



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:56 PM GMT

PDB ID : 4K0V
Title : Structural basis for angiopoietin-1 mediated signaling initiation
Authors : Yu, X.; Seegar, T.C.M.; Dalton, A.C.; Tzvetkova-Robev, D.; Goldgur, Y.;
Nikolov, D.B.; Barton, W.A.
Deposited on : 2013-04-04
Resolution : 4.51 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 ⓘ symbol.

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

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

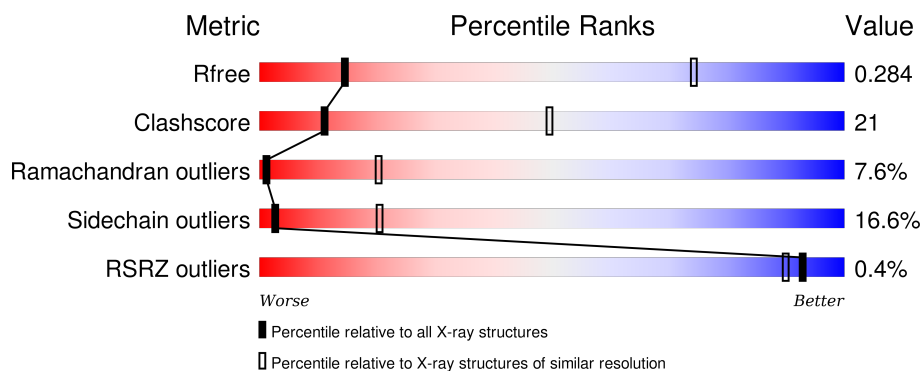
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

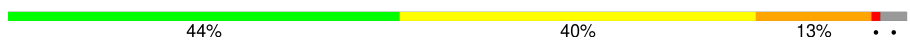

The reported resolution of this entry is 4.51 Å.

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	1071 (5.40-3.60)
Clashscore	102246	1004 (5.40-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	529	 44% 40% 13% . .
2	B	230	 % 52% 35% 7% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5775 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 TEK tyrosine kinase variant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4021	2532	713	736	40			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	GLY	-	EXPRESSION TAG	UNP Q59HG2
A	544	SER	-	EXPRESSION TAG	UNP Q59HG2
A	545	ALA	-	EXPRESSION TAG	UNP Q59HG2
A	546	SER	-	EXPRESSION TAG	UNP Q59HG2
A	547	GLY	-	EXPRESSION TAG	UNP Q59HG2
A	548	LEU	-	EXPRESSION TAG	UNP Q59HG2
A	549	VAL	-	EXPRESSION TAG	UNP Q59HG2
A	550	PRO	-	EXPRESSION TAG	UNP Q59HG2
A	551	ARG	-	EXPRESSION TAG	UNP Q59HG2

- Molecule 2 is a protein called Angiopoietin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1754	1115	304	319	16			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	EXPRESSION TAG	UNP Q15389
B	-3	GLU	-	EXPRESSION TAG	UNP Q15389
B	-2	LEU	-	EXPRESSION TAG	UNP Q15389
B	-1	ALA	-	EXPRESSION TAG	UNP Q15389
B	0	SER	-	EXPRESSION TAG	UNP Q15389
B	220	GLY	-	EXPRESSION TAG	UNP Q15389
B	221	SER	-	EXPRESSION TAG	UNP Q15389

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	LEU	-	EXPRESSION TAG	UNP Q15389
B	223	VAL	-	EXPRESSION TAG	UNP Q15389
B	224	PRO	-	EXPRESSION TAG	UNP Q15389
B	225	ARG	-	EXPRESSION TAG	UNP Q15389

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	189.53Å 189.53Å 334.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.01 – 4.51 30.01 – 4.51	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.01-4.51) 91.9 (30.01-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 4.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.248 , 0.288 0.241 , 0.284	Depositor DCC
R_{free} test set	516 reflections (3.03%)	DCC
Wilson B-factor (Å ²)	141.8	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 178.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 18062 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5775	wwPDB-VP
Average B, all atoms (Å ²)	229.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.56	0/4126	0.79	2/5600 (0.0%)
2	B	0.49	0/1806	0.68	0/2433
All	All	0.54	0/5932	0.76	2/8033 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	500	GLU	N-CA-C	5.41	125.62	111.00
1	A	178	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	467	SER	Peptide

5.2 Too-close contacts [i](#)

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	4021	0	3909	182	0
2	B	1754	0	1642	57	0
All	All	5775	0	5551	235	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 21.

