Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:11 AM GMT

PDB ID	:	2PTK
Title	:	CHICKEN SRC TYROSINE KINASE
Authors	:	Williams, J.C.; Wierenga, R.
Deposited on	:	1997-06-17
Resolution	:	2.35 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:

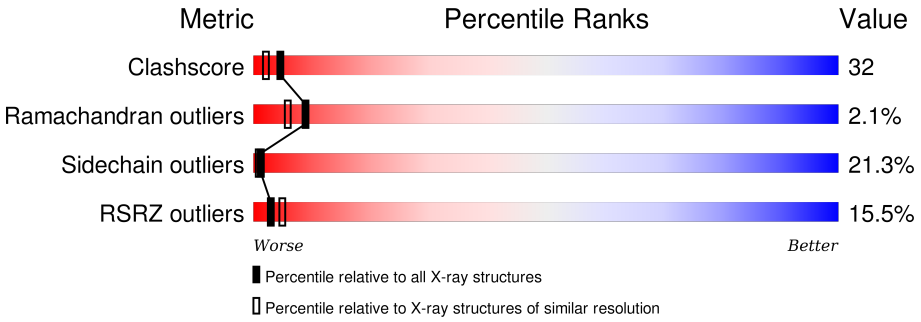
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.35 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))
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	453	15%, 41%, 42%, 11%, 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3702 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 TYROSINE-PROTEIN KINASE TRANSFORMING PROTEIN SRC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	P	S	0	0	0
			3431	2186	581	644	1	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	ASN	THR	CONFLICT	UNP P00523
A	408	GLY	ALA	CONFLICT	UNP P00523
A	527	PTR	TYR	MODIFIED RESIDUE	UNP P00523

- Molecule 2 is water.

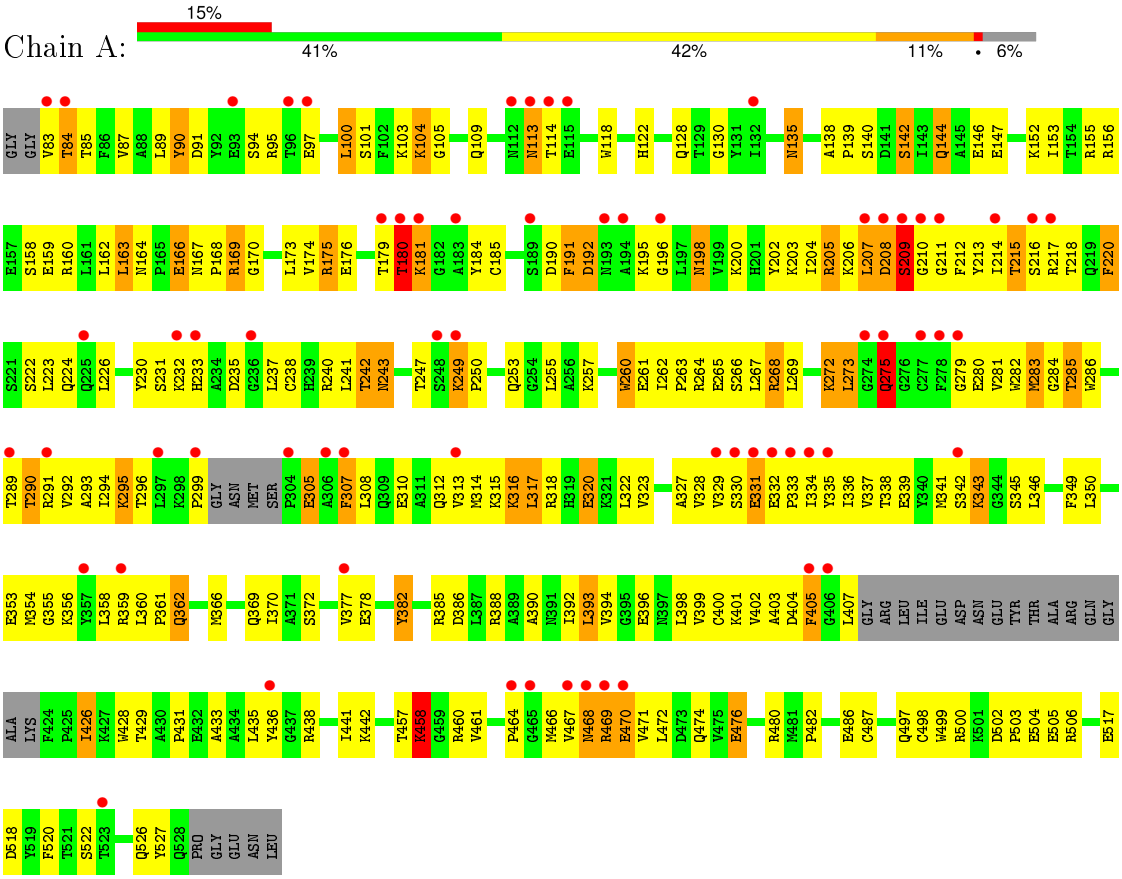
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	271	Total	O	0	0
			271	271		

