Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 08:20 AM EDT

PDB ID	:	1FPR
Title	:	CRYSTAL STRUCTURE OF THE COMPLEX FORMED BETWEEN THE CATALYTIC DOMAIN OF SHP-1 AND AN IN VITRO PEPTIDE SUBSTRATE PY469 DERIVED FROM SHPS-1.
Authors	:	Yang, J.; Cheng, Z.; Niu, Z.; Zhao, Z.J.; Zhou, G.W.
Deposited on	:	2000-08-31
Resolution	:	2.50 Å(reported)

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

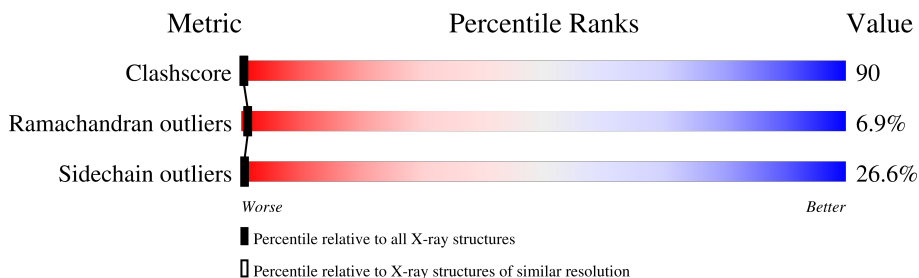|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

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

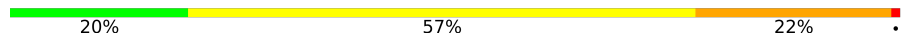The reported resolution of this entry is 2.50 Å.

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
Clashscore		90
Ramachandran outliers		6.9%
Sidechain outliers		26.6%

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	284	20% 57% 22% •
2	B	10	30% 60% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTR	B	1469	-	-	X	-

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2374 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 PROTEIN-TYROSINE PHOSPHATASE 1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2289	1441	402	435	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	SER	CYS	engineered mutation	UNP P29350

- Molecule 2 is a protein called PEPTIDE PY469.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			85	49	10	25	1			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEIN-TYROSINE PHOSPHATASE 1C

Chain A:
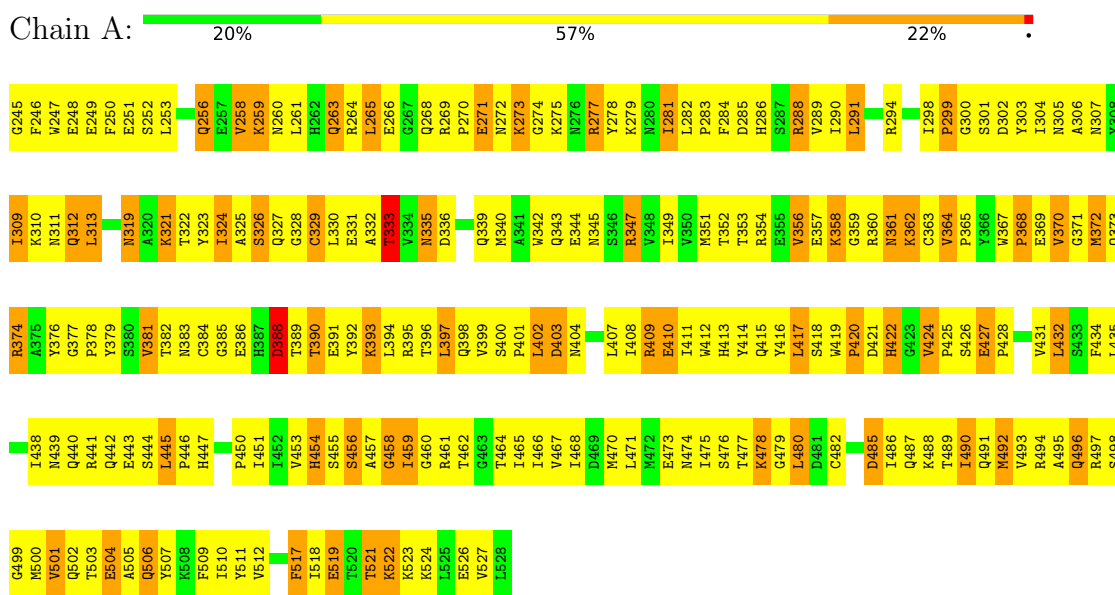
• Molecule 2: PEPTIDE PY469

Chain B:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	111.58Å 45.21Å 56.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2374	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5   Model quality (i)

5.1   Standard geometry (i)

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	0.38	0/2339	0.63	0/3166
2	B	0.45	0/67	1.22	0/88
All	All	0.38	0/2406	0.65	0/3254

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 (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	2289	0	2243	412	0
2	B	85	0	65	59	0
All	All	2374	0	2308	422	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 90.

