:175:GLU:HG2	1.90	0.53
1:A:195:ARG:HB2	1:A:195:ARG:HH11	1.73	0.53
1:B:158:ILE:H	1:B:158:ILE:CD1	1.99	0.53
1:A:311:ASP:O	1:A:314:SER:HB2	2.09	0.53
1:B:311:ASP:O	1:B:314:SER:HB2	2.09	0.52
2:B:1390:627:H361	3:B:1391:SO4:O3	2.08	0.52
1:B:224:LYS:HG2	1:B:225:LEU:HD23	1.91	0.52
1:B:176:HIS:HB2	1:B:179:ARG:HH21	1.74	0.52
1:B:358:ASP:O	1:B:362:ARG:HG3	2.10	0.52
2:A:1390:627:H361	3:A:1391:SO4:O3	2.08	0.52
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.74	0.52
1:A:358:ASP:O	1:A:362:ARG:HG3	2.10	0.52
1:A:387:SER:OG	1:A:388:SER:N	2.42	0.52
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.74	0.52
1:B:227:LYS:HE2	1:B:324:VAL:O	2.11	0.51
1:A:224:LYS:HG2	1:A:225:LEU:HD23	1.91	0.51
1:A:180:ARG:O	1:A:183:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:HIS:HB2	1:A:179:ARG:HH21	1.74	0.51
1:B:180:ARG:O	1:B:183:GLU:HB2	2.11	0.51
1:B:254:HIS:HE1	1:B:274:ASP:OD1	1.93	0.51
1:A:263:LEU:HD12	1:A:273:ALA:HB2	1.92	0.51
1:B:387:SER:OG	1:B:388:SER:N	2.42	0.51
1:A:227:LYS:HE2	1:A:324:VAL:O	2.11	0.51
1:A:254:HIS:HE1	1:A:274:ASP:OD1	1.93	0.50
1:B:263:LEU:HD12	1:B:273:ALA:HB2	1.92	0.50
1:A:230:GLU:CD	1:A:353:THR:HG21	2.32	0.50
1:B:230:GLU:CD	1:B:353:THR:HG21	2.32	0.50
1:A:182:VAL:HG22	1:A:199:TYR:CD2	2.47	0.50
1:B:265:GLY:HA3	1:B:271:LYS:HE2	1.95	0.49
1:A:145:GLY:HA3	1:A:163:VAL:O	2.13	0.49
1:B:182:VAL:HG22	1:B:199:TYR:CD2	2.47	0.49
1:B:207:TYR:O	1:B:208:LEU:HD23	2.13	0.49
1:B:145:GLY:HA3	1:B:163:VAL:O	2.13	0.48
1:A:265:GLY:HA3	1:A:271:LYS:HE2	1.95	0.48
1:B:215:LEU:HG	1:B:265:GLY:O	2.13	0.48
1:A:297:PRO:HB3	1:A:313:TRP:CD1	2.48	0.48
1:B:215:LEU:HB2	1:B:264:LEU:CB	2.43	0.48
1:B:297:PRO:HB3	1:B:313:TRP:CD1	2.48	0.48
1:A:215:LEU:HG	1:A:265:GLY:O	2.13	0.48
1:A:329:PHE:O	1:A:337:THR:HG23	2.13	0.48
1:B:329:PHE:O	1:B:337:THR:HG23	2.13	0.48
1:A:359:LEU:HD11	1:A:377:VAL:HG13	1.96	0.48
1:A:207:TYR:O	1:A:208:LEU:HD23	2.13	0.48
1:B:297:PRO:HB3	1:B:313:TRP:CG	2.49	0.47
1:B:359:LEU:HD11	1:B:377:VAL:HG13	1.96	0.47
1:A:148:TYR:CD1	1:A:148:TYR:N	2.81	0.47
1:B:301:ILE:HD12	1:B:338:TYR:CD1	2.49	0.47
1:A:215:LEU:HB2	1:A:264:LEU:CB	2.43	0.47
1:A:297:PRO:HB3	1:A:313:TRP:CG	2.49	0.47
1:B:148:TYR:N	1:B:148:TYR:CD1	2.81	0.47
1:B:169:LEU:HD22	1:B:174:VAL:HG23	1.97	0.47
1:A:143:LYS:HB2	1:A:144:PHE:CD1	2.50	0.47
1:A:169:LEU:HD22	1:A:174:VAL:HG23	1.97	0.47
1:B:151:ARG:HA	1:B:157:PHE:O	2.15	0.47