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: TYROSINE-PROTEIN KINASE TRANSFORMING PROTEIN SRC

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.56Å 89.25Å 97.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.35 14.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	85.0 (5.00-2.35) 99.8 (14.67-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.21 (at 2.34Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.204 , 0.292 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 124.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 19579 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3702	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: PTR

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	0.39	0/3495	0.59	0/4732

There are no bond length outliers.

There are no bond angle outliers.

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	3431	0	3374	219	0
2	A	271	0	0	12	0
All	All	3702	0	3374	219	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 32.

All (219) 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:435:LEU:HD21	1:A:472:LEU:HD21	1.24	1.15
1:A:268:ARG:HH21	1:A:285:THR:HG21	1.25	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:HG22	1:A:335:TYR:H	1.22	1.01
1:A:355:GLY:HA2	1:A:358:LEU:HD12	1.40	1.00
1:A:255:LEU:HD12	2:A:798:HOH:O	1.61	0.99
1:A:405:PHE:HB2	2:A:751:HOH:O	1.61	0.99
1:A:497:GLN:HE22	1:A:500:ARG:HH21	1.08	0.95
1:A:369:GLN:HE22	1:A:399:VAL:HA	1.41	0.84
1:A:207:LEU:HD13	1:A:213:TYR:HE1	1.46	0.81
1:A:213:TYR:HB2	1:A:215:THR:O	1.80	0.81
1:A:497:GLN:HE22	1:A:500:ARG:NH2	1.78	0.80
1:A:253:GLN:HB3	1:A:318:ARG:NH2	1.97	0.80
1:A:113:ASN:H	1:A:113:ASN:HD22	1.29	0.80
1:A:198:ASN:HD22	1:A:198:ASN:N	1.80	0.80
1:A:497:GLN:NE2	1:A:500:ARG:HH21	1.80	0.79
1:A:466:MET:HE1	1:A:474:GLN:HB2	1.65	0.79
1:A:240:ARG:O	1:A:242:THR:HG22	1.82	0.79
1:A:268:ARG:NH2	1:A:285:THR:HG21	1.99	0.77
1:A:369:GLN:NE2	1:A:400:CYS:H	1.84	0.75
1:A:204:ILE:HG13	1:A:214:ILE:HG13	1.69	0.73
1:A:476:GLU:HG2	2:A:672:HOH:O	1.89	0.73
1:A:502:ASP:HB3	1:A:505:GLU:HG3	1.72	0.72
1:A:329:VAL:CG2	1:A:335:TYR:H	2.02	0.69