All (422) 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)
2:B:1468:THR:O	2:B:1469:PTR:HB3	1.47	1.10
1:A:498:SER:HB2	2:B:1472:LEU:HB2	1.35	1.09
1:A:459:ILE:HD11	2:B:1469:PTR:HD1	1.35	1.07
1:A:486:ILE:HG22	1:A:490:ILE:HD11	1.35	1.06
1:A:428:PRO:HB2	1:A:432:LEU:HD12	1.34	1.06
1:A:364:VAL:HG22	1:A:365:PRO:HD2	1.38	1.05
1:A:398:GLN:HB3	1:A:408:ILE:HD11	1.37	1.05
1:A:381:VAL:CG2	1:A:399:VAL:HG22	1.87	1.03
1:A:425:PRO:HG2	1:A:509:PHE:CE1	1.92	1.03
1:A:278:TYR:CE1	1:A:457:ALA:CB	2.43	1.01
1:A:357:GLU:HG2	1:A:364:VAL:HG23	1.42	1.01
1:A:413:HIS:HE1	1:A:415:GLN:HB2	1.24	1.01
1:A:264:ARG:O	1:A:268:GLN:HG3	1.61	0.99
1:A:278:TYR:HE1	1:A:457:ALA:HB3	1.24	0.97
1:A:432:LEU:HD21	1:A:517:PHE:HB2	1.44	0.96
1:A:381:VAL:HG23	1:A:399:VAL:HG22	0.99	0.96
1:A:360:ARG:CZ	2:B:1465:ASP:HB3	1.97	0.95
1:A:459:ILE:HD11	2:B:1469:PTR:CD1	1.98	0.93
1:A:356:VAL:HG12	1:A:358:LYS:HG2	1.47	0.93
1:A:390:THR:HG22	1:A:391:GLU:HG2	1.50	0.93
1:A:480:LEU:HD21	1:A:521:THR:HG21	1.51	0.93
1:A:395:ARG:HH12	1:A:415:GLN:HE21	0.93	0.91
1:A:374:ARG:HG2	1:A:376:TYR:CZ	2.04	0.91
1:A:417:LEU:HD23	1:A:417:LEU:H	1.35	0.90
1:A:395:ARG:HH12	1:A:415:GLN:NE2	1.70	0.89
1:A:284:PHE:HB3	1:A:286:HIS:CE1	2.07	0.89
1:A:357:GLU:HA	1:A:361:ASN:HA	1.53	0.89
1:A:389:THR:HG22	1:A:390:THR:H	1.39	0.88
1:A:414:TYR:O	1:A:434:PHE:HZ	1.56	0.88
1:A:278:TYR:HE1	1:A:457:ALA:CB	1.81	0.88
1:A:381:VAL:HG23	1:A:399:VAL:CG2	1.96	0.87
1:A:278:TYR:CE1	1:A:457:ALA:HB2	2.08	0.87
1:A:398:GLN:CB	1:A:408:ILE:HD11	2.04	0.87
1:A:413:HIS:CE1	1:A:415:GLN:HB2	2.08	0.86
1:A:263:GLN:OE1	1:A:265:LEU:HD13	1.74	0.86
1:A:281:ILE:HD13	2:B:1472:LEU:HD23	1.56	0.86
1:A:253:LEU:HA	1:A:256:GLN:HG3	1.55	0.86
1:A:445:LEU:HD22	1:A:445:LEU:H	1.40	0.85
1:A:369:GLU:O	1:A:372:MET:HB2	1.76	0.85
1:A:428:PRO:O	1:A:432:LEU:HB2	1.76	0.85
1:A:278:TYR:CE2	2:B:1469:PTR:HB3	2.11	0.85
1:A:480:LEU:HD21	1:A:521:THR:CG2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:SER:HB3	2:B:1473:ASP:O	1.76	0.85
1:A:360:ARG:NH1	2:B:1465:ASP:HB3	1.92	0.84
1:A:522:LYS:HZ3	1:A:522:LYS:HB2	1.43	0.83
1:A:394:LEU:C	1:A:394:LEU:HD23	1.99	0.83
1:A:278:TYR:CE2	2:B:1468:THR:O	2.32	0.83