1:A:301:ILE:HD12	1:A:338:TYR:CD1	2.49	0.47
1:A:200:PHE:HE2	1:A:209:ILE:HD11	1.80	0.46
1:A:151:ARG:HA	1:A:157:PHE:O	2.15	0.46
1:B:360:ILE:HG22	1:B:364:LEU:HD12	1.98	0.46
1:B:143:LYS:HB2	1:B:144:PHE:CD1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:LEU:HD22	1:A:273:ALA:HB1	1.98	0.45
1:A:360:ILE:HG22	1:A:364:LEU:HD12	1.98	0.45
1:B:200:PHE:HE2	1:B:209:ILE:HD11	1.80	0.45
1:B:335:GLN:CD	1:B:335:GLN:H	2.20	0.45
1:A:137:ARG:HH11	1:A:137:ARG:HG3	1.82	0.45
1:A:301:ILE:HD12	1:A:338:TYR:CE1	2.52	0.45
1:B:196:LEU:O	1:B:196:LEU:HG	2.17	0.45
1:A:335:GLN:CD	1:A:335:GLN:H	2.20	0.44
1:A:171:LYS:HD2	1:A:171:LYS:O	2.18	0.44
1:A:176:HIS:O	1:A:180:ARG:HG3	2.18	0.44
1:B:297:PRO:HG3	1:B:310:VAL:HG13	1.99	0.44
1:B:301:ILE:HD12	1:B:338:TYR:CE1	2.52	0.44
1:A:196:LEU:O	1:A:196:LEU:HG	2.17	0.44
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.82	0.44
1:B:176:HIS:O	1:B:180:ARG:HG3	2.18	0.44
1:B:179:ARG:O	1:B:183:GLU:HG2	2.18	0.44
1:B:194:LEU:HD22	1:B:273:ALA:HB1	1.98	0.44
1:A:212:TYR:O	1:A:214:PRO:HD3	2.18	0.44
1:A:179:ARG:O	1:A:183:GLU:HG2	2.18	0.44
1:B:172:ALA:O	1:B:174:VAL:HG13	2.18	0.44
1:B:182:VAL:CG1	1:B:183:GLU:N	2.81	0.44
1:A:297:PRO:HG3	1:A:310:VAL:HG13	1.99	0.44
1:A:317:VAL:HG13	1:A:328:PRO:HD2	2.00	0.44
2:B:1390:627:H221	2:B:1390:627:H10	1.78	0.43
1:B:317:VAL:HG13	1:B:328:PRO:HD2	2.00	0.43
1:B:205:ARG:HG2	1:B:205:ARG:HH11	1.83	0.43
1:A:182:VAL:CG1	1:A:183:GLU:N	2.81	0.43
1:B:212:TYR:O	1:B:214:PRO:HD3	2.18	0.43
1:B:171:LYS:HD2	1:B:171:LYS:O	2.17	0.43
1:A:172:ALA:O	1:A:174:VAL:HG13	2.18	0.43
1:A:194:LEU:HD22	1:A:273:ALA:CB	2.49	0.43
1:A:254:HIS:CE1	1:A:274:ASP:OD1	2.72	0.43
1:A:144:PHE:CD2	1:A:169:LEU:HD23	2.54	0.43
1:A:253:ILE:HG21	1:A:308:GLU:HA	2.01	0.42
1:A:193:ILE:HD11	1:A:243:ALA:HB1	2.01	0.42
1:A:169:LEU:HD11	1:A:178:LEU:HD22	2.01	0.42
1:B:220:ARG:NH1	1:B:223:GLN:NE2	2.67	0.42
2:A:1390:627:H10	2:A:1390:627:H221	1.78	0.42
1:A:205:ARG:HG2	1:A:205:ARG:HH11	1.83	0.42
1:B:220:ARG:HA	1:B:220:ARG:HD2	1.79	0.42
1:B:193:ILE:HD11	1:B:243:ALA:HB1	2.01	0.42
1:B:142:GLY:N	1:B:145:GLY:O	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:ARG:NH1	1:B:205:ARG:HG2	2.35	0.42
1:B:330:GLU:O	1:B:340:ARG:NH1	2.52	0.42
1:A:220:ARG:HA	1:A:220:ARG:HD2	1.79	0.42
1:B:254:HIS:CE1	1:B:274:ASP:OD1	2.72	0.42
1:B:192:ASN:OD1	1:B:239:GLU:HB3	2.19	0.42
1:A:220:ARG:NH1	1:A:223:GLN:NE2	2.67	0.42