1:A:242:THR:OG1	1:A:243:ASN:N	2.23	0.68
1:A:118:TRP:HB2	1:A:257:LYS:HD3	1.74	0.67
1:A:313:VAL:HA	1:A:316:LYS:HD2	1.78	0.66
1:A:164:ASN:HB3	1:A:167:ASN:HD22	1.61	0.66
1:A:89:LEU:O	1:A:104:LYS:HD2	1.95	0.65
1:A:342:SER:HB3	2:A:652:HOH:O	1.97	0.65
1:A:361:PRO:HA	1:A:520:PHE:CE2	2.31	0.65
1:A:327:ALA:HB2	2:A:798:HOH:O	1.95	0.65
1:A:466:MET:HE2	1:A:470:GLU:HB3	1.79	0.64
1:A:345:SER:HA	1:A:393:LEU:HD12	1.79	0.64
1:A:173:LEU:CD1	1:A:175:ARG:HG2	2.27	0.64
1:A:327:ALA:CB	2:A:798:HOH:O	2.46	0.63
1:A:192:ASP:O	1:A:196:GLY:N	2.25	0.63
1:A:164:ASN:OD1	1:A:166:GLU:HG3	1.97	0.63
1:A:198:ASN:N	1:A:198:ASN:ND2	2.46	0.63
1:A:435:LEU:CD2	1:A:472:LEU:HD21	2.16	0.63
1:A:200:LYS:HE2	1:A:238:CYS:HB3	1.79	0.62
1:A:341:MET:HG3	1:A:393:LEU:HB3	1.80	0.62
1:A:264:ARG:NH2	1:A:331:GLU:O	2.33	0.62
1:A:361:PRO:HA	1:A:520:PHE:HE2	1.62	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:MET:CE	1:A:470:GLU:HB3	2.30	0.61
1:A:332:GLU:HA	1:A:333:PRO:C	2.20	0.61
1:A:323:VAL:HB	2:A:737:HOH:O	1.99	0.61
1:A:90:TYR:HB3	1:A:249:LYS:HZ3	1.65	0.61
1:A:332:GLU:HA	1:A:334:ILE:HD12	1.82	0.61
1:A:322:LEU:HG	1:A:405:PHE:CE2	2.35	0.60
1:A:388:ARG:HG3	1:A:390:ALA:H	1.66	0.60
1:A:498:CYS:O	1:A:506:ARG:HD3	2.01	0.59
1:A:329:VAL:HG22	1:A:335:TYR:N	2.06	0.59
1:A:343:LYS:N	1:A:343:LYS:HD2	2.17	0.59
1:A:518:ASP:OD2	1:A:522:SER:HA	2.03	0.59
1:A:316:LYS:O	1:A:318:ARG:HG3	2.03	0.58
1:A:146:GLU:OE1	1:A:146:GLU:HA	2.03	0.58
1:A:231:SER:HA	1:A:241:LEU:O	2.03	0.58
1:A:206:LYS:HE2	1:A:210:GLY:HA2	1.86	0.57
1:A:285:THR:HA	1:A:290:THR:O	2.04	0.57
1:A:486:GLU:HG2	2:A:584:HOH:O	2.03	0.57
1:A:360:LEU:N	1:A:361:PRO:HD2	2.19	0.57
1:A:222:SER:HB2	1:A:224:GLN:OE1	2.04	0.57
1:A:466:MET:HE2	1:A:471:VAL:N	2.20	0.56
1:A:207:LEU:HD13	1:A:213:TYR:CE1	2.34	0.56
1:A:200:LYS:HG3	1:A:238:CYS:SG	2.46	0.56
1:A:346:LEU:O	1:A:350:LEU:HG	2.05	0.56
1:A:100:LEU:HD23	1:A:130:GLY:O	2.06	0.56
1:A:94:SER:N	1:A:101:SER:OG	2.37	0.55
1:A:480:ARG:HE	1:A:499:TRP:HB3	1.72	0.55
1:A:314:MET:HA	1:A:317:LEU:HD12	1.89	0.55
1:A:426:ILE:CD1	1:A:472:LEU:HB2	2.37	0.55
1:A:503:PRO:HA	1:A:506:ARG:HG3	1.88	0.55
1:A:87:VAL:HG12	1:A:138:ALA:O	2.07	0.55