1:A:395:ARG:HH22	1:A:415:GLN:HE22	1.27	0.82
1:A:273:LYS:HE3	1:A:274:GLY:H	1.44	0.82
1:A:278:TYR:CZ	2:B:1469:PTR:CB	2.63	0.82
1:A:504:GLU:O	1:A:507:TYR:HB3	1.79	0.81
1:A:364:VAL:CG2	1:A:365:PRO:HD2	2.11	0.81
1:A:486:ILE:O	1:A:490:ILE:HG13	1.80	0.81
1:A:414:TYR:O	1:A:434:PHE:CZ	2.34	0.80
1:A:395:ARG:NH1	1:A:415:GLN:HE21	1.75	0.80
2:B:1471:ASP:C	2:B:1472:LEU:HG	2.02	0.80
1:A:398:GLN:NE2	1:A:410:GLU:HG3	1.96	0.79
1:A:309:ILE:HD11	1:A:325:ALA:HB2	1.63	0.79
1:A:278:TYR:CE1	1:A:457:ALA:HB3	2.10	0.79
1:A:278:TYR:OH	2:B:1469:PTR:CD2	2.30	0.79
1:A:281:ILE:HD11	1:A:459:ILE:HG21	1.64	0.78
1:A:522:LYS:HB2	1:A:522:LYS:NZ	1.97	0.78
1:A:333:THR:HG22	1:A:336:ASP:HB2	1.66	0.78
1:A:278:TYR:HB2	1:A:281:ILE:HB	1.66	0.78
1:A:360:ARG:NE	2:B:1465:ASP:HA	1.99	0.77
1:A:278:TYR:CZ	2:B:1469:PTR:HB3	2.19	0.77
1:A:386:GLU:CD	1:A:393:LYS:HD3	2.05	0.77
1:A:269:ARG:HB3	1:A:271:GLU:HG2	1.66	0.77
1:A:278:TYR:CZ	2:B:1469:PTR:CG	2.68	0.77
1:A:420:PRO:HG2	1:A:424:VAL:C	2.04	0.77
1:A:457:ALA:O	1:A:459:ILE:HG12	1.84	0.76
1:A:362:LYS:HD3	2:B:1467:LEU:HD11	1.67	0.76
1:A:388:ASP:HA	1:A:393:LYS:HA	1.65	0.76
1:A:445:LEU:HD22	1:A:445:LEU:N	2.00	0.76
1:A:467:VAL:HG12	1:A:471:LEU:CD1	2.16	0.76
1:A:281:ILE:CD1	2:B:1472:LEU:HD23	2.16	0.75
1:A:273:LYS:HG2	1:A:274:GLY:N	2.01	0.74
1:A:485:ASP:HB2	1:A:488:LYS:HB3	1.68	0.74
2:B:1468:THR:O	2:B:1469:PTR:CB	2.33	0.74
1:A:487:GLN:HA	1:A:490:ILE:HD12	1.68	0.73
1:A:309:ILE:O	1:A:310:LYS:HD3	1.88	0.73
1:A:253:LEU:CA	1:A:256:GLN:HG3	2.18	0.72
1:A:499:GLY:O	1:A:502:GLN:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TRP:HZ3	1:A:465:ILE:HD11	1.55	0.72
1:A:467:VAL:HG22	1:A:493:VAL:HG21	1.73	0.71
1:A:378:PRO:C	1:A:402:LEU:HD12	2.11	0.71
1:A:269:ARG:CB	1:A:271:GLU:HG2	2.20	0.71
1:A:386:GLU:OE2	1:A:393:LYS:HD3	1.91	0.70
1:A:284:PHE:HB3	1:A:286:HIS:ND1	2.07	0.70
1:A:325:ALA:HB3	1:A:497:ARG:HD3	1.74	0.70
1:A:391:GLU:O	1:A:417:LEU:HD23	1.91	0.69
1:A:395:ARG:HH22	1:A:415:GLN:NE2	1.89	0.69
1:A:522:LYS:HB3	1:A:527:VAL:HB	1.73	0.69
1:A:422:HIS:ND1	1:A:422:HIS:N	2.39	0.69
1:A:464:THR:HG23	1:A:510:ILE:HD11	1.74	0.69
1:A:284:PHE:CD1	1:A:286:HIS:HE1	2.10	0.69
1:A:291:LEU:HD23	1:A:294:ARG:NH2	2.08	0.69