1:B:144:PHE:CD2	1:B:169:LEU:HD23	2.54	0.42
1:B:194:LEU:HD22	1:B:273:ALA:CB	2.49	0.42
1:A:330:GLU:O	1:A:340:ARG:NH1	2.52	0.42
1:B:253:ILE:HG21	1:B:308:GLU:HA	2.01	0.42
1:B:151:ARG:HD2	1:B:156:LYS:O	2.20	0.42
1:A:225:LEU:O	1:A:226:SER:OG	2.34	0.42
1:B:169:LEU:HD11	1:B:178:LEU:HD22	2.01	0.41
1:A:205:ARG:NH1	1:A:205:ARG:HG2	2.35	0.41
1:A:344:VAL:HG21	1:A:366:HIS:HB2	2.01	0.41
1:A:192:ASN:OD1	1:A:239:GLU:HB3	2.19	0.41
1:A:151:ARG:HD2	1:A:156:LYS:C	2.40	0.41
1:A:230:GLU:CG	1:A:353:THR:HG21	2.51	0.41
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.88	0.41
1:B:230:GLU:CG	1:B:353:THR:HG21	2.51	0.41
1:A:244:LEU:HD13	1:A:311:ASP:HB3	2.02	0.41
1:B:309:LYS:HA	1:B:309:LYS:HD3	1.81	0.41
1:A:166:LYS:O	1:A:169:LEU:HB2	2.21	0.41
1:A:151:ARG:HD2	1:A:156:LYS:O	2.20	0.41
1:A:380:HIS:ND1	1:A:381:PRO:HD2	2.36	0.41
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.87	0.41
1:B:244:LEU:HD13	1:B:311:ASP:HB3	2.02	0.41
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.81	0.41
1:B:344:VAL:HG21	1:B:366:HIS:HB2	2.01	0.41
1:B:225:LEU:O	1:B:226:SER:OG	2.34	0.41
1:B:380:HIS:ND1	1:B:381:PRO:HD2	2.36	0.41
1:B:264:LEU:HA	1:B:269:GLU:O	2.21	0.40
1:A:157:PHE:CD2	1:A:159:LEU:HD23	2.56	0.40
1:B:151:ARG:HD2	1:B:156:LYS:C	2.40	0.40
1:B:380:HIS:HA	1:B:381:PRO:HD3	1.95	0.40
1:A:184:ILE:O	1:A:186:SER:N	2.54	0.40
1:B:184:ILE:O	1:B:186:SER:N	2.54	0.40
1:B:166:LYS:O	1:B:169:LEU:HB2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:GLN:OE1	1:B:223:GLN:OE1[1_455]	1.76	0.44
1:A:224:LYS:O	1:B:370:GLN:NE2[3_655]	1.98	0.22
1:A:370:GLN:NE2	1:B:224:LYS:O[2_664]	1.99	0.21

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	244/280 (87%)	216 (88%)	23 (9%)	5 (2%)	11	48
1	B	244/280 (87%)	216 (88%)	23 (9%)	5 (2%)	11	48
All	All	488/560 (87%)	432 (88%)	46 (9%)	10 (2%)	11	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	GLU
1	B	308	GLU
1	A	185	GLN
1	A	203	ALA
1	B	185	GLN
1	B	203	ALA
1	A	289	LEU
1	B	289	LEU
1	A	184	ILE
1	B	184	ILE

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	219/247 (89%)	206 (94%)	13 (6%)	28	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	219/247 (89%)	206 (94%)	13 (6%)	28	70
All	All	438/494 (89%)	412 (94%)	26 (6%)	28	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	TRP
1	A	144	PHE
1	A	148	TYR
1	A	158	ILE
1	A	159	LEU
1	A	175	GLU
1	A	195	ARG
1	A	211	GLU
1	A	230	GLU