1:A:253:GLN:HB3	1:A:318:ARG:HH22	1.71	0.54
1:A:292:VAL:HB	1:A:337:VAL:HG13	1.89	0.54
1:A:230:TYR:CD1	1:A:237:LEU:HD22	2.44	0.53
1:A:208:ASP:C	1:A:210:GLY:H	2.11	0.53
1:A:308:LEU:O	1:A:312:GLN:HG2	2.09	0.53
1:A:426:ILE:HD11	1:A:472:LEU:H	1.73	0.53
1:A:467:VAL:HG22	1:A:470:GLU:OE1	2.09	0.53
1:A:307:PHE:CE1	1:A:334:ILE:HG21	2.43	0.53
1:A:262:ILE:CD1	1:A:267:LEU:HD21	2.39	0.52
1:A:355:GLY:HA2	1:A:358:LEU:CD1	2.28	0.52
1:A:369:GLN:HE22	1:A:400:CYS:H	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ARG:HB3	1:A:213:TYR:CE1	2.44	0.52
1:A:377:VAL:HG13	1:A:382:TYR:HB3	1.92	0.52
1:A:284:GLY:HA3	1:A:294:ILE:CD1	2.39	0.52
1:A:226:LEU:HG	1:A:230:TYR:CE2	2.45	0.52
1:A:261:GLU:HA	1:A:328:VAL:O	2.09	0.52
1:A:255:LEU:HD13	1:A:286:TRP:CD2	2.45	0.51
1:A:378:GLU:HG3	1:A:441:ILE:HG12	1.91	0.51
1:A:269:LEU:N	1:A:269:LEU:HD12	2.25	0.51
1:A:386:ASP:CG	1:A:388:ARG:HH21	2.14	0.51
1:A:273:LEU:HD12	1:A:281:VAL:O	2.11	0.51
1:A:170:GLY:HA3	1:A:242:THR:HG23	1.93	0.51
1:A:369:GLN:O	1:A:372:SER:HB3	2.11	0.51
1:A:262:ILE:HD11	1:A:267:LEU:HD21	1.92	0.51
1:A:176:GLU:HG2	1:A:184:TYR:HE1	1.75	0.51
1:A:262:ILE:HB	1:A:263:PRO:HD2	1.92	0.50
1:A:160:ARG:CZ	1:A:160:ARG:HB2	2.41	0.50
1:A:206:LYS:HB2	1:A:212:PHE:CE1	2.47	0.50
1:A:231:SER:O	1:A:240:ARG:NE	2.45	0.50
1:A:202:TYR:HH	1:A:238:CYS:H	1.59	0.50
1:A:358:LEU:HD23	1:A:362:GLN:HG2	1.93	0.50
1:A:320:GLU:O	1:A:401:LYS:HE2	2.12	0.49
1:A:206:LYS:HD3	1:A:212:PHE:CZ	2.48	0.49
1:A:293:ALA:O	1:A:337:VAL:HA	2.13	0.49
1:A:84:THR:CG2	1:A:84:THR:O	2.60	0.49
1:A:435:LEU:HD21	1:A:472:LEU:CD2	2.17	0.49
1:A:174:VAL:HG11	1:A:223:LEU:HD22	1.95	0.49
1:A:343:LYS:HB2	1:A:394:VAL:O	2.12	0.49
1:A:156:ARG:HG3	1:A:517:GLU:HG2	1.95	0.49
1:A:156:ARG:CD	1:A:517:GLU:HG2	2.43	0.48
1:A:220:PHE:CD1	1:A:220:PHE:N	2.81	0.48
1:A:208:ASP:CG	1:A:209:SER:N	2.67	0.48
1:A:359:ARG:HG2	1:A:362:GLN:OE1	2.14	0.48
1:A:220:PHE:CD1	1:A:226:LEU:HB2	2.49	0.48
1:A:230:TYR:HB3	1:A:241:LEU:HG	1.95	0.47
1:A:284:GLY:HA3	1:A:294:ILE:HD11	1.96	0.47
1:A:334:ILE:HD12	1:A:334:ILE:N	2.30	0.47
1:A:429:THR:HG22	1:A:433:ALA:HB3	1.97	0.47
1:A:355:GLY:O	1:A:458:LYS:HD2	2.13	0.47