1:A:467:VAL:HG12	1:A:471:LEU:HD12	1.75	0.69
1:A:277:ARG:HG3	1:A:330:LEU:HD13	1.75	0.69
1:A:498:SER:CB	2:B:1472:LEU:HB2	2.19	0.69
1:A:259:LYS:HE3	2:B:1472:LEU:CD1	2.23	0.68
1:A:386:GLU:HB2	1:A:393:LYS:HD3	1.74	0.68
1:A:284:PHE:CB	1:A:286:HIS:CE1	2.77	0.68
1:A:264:ARG:NH1	1:A:282:LEU:HB2	2.08	0.68
1:A:417:LEU:HD23	1:A:417:LEU:N	2.06	0.68
1:A:389:THR:HG22	1:A:390:THR:N	2.08	0.68
1:A:324:ILE:O	1:A:324:ILE:HG22	1.92	0.67
1:A:386:GLU:HB3	1:A:395:ARG:HG2	1.75	0.67
1:A:498:SER:HB2	2:B:1473:ASP:H	1.59	0.67
1:A:522:LYS:HZ3	1:A:522:LYS:CB	2.07	0.67
1:A:395:ARG:NH2	1:A:415:GLN:HE22	1.92	0.67
1:A:390:THR:CG2	1:A:391:GLU:HG2	2.22	0.67
1:A:309:ILE:HD11	1:A:325:ALA:CB	2.25	0.67
1:A:428:PRO:HG3	1:A:512:VAL:HG12	1.75	0.67
1:A:245:GLY:HA3	1:A:248:GLU:CD	2.15	0.67
1:A:340:MET:O	1:A:344:GLU:HG2	1.95	0.67
1:A:395:ARG:NH1	1:A:415:GLN:NE2	2.39	0.67
1:A:455:SER:HB2	2:B:1469:PTR:O2P	1.95	0.67
1:A:311:ASN:ND2	1:A:313:LEU:HB2	2.11	0.66
1:A:392:TYR:HA	1:A:417:LEU:HD23	1.75	0.66
1:A:392:TYR:HA	1:A:417:LEU:CD2	2.25	0.66
1:A:459:ILE:CD1	2:B:1469:PTR:HD1	2.21	0.65
1:A:347:ARG:HG2	1:A:347:ARG:HH11	1.61	0.65
1:A:420:PRO:HD2	1:A:425:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASN:O	1:A:443:GLU:HG3	1.97	0.65
1:A:259:LYS:NZ	2:B:1472:LEU:HD13	2.12	0.65
1:A:281:ILE:HD11	1:A:459:ILE:CG2	2.26	0.65
1:A:277:ARG:HE	1:A:330:LEU:HD13	1.61	0.64
1:A:322:THR:OG1	1:A:450:PRO:HA	1.96	0.64
1:A:372:MET:HE2	1:A:372:MET:HA	1.78	0.64
1:A:431:VAL:HA	1:A:434:PHE:HB3	1.79	0.64
1:A:356:VAL:HG12	1:A:358:LYS:CG	2.26	0.64
1:A:373:GLN:HB2	1:A:382:THR:HG22	1.79	0.64
1:A:370:VAL:HG13	1:A:385:GLY:HA2	1.80	0.64
1:A:416:TYR:CE2	1:A:431:VAL:HG12	2.33	0.64
1:A:281:ILE:HD13	2:B:1472:LEU:CD2	2.28	0.64
1:A:311:ASN:HD21	1:A:313:LEU:HB2	1.63	0.63
1:A:321:LYS:HD3	1:A:451:ILE:CD1	2.28	0.63
1:A:269:ARG:HB3	1:A:271:GLU:CG	2.29	0.63
1:A:357:GLU:O	1:A:360:ARG:C	2.37	0.63
1:A:277:ARG:NE	1:A:330:LEU:HD13	2.13	0.63
1:A:398:GLN:HA	1:A:409:ARG:O	1.99	0.63
1:A:345:ASN:HD21	1:A:347:ARG:NH1	1.96	0.63
1:A:404:ASN:HD22	1:A:407:LEU:HB2	1.63	0.63
1:A:277:ARG:NH2	1:A:362:LYS:O	2.32	0.63
1:A:253:LEU:HA	1:A:256:GLN:CG	2.28	0.62
1:A:404:ASN:ND2	1:A:407:LEU:HB2	2.13	0.62