1	A	231	GLN
1	A	245	SER
1	A	251	ARG
1	A	353	THR
1	B	128	TRP
1	B	144	PHE
1	B	148	TYR
1	B	158	ILE
1	B	159	LEU
1	B	175	GLU
1	B	195	ARG
1	B	211	GLU
1	B	230	GLU
1	B	231	GLN
1	B	245	SER
1	B	251	ARG
1	B	353	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	177	GLN
1	A	185	GLN
1	A	192	ASN
1	A	223	GLN

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Mol	Chain	Res	Type
1	A	231	GLN
1	A	242	ASN
1	A	254	HIS
1	A	367	ASN
1	A	386	ASN
1	B	154	GLN
1	B	177	GLN
1	B	185	GLN
1	B	192	ASN
1	B	223	GLN
1	B	231	GLN
1	B	242	ASN
1	B	254	HIS
1	B	367	ASN
1	B	386	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	627	A	1390	-	39,39,39	3.00	20 (51%)	52,55,55	2.42	15 (28%)
3	SO4	A	1391	-	4,4,4	2.43	4 (100%)	6,6,6	0.44	0
2	627	B	1390	-	39,39,39	3.00	18 (46%)	52,55,55	2.42	15 (28%)
3	SO4	B	1391	-	4,4,4	2.43	4 (100%)	6,6,6	0.44	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	627	A	1390	-	-	0/21/45/45	0/3/5/5
3	SO4	A	1391	-	-	0/0/0/0	0/0/0/0
2	627	B	1390	-	-	0/21/45/45	0/3/5/5
3	SO4	B	1391	-	-	0/0/0/0	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1390	627	C15-C14	7.56	1.48	1.38
2	A	1390	627	C15-C14	7.54	1.48	1.38
2	A	1390	627	C16-C13	7.38	1.50	1.38
2	B	1390	627	C16-C13	7.36	1.50	1.38
2	A	1390	627	C13-N2	-5.68	1.32	1.38
2	B	1390	627	C13-N2	-5.66	1.32	1.38
2	A	1390	627	C16-N1	5.35	1.47	1.39
2	B	1390	627	C16-N1	5.29	1.47	1.39
2	A	1390	627	C20-C25	5.07	1.61	1.54
2	B	1390	627	C20-C25	5.07	1.61	1.54
2	B	1390	627	C14-C13	-4.50	1.34	1.41
2	A	1390	627	C14-C13	-4.49	1.34	1.41
2	B	1390	627	C15-N1	4.20	1.46	1.39
2	A	1390	627	C15-N1	4.19	1.46	1.39
2	A	1390	627	C18-N17	3.85	1.52	1.46
2	B	1390	627	C18-N17	3.80	1.52	1.46
2	A	1390	627	C24-N17	3.13	1.47	1.38
2	B	1390	627	C24-N17	3.11	1.47	1.38
2	B	1390	627	C11-C24	3.02	1.45	1.39
2	A	1390	627	C11-C24	3.01	1.45	1.39
2	A	1390	627	C10-C24	2.97	1.45	1.39
2	B	1390	627	C10-C24	2.96	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1390	627	C12-C7	2.78	1.44	1.39
2	A	1390	627	C12-C7	2.77	1.44	1.39
2	B	1390	627	C22-N17	2.74	1.50	1.46
2	A	1390	627	C22-N17	2.68	1.50	1.46
2	B	1390	627	C29-C27	2.67	1.43	1.39
2	A	1390	627	C29-C27	2.67	1.43	1.39
3	A	1391	SO4	O2-S	2.63	1.55	1.47
3	B	1391	SO4	O2-S	2.63	1.55	1.47
2	B	1390	627	O34-C20	2.56	1.46	1.41
2	A	1390	627	O34-C20	2.51	1.46	1.41
3	B	1391	SO4	O4-S	2.48	1.55	1.47
3	A	1391	SO4	O4-S	2.47	1.55	1.47