1:A:392:ILE:HD13	1:A:402:VAL:HA	1.95	0.47
1:A:323:VAL:HG21	2:A:628:HOH:O	2.14	0.47
1:A:214:ILE:HD12	1:A:230:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:OD2	1:A:388:ARG:NH2	2.49	0.46
1:A:203:LYS:HE3	1:A:205:ARG:NH2	2.30	0.46
1:A:249:LYS:HG3	2:A:605:HOH:O	2.15	0.46
1:A:156:ARG:HD3	1:A:517:GLU:HG2	1.97	0.46
1:A:500:ARG:HH11	1:A:505:GLU:HB3	1.81	0.46
1:A:442:LYS:HB3	1:A:503:PRO:HB3	1.96	0.46
1:A:170:GLY:HA3	1:A:242:THR:CG2	2.46	0.46
1:A:231:SER:HA	1:A:241:LEU:HB2	1.98	0.46
1:A:339:GLU:OE2	1:A:401:LYS:NZ	2.45	0.46
1:A:90:TYR:HA	1:A:104:LYS:HB2	1.98	0.46
1:A:272:LYS:HE2	1:A:275:GLN:HE22	1.80	0.46
1:A:482:PRO:HD2	2:A:622:HOH:O	2.16	0.46
1:A:90:TYR:HB3	1:A:249:LYS:NZ	2.31	0.45
1:A:269:LEU:H	1:A:269:LEU:HD12	1.80	0.45
1:A:261:GLU:OE1	1:A:330:SER:N	2.48	0.45
1:A:155:ARG:O	1:A:158:SER:OG	2.34	0.45
1:A:497:GLN:NE2	1:A:500:ARG:HE	2.14	0.45
1:A:226:LEU:HG	1:A:230:TYR:HE2	1.82	0.45
1:A:431:PRO:HA	2:A:695:HOH:O	2.17	0.45
1:A:526:GLN:OE1	1:A:526:GLN:HA	2.15	0.45
1:A:460:ARG:NE	1:A:464:PRO:HG3	2.31	0.45
1:A:313:VAL:HA	1:A:316:LYS:CD	2.46	0.45
1:A:263:PRO:O	1:A:266:SER:OG	2.32	0.45
1:A:198:ASN:HD22	1:A:198:ASN:H	1.60	0.45
1:A:181:LYS:HD3	1:A:181:LYS:HA	1.74	0.45
1:A:467:VAL:O	1:A:468:ASN:C	2.54	0.45
1:A:349:PHE:CE2	1:A:358:LEU:HD11	2.51	0.45
1:A:342:SER:OG	1:A:343:LYS:HD2	2.17	0.44
1:A:329:VAL:O	1:A:334:ILE:HG23	2.18	0.44
1:A:359:ARG:HB2	1:A:361:PRO:HD2	1.98	0.44
1:A:402:VAL:O	1:A:405:PHE:CE2	2.70	0.44
1:A:206:LYS:HB2	1:A:212:PHE:HE1	1.82	0.44
1:A:207:LEU:HA	1:A:207:LEU:HD12	1.79	0.44
1:A:323:VAL:O	1:A:405:PHE:HZ	2.00	0.44
1:A:341:MET:HG3	1:A:393:LEU:CB	2.48	0.44
1:A:100:LEU:HD22	1:A:130:GLY:N	2.33	0.44
1:A:184:TYR:CD2	1:A:223:LEU:HD11	2.52	0.44
1:A:169:ARG:HD2	1:A:191:PHE:HB3	1.99	0.44
1:A:206:LYS:C	1:A:206:LYS:HD2	2.37	0.44
1:A:480:ARG:NE	1:A:499:TRP:HB3	2.32	0.44
1:A:179:THR:O	1:A:181:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:O	1:A:370:ILE:HG13	2.16	0.44
1:A:185:CYS:SG	1:A:527:PTR:HE1	2.58	0.43
1:A:269:LEU:CD1	1:A:269:LEU:H	2.31	0.43
1:A:269:LEU:HD23	1:A:282:TRP:CD1	2.53	0.43
1:A:144:GLN:HB2	1:A:144:GLN:HE21	1.61	0.43