All (235) 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:373:SER:OG	1:A:374:GLY:N	2.04	0.89
1:A:463:ILE:HD11	1:A:481:LEU:HD11	1.58	0.86
2:B:156:CYS:HB2	2:B:172:ALA:HA	1.57	0.86
1:A:450:ALA:HA	1:A:530:PRO:HB3	1.60	0.83
2:B:59:GLN:NE2	2:B:181:MET:SD	2.52	0.83
1:A:197:ASN:HB3	1:A:199:PHE:H	1.45	0.81
1:A:371:LYS:HG3	1:A:406:VAL:HG22	1.65	0.78
1:A:50:ARG:CZ	1:A:438:ASN:HD21	1.98	0.77
1:A:59:ARG:NH2	1:A:95:LYS:O	2.18	0.77
1:A:155:ILE:HG22	1:A:162:ILE:HD12	1.68	0.73
2:B:71:ASN:ND2	2:B:73:SER:OG	2.19	0.73
1:A:58:GLY:HA2	1:A:72:LEU:HD21	1.72	0.71
1:A:402:ASP:OD1	1:A:403:HIS:ND1	2.22	0.70
2:B:108:SER:HG	2:B:129:HIS:HE2	1.37	0.70
1:A:24:MET:SD	1:A:106:VAL:HG21	2.33	0.69
1:A:68:HIS:HB3	1:A:95:LYS:HD3	1.76	0.68
1:A:482:LEU:HD23	1:A:514:GLU:HB2	1.77	0.67
1:A:462:VAL:HG22	1:A:501:ILE:HG12	1.75	0.67
1:A:482:LEU:HA	1:A:491:ALA:HB1	1.77	0.66
1:A:445:PRO:HD3	1:A:519:LEU:HG	1.76	0.65
1:A:468:GLU:H	1:A:469:PRO:HD2	1.61	0.65
1:A:33:PRO:HA	1:A:117:LYS:HD2	1.79	0.65
1:A:130:THR:HG22	1:A:205:ARG:HB3	1.79	0.64
1:A:465:ILE:HB	1:A:498:THR:O	1.97	0.64
1:A:244:PRO:HD3	1:A:281:LEU:HD11	1.78	0.64
1:A:156:TYR:HB2	1:A:190:SER:HB2	1.80	0.64
1:A:126:PRO:HD3	1:A:202:ALA:HB1	1.80	0.64
1:A:359:ILE:HB	1:A:439:ILE:HA	1.79	0.64
1:A:150:GLU:HG3	1:A:167:ARG:HD3	1.80	0.63
2:B:147:SER:HB2	2:B:170:PHE:HD2	1.64	0.63
1:A:366:PHE:HB3	1:A:411:ILE:HD12	1.80	0.62
1:A:270:GLY:O	1:A:273:GLY:N	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:H	1:A:72:LEU:HD23	1.65	0.62
1:A:465:ILE:HG12	1:A:515:LEU:HD22	1.82	0.61
2:B:25:ILE:HB	2:B:28:MET:HG3	1.80	0.61
1:A:348:MET:HG3	1:A:375:TRP:H	1.64	0.61
2:B:140:ILE:HD13	2:B:171:ASP:HB2	1.83	0.61
1:A:52:HIS:HB3	1:A:82:TRP:CE2	2.35	0.60
1:A:513:TYR:O	1:A:531:GLY:HA2	2.01	0.60
2:B:40:VAL:O	2:B:42:GLY:N	2.35	0.60
2:B:178:LEU:HG	2:B:210:THR:HG21	1.84	0.60
1:A:59:ARG:HH12	1:A:70:ASP:HB3	1.66	0.60
1:A:234:HIS:CE1	1:A:236:ASP:HB2	2.37	0.59
1:A:32:LEU:O	1:A:117:LYS:NZ	2.36	0.58
1:A:241:ILE:HD13	1:A:282:PRO:HB2	1.84	0.58
2:B:78:LEU:HD23	2:B:83:ILE:HG13	1.86	0.58
1:A:492:TRP:O	1:A:493:GLN:HB2	2.03	0.58
1:A:136:GLY:HA2	1:A:180:HIS:HA	1.86	0.58
1:A:483:TYR:CD1	1:A:491:ALA:HA	2.39	0.57
1:A:67:GLN:NE2	1:A:99:ALA:H	2.02	0.57
1:A:59:ARG:NH1	1:A:70:ASP:HB3	2.20	0.57
1:A:348:MET:O	1:A:376:PRO:HD2	2.05	0.57
1:A:451:PRO:O	1:A:532:PRO:HG3	2.04	0.56
1:A:451:PRO:HD2	1:A:531:GLY:H	1.70	0.56
1:A:489:TYR:HD1	1:A:490:GLU:H	1.54	0.56
1:A:35:VAL:HG11	1:A:93:ALA:HB1	1.86	0.56
1:A:310:ASP:HB2	1:A:312:LYS:HG3	1.87	0.56
2:B:145:ASP:N	2:B:145:ASP:OD1	2.37	0.56
1:A:33:PRO:HG3	1:A:129:LEU:HD21	1.88	0.56