3	A	1391	SO4	O1-S	2.43	1.55	1.47
3	B	1391	SO4	O1-S	2.42	1.54	1.47
3	B	1391	SO4	O3-S	2.20	1.54	1.47
3	A	1391	SO4	O3-S	2.19	1.54	1.47
2	B	1390	627	C7-C6	2.15	1.52	1.49
2	A	1390	627	C7-C6	2.10	1.52	1.49
2	A	1390	627	C14-C3	-2.09	1.42	1.47
2	B	1390	627	C14-C3	-2.08	1.42	1.47
2	A	1390	627	C27-C20	2.06	1.55	1.51
2	B	1390	627	C27-C20	2.04	1.55	1.51
2	A	1390	627	C10-C9	2.03	1.42	1.38
2	A	1390	627	C28-C27	2.01	1.42	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1390	627	N5-C3-N4	-7.11	117.83	129.58
2	B	1390	627	N5-C3-N4	-7.10	117.84	129.58
2	A	1390	627	C14-C3-N5	5.72	135.14	122.95
2	B	1390	627	C14-C3-N5	5.71	135.14	122.95
2	B	1390	627	C16-N1-C15	5.44	110.33	108.13
2	A	1390	627	C16-N1-C15	5.38	110.30	108.13
2	A	1390	627	C13-N2-N4	5.26	112.35	109.23
2	B	1390	627	C13-N2-N4	5.23	112.33	109.23
2	A	1390	627	C14-C13-N2	-5.09	108.29	112.68
2	B	1390	627	C14-C13-N2	-5.07	108.31	112.68
2	A	1390	627	C21-C22-N17	4.96	119.96	110.62
2	B	1390	627	C21-C22-N17	4.95	119.94	110.62
2	B	1390	627	C19-C18-N17	4.69	119.45	110.62
2	A	1390	627	C19-C18-N17	4.66	119.40	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1390	627	C6-N5-C3	3.84	128.60	123.12
2	B	1390	627	C6-N5-C3	3.82	128.58	123.12
2	B	1390	627	C14-C15-N1	-2.97	102.22	111.00
2	A	1390	627	C14-C15-N1	-2.96	102.26	111.00
2	B	1390	627	C16-C13-C14	-2.69	106.96	111.12
2	A	1390	627	C16-C13-C14	-2.68	106.98	111.12
2	A	1390	627	C18-C19-N20	2.48	113.56	110.82
2	B	1390	627	C18-C19-N20	2.45	113.53	110.82
2	A	1390	627	C36-O34-C20	2.44	115.28	112.81
2	B	1390	627	C36-O34-C20	2.44	115.28	112.81
2	B	1390	627	C10-C24-N17	2.43	124.84	121.37
2	B	1390	627	C15-C14-C13	2.42	114.86	111.12
2	A	1390	627	C15-C14-C13	2.41	114.85	111.12
2	A	1390	627	C10-C24-N17	2.40	124.80	121.37
2	A	1390	627	C22-C21-N20	2.07	113.11	110.82
2	B	1390	627	C22-C21-N20	2.07	113.11	110.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/280 (89%)	-0.26	0	100	100	33, 62, 107, 138	0
1	B	250/280 (89%)	-0.23	0	100	100	33, 62, 107, 138	0
All	All	500/560 (89%)	-0.25	0	100	100	33, 62, 108, 138	0

There are no RSRZ outliers to report.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	627	A	1390	35/35	0.23	0.88	51,51,51,51	0
2	627	B	1390	35/35	0.23	0.67	51,51,51,51	0
3	SO4	A	1391	5/5	0.17	-0.79	73,73,73,73	0
3	SO4	B	1391	5/5	0.15	-1.28	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.