1:A:310:GLU:O	1:A:314:MET:HG3	2.19	0.43
1:A:269:LEU:HD23	1:A:282:TRP:CG	2.54	0.43
1:A:503:PRO:O	1:A:506:ARG:HG3	2.19	0.43
1:A:113:ASN:HD22	1:A:113:ASN:N	2.04	0.43
1:A:153:ILE:HG23	1:A:175:ARG:HD3	2.01	0.43
1:A:369:GLN:HE22	1:A:399:VAL:CA	2.21	0.43
1:A:426:ILE:HD12	1:A:472:LEU:HD12	2.00	0.42
1:A:360:LEU:N	1:A:361:PRO:CD	2.82	0.42
1:A:500:ARG:NH1	1:A:505:GLU:HB3	2.34	0.42
1:A:159:GLU:O	1:A:163:LEU:HB2	2.18	0.42
1:A:426:ILE:HD11	1:A:472:LEU:HB2	2.00	0.42
1:A:87:VAL:HG23	1:A:105:GLY:O	2.18	0.42
1:A:169:ARG:HG2	1:A:190:ASP:HA	2.01	0.42
1:A:279:GLY:HA3	1:A:296:THR:O	2.19	0.42
1:A:305:GLU:HG3	1:A:305:GLU:H	1.72	0.42
1:A:323:VAL:HG22	1:A:403:ALA:HA	2.01	0.42
1:A:457:THR:HB	1:A:460:ARG:HB3	2.01	0.42
1:A:362:GLN:HG3	1:A:398:LEU:CD1	2.50	0.42
1:A:497:GLN:HE22	1:A:500:ARG:HE	1.68	0.42
1:A:113:ASN:H	1:A:113:ASN:ND2	2.07	0.42
1:A:497:GLN:HE22	1:A:500:ARG:CZ	2.30	0.42
1:A:158:SER:O	1:A:162:LEU:HD12	2.20	0.42
1:A:232:LYS:C	1:A:233:HIS:ND1	2.73	0.42
1:A:139:PRO:HB2	1:A:142:SER:HB3	2.01	0.41
1:A:249:LYS:HG2	1:A:249:LYS:H	1.41	0.41
1:A:435:LEU:O	1:A:436:TYR:CG	2.74	0.41
1:A:167:ASN:HA	1:A:168:PRO:HD2	1.92	0.41
1:A:260:TRP:O	1:A:327:ALA:HB1	2.21	0.41
1:A:442:LYS:O	1:A:506:ARG:NH1	2.53	0.41
1:A:261:GLU:OE2	1:A:329:VAL:HA	2.21	0.41
1:A:180:THR:O	1:A:180:THR:OG1	2.31	0.41
1:A:316:LYS:H	1:A:316:LYS:HG3	1.63	0.41
1:A:336:ILE:HG22	1:A:338:THR:HG23	2.02	0.41
1:A:359:ARG:H	1:A:359:ARG:HG2	1.72	0.41
1:A:196:GLY:O	1:A:198:ASN:ND2	2.54	0.41
1:A:90:TYR:CZ	1:A:250:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:O	1:A:163:LEU:N	2.50	0.41
1:A:216:SER:C	1:A:218:THR:H	2.25	0.41
1:A:109:GLN:NE2	1:A:122:HIS:ND1	2.68	0.40
1:A:388:ARG:HB2	1:A:428:TRP:NE1	2.36	0.40
1:A:208:ASP:C	1:A:210:GLY:N	2.75	0.40
1:A:135:ASN:HD22	1:A:135:ASN:H	1.68	0.40
1:A:283:MET:CG	1:A:283:MET:O	2.70	0.40
1:A:206:LYS:O	1:A:207:LEU:C	2.59	0.40
1:A:220:PHE:CE1	1:A:226:LEU:HD12	2.57	0.40
1:A:469:ARG:HA	1:A:469:ARG:HD3	1.72	0.40
1:A:299:PRO:HD3	1:A:333:PRO:HB3	2.02	0.40
1:A:281:VAL:HG22	1:A:295:LYS:HG2	2.03	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	419/453 (92%)	364 (87%)	46 (11%)	9 (2%)	9 6