1:A:535:ARG:HG2	1:A:536:PHE:H	1.71	0.56
1:A:510:ARG:HA	1:A:534:ARG:O	2.06	0.55
2:B:190:GLY:HA2	2:B:204:SER:HB2	1.89	0.55
1:A:25:ASP:HB3	1:A:47:SER:HB2	1.89	0.55
1:A:355:LEU:HD12	1:A:356:PRO:CD	2.37	0.55
1:A:529:HIS:H	1:A:530:PRO:HD2	1.72	0.54
1:A:350:PRO:HG3	1:A:428:THR:HG23	1.89	0.53
1:A:232:VAL:HG11	1:A:284:PRO:O	2.09	0.53
1:A:380:ASN:HB3	1:A:398:PHE:CD1	2.43	0.53
1:A:373:SER:HG	1:A:374:GLY:H	1.50	0.53
1:A:154:VAL:HG22	1:A:192:ARG:O	2.09	0.53
1:A:359:ILE:HG21	1:A:439:ILE:HG12	1.90	0.53
1:A:369:ILE:HG12	1:A:408:ILE:HG22	1.90	0.53
1:A:186:ALA:HB1	1:A:206:LEU:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:NZ	1:A:170:VAL:O	2.40	0.52
1:A:23:ALA:HB3	1:A:24:MET:SD	2.48	0.52
1:A:153:ALA:HB3	1:A:165:VAL:HB	1.92	0.52
2:B:29:PRO:O	2:B:30:GLU:HB2	2.09	0.52
2:B:24:TYR:CD2	2:B:31:PRO:HB3	2.45	0.51
2:B:62:TRP:O	2:B:66:LYS:N	2.43	0.51
1:A:397:ASP:HB3	1:A:408:ILE:HD11	1.93	0.51
1:A:307:TYR:HB2	1:A:324:ASP:O	2.10	0.51
1:A:128:THR:O	1:A:204:THR:OG1	2.25	0.51
1:A:400:HIS:ND1	1:A:401:THR:O	2.44	0.51
1:A:535:ARG:HG2	1:A:536:PHE:N	2.25	0.51
1:A:279:PHE:HE1	1:A:290:ALA:HB2	1.76	0.51
1:A:423:VAL:HG13	1:A:435:LYS:O	2.10	0.51
1:A:182:GLN:O	1:A:185:ASP:HB3	2.11	0.51
1:A:23:ALA:HB1	1:A:106:VAL:HG11	1.94	0.51
1:A:422:TRP:CD1	1:A:439:ILE:HD12	2.46	0.51
1:A:423:VAL:HG22	1:A:436:PRO:HB3	1.92	0.50
2:B:47:VAL:HG22	2:B:213:MET:HE2	1.93	0.50
1:A:107:ARG:HD2	1:A:389:ASP:OD1	2.11	0.50
1:A:131:MET:HB3	1:A:206:LEU:HD23	1.94	0.50
2:B:66:LYS:NZ	2:B:118:GLU:OE1	2.23	0.50
1:A:483:TYR:HE2	1:A:502:VAL:HG11	1.76	0.50
1:A:50:ARG:NH2	1:A:438:ASN:HD21	2.10	0.50
1:A:359:ILE:HG22	1:A:360:GLU:N	2.27	0.50
2:B:4:PHE:CE1	2:B:10:VAL:HG22	2.48	0.49
1:A:401:THR:OG1	1:A:402:ASP:N	2.44	0.49
2:B:80:ASN:HB3	2:B:122:TYR:CD2	2.48	0.49
1:A:197:ASN:HB3	1:A:200:THR:H	1.77	0.49
1:A:161:PHE:HE1	2:B:191:LYS:HD3	1.77	0.49
2:B:159:LYS:HB3	2:B:162:LEU:HD12	1.95	0.49
1:A:480:LYS:HD2	1:A:492:TRP:HZ3	1.78	0.49
2:B:8:ALA:O	2:B:12:GLN:HG2	2.13	0.49
1:A:43:THR:HG23	1:A:85:LYS:HB3	1.95	0.48
1:A:59:ARG:HB2	1:A:61:PHE:CE1	2.47	0.48
1:A:68:HIS:ND1	1:A:95:LYS:HD2	2.28	0.48
1:A:387:LYS:O	1:A:390:GLY:N	2.46	0.48
2:B:100:ASP:OD2	2:B:201:LYS:HE2	2.14	0.48
2:B:150:ASP:OD1	2:B:150:ASP:N	2.45	0.48
2:B:164:LEU:HB3	2:B:177:ASN:HD22	1.79	0.48
2:B:184:THR:OG1	2:B:187:GLN:OE1	2.30	0.48
1:A:192:ARG:NE	1:A:197:ASN:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:VAL:HG12	1:A:500:GLU:OE2	2.13	0.48
1:A:451:PRO:HB3	1:A:515:LEU:HD11	1.95	0.48
1:A:345:ILE:O	1:A:345:ILE:HD12	2.14	0.48
1:A:375:TRP:C	1:A:377:LEU:N	2.67	0.47
1:A:165:VAL:HG11	1:A:170:VAL:HA	1.95	0.47