1:A:498:SER:HB2	2:B:1473:ASP:N	2.14	0.62
1:A:339:GLN:HA	1:A:379:TYR:HE1	1.63	0.62
1:A:424:VAL:HG22	1:A:425:PRO:HD2	1.81	0.62
1:A:453:VAL:O	1:A:454:HIS:HB3	1.99	0.62
2:B:1471:ASP:OD1	2:B:1472:LEU:N	2.32	0.62
1:A:277:ARG:HG3	1:A:330:LEU:CD1	2.30	0.62
1:A:461:ARG:O	1:A:465:ILE:HG12	2.00	0.62
1:A:277:ARG:NH1	1:A:456:SER:CB	2.63	0.62
1:A:281:ILE:HG22	1:A:281:ILE:O	2.00	0.62
1:A:347:ARG:O	1:A:411:ILE:HG23	2.00	0.62
1:A:335:ASN:HD22	1:A:377:GLY:N	1.99	0.61
1:A:467:VAL:HG12	1:A:471:LEU:HD11	1.82	0.61
1:A:277:ARG:NH1	1:A:456:SER:HB3	2.15	0.61
1:A:356:VAL:HB	1:A:362:LYS:HG2	1.82	0.61
1:A:322:THR:O	1:A:451:ILE:N	2.32	0.61
1:A:417:LEU:N	1:A:417:LEU:CD2	2.63	0.60
1:A:435:LEU:O	1:A:439:ASN:CG	2.40	0.60
1:A:479:GLY:O	1:A:482:CYS:SG	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1471:ASP:C	2:B:1471:ASP:OD1	2.39	0.60
1:A:394:LEU:C	1:A:394:LEU:CD2	2.69	0.60
1:A:360:ARG:HG3	1:A:361:ASN:H	1.65	0.60
1:A:462:THR:O	1:A:466:ILE:HG12	2.01	0.60
1:A:259:LYS:HZ3	1:A:259:LYS:HB2	1.65	0.60
1:A:347:ARG:HA	1:A:411:ILE:HG13	1.82	0.60
1:A:491:GLN:OE1	1:A:494:ARG:NH1	2.34	0.60
1:A:358:LYS:HD3	1:A:362:LYS:HE3	1.82	0.60
1:A:386:GLU:CB	1:A:393:LYS:HD3	2.32	0.60
1:A:393:LYS:HG2	1:A:394:LEU:H	1.67	0.60
1:A:461:ARG:HG3	2:B:1469:PTR:O1P	2.02	0.60
1:A:522:LYS:NZ	1:A:522:LYS:CB	2.57	0.59
1:A:390:THR:HG23	1:A:391:GLU:OE1	2.01	0.59
1:A:284:PHE:O	1:A:288:ARG:HB3	2.02	0.59
1:A:435:LEU:O	1:A:439:ASN:OD1	2.21	0.59
1:A:486:ILE:CG2	1:A:490:ILE:HD11	2.21	0.59
1:A:277:ARG:NH2	1:A:328:GLY:O	2.36	0.58
1:A:289:VAL:O	1:A:304:ILE:HG22	2.03	0.58
1:A:311:ASN:HD21	1:A:313:LEU:CB	2.17	0.58
1:A:259:LYS:HZ1	2:B:1472:LEU:HD13	1.69	0.58
1:A:278:TYR:OH	2:B:1469:PTR:CG	2.52	0.58
1:A:373:GLN:CB	1:A:382:THR:HG22	2.34	0.58
1:A:294:ARG:NE	1:A:301:SER:O	2.37	0.58
1:A:374:ARG:HG2	1:A:376:TYR:CE1	2.38	0.57
2:B:1466:THR:OG1	2:B:1467:LEU:N	2.37	0.57
1:A:503:THR:OG1	1:A:506:GLN:HG3	2.04	0.57
1:A:459:ILE:HD11	2:B:1469:PTR:CE1	2.33	0.57
1:A:464:THR:HG23	1:A:510:ILE:CD1	2.33	0.57
1:A:253:LEU:C	1:A:256:GLN:HG3	2.25	0.57
1:A:321:LYS:HD3	1:A:451:ILE:HD11	1.87	0.57
1:A:358:LYS:O	1:A:360:ARG:N	2.33	0.57
1:A:306:ALA:HA	1:A:497:ARG:NH1	2.20	0.56