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	SER
1	A	211	GLY
1	A	275	GLN
1	A	458	LYS
1	A	191	PHE
1	A	317	LEU
1	A	180	THR
1	A	260	TRP
1	A	396	GLU

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	371/391 (95%)	292 (79%)	79 (21%)	1 1

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	84	THR
1	A	85	THR
1	A	90	TYR
1	A	91	ASP
1	A	95	ARG
1	A	97	GLU
1	A	100	LEU
1	A	103	LYS
1	A	104	LYS
1	A	113	ASN
1	A	114	THR
1	A	128	GLN
1	A	135	ASN
1	A	140	SER
1	A	142	SER
1	A	144	GLN
1	A	147	GLU
1	A	152	LYS
1	A	163	LEU
1	A	166	GLU
1	A	169	ARG
1	A	175	ARG
1	A	180	THR
1	A	181	LYS
1	A	192	ASP
1	A	195	LYS
1	A	198	ASN
1	A	205	ARG
1	A	207	LEU

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Mol	Chain	Res	Type
1	A	208	ASP
1	A	209	SER
1	A	215	THR
1	A	217	ARG
1	A	220	PHE
1	A	235	ASP
1	A	242	THR
1	A	243	ASN
1	A	247	THR
1	A	249	LYS
1	A	265	GLU
1	A	268	ARG
1	A	272	LYS
1	A	273	LEU
1	A	275	GLN
1	A	280	GLU
1	A	283	MET
1	A	285	THR
1	A	289	THR
1	A	290	THR
1	A	291	ARG
1	A	295	LYS
1	A	305	GLU
1	A	307	PHE
1	A	315	LYS
1	A	316	LYS
1	A	320	GLU
1	A	331	GLU
1	A	343	LYS
1	A	353	GLU
1	A	354	MET
1	A	356	LYS
1	A	362	GLN
1	A	382	TYR
1	A	385	ARG
1	A	393	LEU
1	A	404	ASP
1	A	405	PHE
1	A	407	LEU
1	A	426	ILE
1	A	438	ARG
1	A	458	LYS

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Mol	Chain	Res	Type
1	A	461	VAL
1	A	468	ASN
1	A	469	ARG
1	A	470	GLU
1	A	476	GLU
1	A	487	CYS
1	A	504	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	113	ASN
1	A	135	ASN
1	A	144	GLN
1	A	167	ASN
1	A	198	ASN
1	A	275	GLN
1	A	369	GLN
1	A	468	ASN
1	A	497	GLN
1	A	513	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$
1	PTR	A	527	1	14,16,17	2.34	1 (7%)	18,22,24	1.04	1 (5%)

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
1	PTR	A	527	1	-	0/9/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	PTR	OH-CZ	8.30	1.60	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	PTR	O3P-P-OH	3.29	117.01	105.22

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
1	A	527	PTR	1	0

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

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	425/453 (93%)	0.85	66 (15%) 3 5	20, 49, 86, 99	2 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	PHE	9.9
1	A	210	GLY	9.1
1	A	208	ASP	6.8
1	A	207	LEU	6.8
1	A	357	TYR	5.7
1	A	277	CYS	5.6
1	A	469	ARG	5.2
1	A	331	GLU	4.9
1	A	304	PRO	4.9
1	A	299	PRO	4.7
1	A	179	THR	4.7
1	A	436	TYR	4.5
1	A	83	VAL	4.4
1	A	112	ASN	4.3
1	A	93	GLU	4.1
1	A	209	SER	4.1
1	A	217	ARG	4.0
1	A	274	GLY	3.8
1	A	97	GLU	3.7
1	A	291	ARG	3.7
1	A	236	GLY	3.6
1	A	297	LEU	3.6
1	A	465	GLY	3.6
1	A	115	GLU	3.5
1	A	307	PHE	3.4
1	A	333	PRO	3.3
1	A	113	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	114	THR	3.2
1	A	194	ALA	3.2
1	A	289	THR	3.2
1	A	248	SER	3.1
1	A	275	GLN	3.1
1	A	216	SER	3.1
1	A	180	THR	3.1
1	A	405	PHE	3.0
1	A	359	ARG	3.0
1	A	332	GLU	2.9
1	A	523	THR	2.8
1	A	467	VAL	2.7
1	A	181	LYS	2.7
1	A	233	HIS	2.6
1	A	214	ILE	2.6
1	A	306	ALA	2.6
1	A	196	GLY	2.5
1	A	225	GLN	2.5
1	A	377	VAL	2.5
1	A	193	ASN	2.4
1	A	132	ILE	2.4
1	A	313	VAL	2.4
1	A	84	THR	2.3
1	A	96	THR	2.3
1	A	211	GLY	2.2
1	A	468	ASN	2.2
1	A	279	GLY	2.2
1	A	232	LYS	2.2
1	A	464	PRO	2.2
1	A	189	SER	2.2
1	A	470	GLU	2.2
1	A	249	LYS	2.1
1	A	334	ILE	2.1
1	A	406	GLY	2.1
1	A	335	TYR	2.1
1	A	330	SER	2.1
1	A	342	SER	2.0
1	A	329	VAL	2.0
1	A	183	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PTR	A	527	16/17	0.92	0.19	-	32,37,49,53	0

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.