1:A:68:HIS:HB3	1:A:95:LYS:CD	2.44	0.47
1:A:484:LYS:HE3	1:A:512:GLU:OE1	2.15	0.47
1:A:473:ASP:O	1:A:519:LEU:HD21	2.14	0.47
1:A:387:LYS:HG3	1:A:422:TRP:CZ3	2.49	0.47
2:B:149:LYS:O	2:B:162:LEU:HD21	2.14	0.47
1:A:125:LEU:HA	1:A:126:PRO:HD2	1.64	0.47
2:B:68:GLY:HA3	2:B:78:LEU:O	2.15	0.47
2:B:115:ILE:HD12	2:B:122:TYR:HB3	1.96	0.47
1:A:151:GLU:OE2	2:B:157:MET:HE3	2.15	0.47
2:B:181:MET:HB2	2:B:193:ASN:O	2.15	0.47
1:A:387:LYS:HD2	1:A:393:LEU:HD11	1.97	0.47
1:A:46:ALA:HB3	1:A:82:TRP:HD1	1.80	0.47
2:B:162:LEU:HG	2:B:162:LEU:H	1.45	0.47
1:A:209:ARG:CB	1:A:235:GLU:HG2	2.45	0.47
1:A:292:GLY:HA2	1:A:325:ARG:O	2.14	0.47
1:A:366:PHE:O	1:A:368:PRO:HD3	2.15	0.47
1:A:76:GLN:HE21	1:A:82:TRP:HZ3	1.63	0.47
1:A:416:PRO:N	1:A:417:PRO:HD2	2.30	0.47
1:A:147:LEU:O	1:A:193:TYR:HE1	1.97	0.47
1:A:447:PRO:HB3	1:A:467:SER:OG	2.15	0.47
1:A:480:LYS:HD2	1:A:492:TRP:CZ3	2.50	0.46
1:A:364:GLY:O	1:A:414:ILE:HG22	2.15	0.46
1:A:155:ILE:CG2	1:A:162:ILE:HD12	2.44	0.46
2:B:200:PHE:CE2	2:B:201:LYS:HG2	2.49	0.46
1:A:162:ILE:O	2:B:192:LEU:HD12	2.16	0.46
2:B:100:ASP:OD1	2:B:104:ASN:HB2	2.15	0.46
1:A:197:ASN:C	1:A:199:PHE:H	2.18	0.46
2:B:98:LEU:HD22	2:B:207:LEU:HD13	1.98	0.46
2:B:183:TYR:CE2	2:B:191:LYS:HB3	2.51	0.46
1:A:153:ALA:O	1:A:164:SER:HB2	2.15	0.45
1:A:352:ILE:HD11	1:A:426:VAL:HG23	1.98	0.45
1:A:426:VAL:HB	1:A:433:VAL:HG23	1.99	0.45
1:A:345:ILE:HD11	1:A:375:TRP:CZ2	2.51	0.45
1:A:375:TRP:C	1:A:377:LEU:H	2.20	0.45
2:B:187:GLN:O	2:B:189:HIS:N	2.50	0.45
1:A:312:LYS:HB3	1:A:312:LYS:HE2	1.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:HG22	1:A:116:MET:H	1.82	0.45
1:A:163:HIS:HB2	2:B:203:PRO:HB2	1.99	0.45
1:A:34:LEU:HD23	1:A:118:MET:HG3	1.99	0.45
1:A:468:GLU:H	1:A:469:PRO:CD	2.29	0.45
1:A:32:LEU:HD22	1:A:297:GLN:NE2	2.32	0.45
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.72	0.45
1:A:197:ASN:HB3	1:A:199:PHE:N	2.24	0.44
2:B:84:PHE:CZ	2:B:117:ASN:HB3	2.52	0.44
1:A:466:SER:H	1:A:515:LEU:CD1	2.30	0.44
1:A:28:LEU:HD23	1:A:102:CYS:SG	2.58	0.44
2:B:25:ILE:HD12	2:B:82:PHE:HD2	1.82	0.44
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.70	0.44
1:A:377:LEU:HA	1:A:378:PRO:HD2	1.62	0.44
2:B:68:GLY:HA2	2:B:77:TRP:HD1	1.83	0.44
2:B:17:LYS:HG3	2:B:18:SER:N	2.33	0.44
2:B:96:ILE:HG12	2:B:212:MET:HG2	1.99	0.44
1:A:275:LYS:HG3	1:A:293:TRP:CZ3	2.52	0.44
1:A:476:ILE:HG12	1:A:517:VAL:CG1	2.48	0.44
1:A:119:ARG:HE	1:A:200:THR:HA	1.82	0.44
1:A:448:LEU:CB	1:A:469:PRO:HB2	2.48	0.43
1:A:67:GLN:HE22	1:A:99:ALA:H	1.62	0.43
1:A:157:LYS:HG2	1:A:158:ASN:N	2.32	0.43
2:B:124:LEU:HB2	2:B:169:TRP:CD1	2.53	0.43
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.67	0.43