1:A:441:ARG:O	1:A:445:LEU:HD22	2.05	0.56
1:A:519:GLU:O	1:A:523:LYS:HE3	2.05	0.56
1:A:284:PHE:CB	1:A:286:HIS:HE1	2.18	0.56
1:A:398:GLN:CD	1:A:410:GLU:HG3	2.26	0.56
1:A:457:ALA:O	1:A:459:ILE:CG1	2.53	0.56
1:A:519:GLU:O	1:A:523:LYS:HB2	2.04	0.56
1:A:395:ARG:NH2	1:A:415:GLN:NE2	2.53	0.56
1:A:266:GLU:HG3	1:A:288:ARG:CZ	2.36	0.56
1:A:442:GLN:HA	1:A:445:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:O	1:A:412:TRP:N	2.36	0.56
1:A:351:MET:CE	1:A:353:THR:O	2.54	0.56
1:A:428:PRO:HA	1:A:509:PHE:CZ	2.41	0.55
1:A:252:SER:O	1:A:256:GLN:HG2	2.06	0.55
1:A:294:ARG:HG3	1:A:302:ASP:HA	1.89	0.55
1:A:331:GLU:HG3	1:A:364:VAL:HG11	1.88	0.55
1:A:351:MET:HE2	1:A:353:THR:O	2.06	0.55
1:A:245:GLY:HA3	1:A:248:GLU:OE1	2.06	0.55
1:A:431:VAL:HA	1:A:434:PHE:CB	2.36	0.55
1:A:445:LEU:H	1:A:445:LEU:CD2	2.15	0.54
1:A:502:GLN:NE2	2:B:1471:ASP:O	2.39	0.54
1:A:313:LEU:HD11	1:A:485:ASP:OD2	2.08	0.54
1:A:339:GLN:OE1	1:A:343:GLN:OE1	2.25	0.54
1:A:467:VAL:O	1:A:471:LEU:HD12	2.07	0.54
1:A:360:ARG:CZ	2:B:1465:ASP:CB	2.80	0.54
1:A:384:CYS:N	1:A:396:THR:O	2.28	0.54
1:A:420:PRO:C	1:A:422:HIS:H	2.10	0.54
1:A:506:GLN:O	1:A:510:ILE:HD12	2.08	0.54
1:A:386:GLU:OE2	1:A:393:LYS:HE2	2.08	0.53
1:A:490:ILE:HG23	1:A:501:VAL:HG21	1.90	0.53
1:A:291:LEU:HB2	1:A:302:ASP:HA	1.90	0.53
1:A:281:ILE:CD1	1:A:459:ILE:HG21	2.37	0.53
1:A:494:ARG:C	1:A:496:GLN:H	2.12	0.53
1:A:401:PRO:HB2	1:A:403:ASP:OD2	2.09	0.53
1:A:345:ASN:HA	1:A:409:ARG:NH1	2.24	0.53
1:A:378:PRO:O	1:A:402:LEU:HD12	2.08	0.53
1:A:386:GLU:HB2	1:A:393:LYS:CG	2.39	0.53
1:A:278:TYR:CE1	2:B:1469:PTR:CB	2.92	0.53
1:A:388:ASP:OD1	1:A:388:ASP:N	2.41	0.53
1:A:504:GLU:HA	1:A:504:GLU:OE2	2.05	0.53
1:A:328:GLY:HA3	1:A:455:SER:O	2.09	0.53
1:A:272:ASN:ND2	1:A:275:LYS:HD2	2.24	0.52
1:A:371:GLY:O	1:A:372:MET:HE3	2.09	0.52
1:A:522:LYS:HB3	1:A:527:VAL:CB	2.39	0.52
2:B:1466:THR:O	2:B:1467:LEU:HD22	2.09	0.52
1:A:357:GLU:O	1:A:358:LYS:C	2.47	0.52
1:A:386:GLU:HB2	1:A:393:LYS:CD	2.39	0.52
1:A:305:ASN:OD1	1:A:497:ARG:NH2	2.37	0.52
1:A:471:LEU:O	1:A:475:ILE:HD12	2.09	0.52
1:A:306:ALA:HB2	1:A:326:SER:HB3	1.91	0.52