1:A:145:LYS:NZ	1:A:171:PRO:O	2.35	0.43
1:A:131:MET:O	1:A:207:ILE:HG13	2.19	0.43
2:B:183:TYR:HB2	2:B:206:SER:CB	2.49	0.43
1:A:163:HIS:CG	1:A:164:SER:N	2.87	0.43
1:A:456:THR:HG22	1:A:457:GLY:N	2.32	0.43
1:A:156:TYR:O	1:A:190:SER:N	2.47	0.43
1:A:133:VAL:O	1:A:208:VAL:HA	2.19	0.43
1:A:245:GLY:O	1:A:255:CYS:HB2	2.19	0.43
1:A:76:GLN:NE2	1:A:82:TRP:HZ3	2.17	0.43
2:B:121:ASN:HB3	2:B:145:ASP:HB3	2.00	0.43
1:A:47:SER:OG	1:A:266:GLU:OE2	2.36	0.43
2:B:25:ILE:HB	2:B:28:MET:CG	2.46	0.42
1:A:90:ARG:HE	1:A:90:ARG:HB3	1.48	0.42
1:A:30:ASN:HA	1:A:42:LEU:HD12	2.01	0.42
1:A:448:LEU:CD2	1:A:469:PRO:HB2	2.48	0.42
2:B:138:SER:HB2	2:B:197:TRP:CE2	2.53	0.42
1:A:225:THR:HG22	1:A:250:THR:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HB	2:B:28:MET:HB2	2.01	0.42
1:A:442:LYS:HD2	1:A:442:LYS:HA	1.74	0.42
1:A:386:VAL:HG22	1:A:423:VAL:O	2.20	0.42
1:A:74:VAL:HG12	1:A:84:LYS:HB3	2.02	0.42
1:A:194:ILE:HG23	1:A:195:GLY:H	1.84	0.42
1:A:444:LEU:H	1:A:444:LEU:HG	1.65	0.42
1:A:450:ALA:O	1:A:466:SER:HB2	2.20	0.42
1:A:52:HIS:HB3	1:A:82:TRP:CD2	2.55	0.42
1:A:456:THR:HG22	1:A:457:GLY:H	1.85	0.42
1:A:216:TRP:CE2	1:A:238:GLY:HA3	2.55	0.42
1:A:482:LEU:HD12	1:A:491:ALA:CB	2.50	0.42
1:A:65:MET:HG2	1:A:158:ASN:O	2.20	0.42
2:B:56:LEU:HD21	2:B:69:PHE:CD1	2.55	0.42
1:A:33:PRO:HD2	1:A:297:GLN:NE2	2.35	0.41
1:A:40:THR:OG1	1:A:117:LYS:HE3	2.20	0.41
1:A:360:GLU:HA	1:A:440:SER:O	2.19	0.41
1:A:235:GLU:H	1:A:235:GLU:HG3	1.59	0.41
1:A:478:SER:HB3	1:A:518:GLN:OE1	2.18	0.41
1:A:197:ASN:CB	1:A:200:THR:H	2.33	0.41
1:A:274:CYS:C	1:A:276:SER:H	2.23	0.41
1:A:50:ARG:NH1	1:A:438:ASN:HD21	2.17	0.41
1:A:445:PRO:HB2	1:A:517:VAL:HB	2.02	0.41
1:A:422:TRP:HB2	1:A:437:PHE:CE1	2.55	0.41
1:A:215:LYS:HE3	1:A:220:CYS:O	2.19	0.41
1:A:362:ASN:OD1	1:A:519:LEU:HD12	2.21	0.41
1:A:480:LYS:HD3	1:A:494:HIS:CE1	2.55	0.41
2:B:201:LYS:HA	2:B:201:LYS:HD2	1.79	0.41
1:A:113:ILE:HD13	1:A:280:CYS:O	2.21	0.41
2:B:112:ARG:HB2	2:B:127:LYS:HB3	2.02	0.41
1:A:33:PRO:HD3	1:A:278:VAL:HG21	2.03	0.41
2:B:51:ARG:HA	2:B:75:GLU:HG2	2.01	0.41
1:A:162:ILE:HB	1:A:163:HIS:H	1.41	0.41
1:A:135:LYS:HE3	1:A:182:GLN:OE1	2.20	0.41
2:B:94:LEU:HD12	2:B:213:MET:O	2.21	0.40
1:A:476:ILE:HG12	1:A:517:VAL:HG11	2.04	0.40
1:A:49:TRP:CH2	1:A:436:PRO:HG3	2.55	0.40
2:B:107:TYR:HE2	2:B:109:GLN:NE2	2.19	0.40
1:A:124:PHE:CE1	1:A:174:LEU:HD12	2.56	0.40
2:B:159:LYS:CB	2:B:162:LEU:HD12	2.52	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	512/529 (97%)	396 (77%)	71 (14%)	45 (9%)	1	17
2	B	215/230 (94%)	179 (83%)	26 (12%)	10 (5%)	3	32
All	All	727/759 (96%)	575 (79%)	97 (13%)	55 (8%)	1	20