1:A:371:GLY:O	1:A:372:MET:CE	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD11	1:A:441:ARG:HH21	1.75	0.52
1:A:347:ARG:HE	1:A:409:ARG:HD3	1.75	0.51
1:A:278:TYR:CE1	2:B:1469:PTR:CG	2.93	0.51
1:A:504:GLU:OE2	1:A:507:TYR:HB3	2.10	0.51
1:A:278:TYR:CE1	2:B:1469:PTR:CD1	2.94	0.51
1:A:428:PRO:HG3	1:A:512:VAL:CG1	2.40	0.51
1:A:460:GLY:HA3	1:A:506:GLN:HE22	1.75	0.51
1:A:492:MET:HE3	1:A:493:VAL:HG23	1.92	0.51
1:A:349:ILE:CD1	1:A:411:ILE:HG21	2.41	0.51
1:A:468:ILE:HG13	1:A:510:ILE:HG12	1.92	0.51
1:A:327:GLN:HG3	1:A:457:ALA:HA	1.93	0.51
1:A:485:ASP:O	1:A:489:THR:OG1	2.28	0.51
1:A:360:ARG:CG	1:A:361:ASN:H	2.23	0.51
1:A:426:SER:C	1:A:427:GLU:HG3	2.30	0.50
1:A:466:ILE:O	1:A:470:MET:HG3	2.12	0.50
1:A:269:ARG:C	1:A:271:GLU:H	2.13	0.50
1:A:419:TRP:CD1	1:A:420:PRO:HD2	2.46	0.50
1:A:258:VAL:HA	1:A:261:LEU:HG	1.92	0.50
1:A:416:TYR:CZ	1:A:431:VAL:HG12	2.46	0.50
1:A:347:ARG:C	1:A:411:ILE:HG23	2.32	0.50
1:A:376:TYR:HE1	1:A:381:VAL:HG12	1.76	0.50
1:A:441:ARG:O	1:A:445:LEU:CD2	2.59	0.50
1:A:454:HIS:ND1	1:A:454:HIS:C	2.64	0.50
2:B:1468:THR:HG22	2:B:1469:PTR:N	2.26	0.50
1:A:420:PRO:O	1:A:422:HIS:N	2.44	0.50
1:A:278:TYR:CE1	2:B:1469:PTR:HB2	2.48	0.49
1:A:275:LYS:HD3	1:A:303:TYR:HD2	1.76	0.49
1:A:324:ILE:HG22	1:A:326:SER:OG	2.12	0.49
1:A:281:ILE:HA	2:B:1472:LEU:HD21	1.94	0.49
1:A:245:GLY:O	1:A:249:GLU:HG2	2.12	0.49
1:A:364:VAL:HG22	1:A:365:PRO:CD	2.27	0.49
1:A:259:LYS:CE	2:B:1472:LEU:HD13	2.42	0.49
1:A:329:CYS:HB2	1:A:364:VAL:N	2.28	0.49
1:A:345:ASN:O	1:A:347:ARG:HD3	2.11	0.49
1:A:259:LYS:CE	2:B:1472:LEU:CD1	2.89	0.49
1:A:455:SER:CB	2:B:1469:PTR:O2P	2.59	0.49
1:A:498:SER:CB	2:B:1473:ASP:O	2.55	0.49
1:A:420:PRO:HG2	1:A:424:VAL:O	2.12	0.49
1:A:420:PRO:C	1:A:422:HIS:N	2.65	0.48
1:A:473:GLU:O	1:A:477:THR:HB	2.13	0.48
1:A:459:ILE:O	1:A:500:MET:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:HG21	1:A:517:PHE:HE2	1.78	0.48
1:A:480:LEU:HD21	1:A:521:THR:HG22	1.88	0.48
1:A:333:THR:HG22	1:A:336:ASP:CB	2.41	0.48
1:A:459:ILE:HG13	1:A:460:GLY:H	1.78	0.48
1:A:252:SER:C	1:A:256:GLN:HE21	2.16	0.48
1:A:284:PHE:CG	1:A:286:HIS:HE1	2.32	0.48
1:A:522:LYS:HD2	1:A:527:VAL:HG11	1.96	0.48
1:A:269:ARG:HB2	1:A:271:GLU:HG2	1.96	0.48
1:A:357:GLU:CA	1:A:361:ASN:HA	2.37	0.48