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	PRO
1	A	106	VAL
1	A	111	ILE
1	A	121	GLN
1	A	194	ILE
1	A	276	SER
1	A	412	HIS
1	A	445	PRO
1	A	458	HIS
1	A	466	SER
1	A	485	PRO
1	A	486	VAL
1	A	491	ALA
1	A	492	TRP
1	A	521	ARG
1	A	529	HIS
1	A	530	PRO
2	B	171	ASP
2	B	41	ASN
2	B	188	ASN
1	A	32	LEU
1	A	93	ALA
1	A	271	GLN
1	A	275	LYS
1	A	373	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	446	LYS
1	A	493	GLN
1	A	506	TYR
1	A	532	PRO
2	B	158	CYS
1	A	24	MET
1	A	128	THR
1	A	376	PRO
2	B	30	GLU
2	B	31	PRO
2	B	165	THR
1	A	81	GLU
1	A	126	PRO
1	A	220	CYS
1	A	312	LYS
1	A	404	PHE
1	A	468	GLU
1	A	490	GLU
2	B	123	ARG
2	B	193	ASN
1	A	162	ILE
2	B	13	ALA
1	A	525	GLY
1	A	378	PRO
1	A	436	PRO
1	A	475	PRO
1	A	509	PRO
1	A	377	LEU
1	A	526	GLY
1	A	282	PRO

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	446/457 (98%)	363 (81%)	83 (19%)	2 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	182/192 (95%)	161 (88%)	21 (12%)	7	35
All	All	628/649 (97%)	524 (83%)	104 (17%)	3	20

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	29	ILE
1	A	42	LEU
1	A	43	THR
1	A	49	TRP
1	A	50	ARG
1	A	56	THR
1	A	62	GLU
1	A	65	MET
1	A	87	VAL
1	A	90	ARG
1	A	94	SER
1	A	95	LYS
1	A	96	ILE
1	A	101	PHE
1	A	106	VAL
1	A	109	GLU
1	A	112	ARG
1	A	115	THR
1	A	116	MET
1	A	123	SER
1	A	147	LEU
1	A	148	ILE
1	A	150	GLU
1	A	161	PHE
1	A	168	HIS
1	A	173	ILE
1	A	180	HIS
1	A	184	GLN
1	A	194	ILE
1	A	204	THR
1	A	206	LEU
1	A	207	ILE
1	A	219	GLU
1	A	223	LEU
1	A	227	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	234	HIS
1	A	235	GLU
1	A	236	ASP
1	A	255	CYS
1	A	257	LEU
1	A	267	ARG
1	A	269	SER
1	A	288	SER
1	A	311	CYS
1	A	315	CYS
1	A	316	SER
1	A	319	ASN
1	A	325	ARG
1	A	336	GLN
1	A	338	LEU
1	A	341	GLU
1	A	349	THR
1	A	351	LYS
1	A	355	LEU
1	A	357	ASP
1	A	358	HIS
1	A	363	SER
1	A	367	ASN
1	A	373	SER
1	A	385	LEU
1	A	386	VAL
1	A	387	LYS
1	A	391	THR
1	A	401	THR
1	A	402	ASP
1	A	403	HIS
1	A	404	PHE
1	A	411	ILE
1	A	433	VAL
1	A	458	HIS
1	A	481	LEU
1	A	483	TYR
1	A	488	HIS
1	A	489	TYR
1	A	496	GLN
1	A	497	VAL
1	A	498	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	502	VAL
1	A	510	ARG
1	A	519	LEU
1	A	534	ARG
1	A	536	PHE
2	B	4	PHE
2	B	5	ARG
2	B	25	ILE
2	B	48	ILE
2	B	49	GLN
2	B	55	SER
2	B	73	SER
2	B	108	SER
2	B	114	HIS
2	B	124	LEU
2	B	138	SER
2	B	139	LEU
2	B	145	ASP
2	B	150	ASP
2	B	162	LEU
2	B	181	MET
2	B	192	LEU
2	B	196	LYS
2	B	201	LYS
2	B	213	MET
2	B	218	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	297	GLN
1	A	318	ASN
1	A	438	ASN
1	A	449	ASN
2	B	59	GLN
2	B	71	ASN
2	B	109	GLN
2	B	142	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	514/529 (97%)	-0.25	1 (0%) 95 94	184, 225, 272, 309	0
2	B	217/230 (94%)	-0.18	2 (0%) 85 80	194, 228, 268, 281	1 (0%)
All	All	731/759 (96%)	-0.23	3 (0%) 93 90	184, 226, 271, 309	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ARG	2.4
2	B	219	PHE	2.2
2	B	218	ASP	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.