1:A:311:ASN:ND2	1:A:313:LEU:CB	2.76	0.47
1:A:383:ASN:HA	1:A:397:LEU:HD23	1.95	0.47
1:A:474:ASN:O	1:A:478:LYS:N	2.38	0.47
1:A:288:ARG:NH2	1:A:290:ILE:HG12	2.29	0.47
1:A:289:VAL:HG11	1:A:340:MET:HG3	1.96	0.47
1:A:361:ASN:HB2	1:A:364:VAL:HB	1.97	0.47
1:A:263:GLN:CD	1:A:265:LEU:HD13	2.33	0.47
1:A:278:TYR:CD1	1:A:457:ALA:CB	2.96	0.47
1:A:321:LYS:HG2	1:A:323:TYR:CZ	2.50	0.47
1:A:354:ARG:CZ	1:A:356:VAL:HG22	2.45	0.47
1:A:360:ARG:HD2	1:A:361:ASN:ND2	2.29	0.47
1:A:306:ALA:CA	1:A:497:ARG:NH1	2.78	0.47
1:A:349:ILE:HD12	1:A:411:ILE:HG21	1.96	0.47
1:A:486:ILE:O	1:A:490:ILE:CG1	2.58	0.47
1:A:345:ASN:ND2	1:A:347:ARG:NH1	2.63	0.47
1:A:360:ARG:CD	2:B:1465:ASP:HA	2.45	0.47
1:A:259:LYS:HE3	2:B:1472:LEU:HD13	1.95	0.46
1:A:490:ILE:HG13	1:A:490:ILE:H	1.57	0.46
1:A:519:GLU:HG2	1:A:523:LYS:HE3	1.96	0.46
1:A:393:LYS:HG2	1:A:394:LEU:N	2.29	0.46
1:A:321:LYS:HG3	1:A:322:THR:N	2.31	0.46
1:A:357:GLU:O	1:A:360:ARG:N	2.49	0.46
1:A:386:GLU:OE2	1:A:393:LYS:CD	2.60	0.46
1:A:471:LEU:HD21	1:A:486:ILE:HD13	1.97	0.46
1:A:347:ARG:HH11	1:A:347:ARG:CG	2.29	0.46
1:A:457:ALA:O	1:A:459:ILE:N	2.49	0.46
1:A:325:ALA:CB	1:A:497:ARG:HD3	2.45	0.46
1:A:342:TRP:HD1	1:A:379:TYR:HH	1.63	0.46
1:A:419:TRP:CZ3	1:A:465:ILE:HD11	2.44	0.46
1:A:304:ILE:HD13	1:A:340:MET:HB2	1.98	0.45
1:A:441:ARG:O	1:A:444:SER:N	2.32	0.45
1:A:519:GLU:O	1:A:519:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1467:LEU:O	2:B:1468:THR:OG1	2.30	0.45
1:A:394:LEU:HD12	1:A:414:TYR:CE1	2.51	0.45
1:A:462:THR:O	1:A:466:ILE:CG1	2.64	0.45
1:A:504:GLU:OE2	1:A:507:TYR:CD2	2.70	0.45
1:A:283:PRO:CB	1:A:307:ASN:OD1	2.64	0.45
1:A:459:ILE:HB	1:A:502:GLN:HE21	1.82	0.45
1:A:474:ASN:O	1:A:478:LYS:HB2	2.17	0.45
1:A:246:PHE:HD2	1:A:247:TRP:CD1	2.35	0.45
1:A:356:VAL:O	1:A:358:LYS:HG2	2.16	0.45
1:A:412:TRP:CE3	1:A:441:ARG:CZ	3.00	0.45
1:A:250:PHE:C	1:A:252:SER:H	2.20	0.45
1:A:272:ASN:HD21	1:A:300:GLY:HA3	1.82	0.45
1:A:361:ASN:O	1:A:362:LYS:C	2.52	0.45
1:A:367:TRP:CZ3	1:A:413:HIS:NE2	2.85	0.44
1:A:425:PRO:HG2	1:A:509:PHE:HE1	1.70	0.44
1:A:473:GLU:O	1:A:477:THR:CB	2.65	0.44
1:A:498:SER:HA	2:B:1473:ASP:C	2.38	0.44
1:A:498:SER:CB	2:B:1473:ASP:H	2.28	0.44
1:A:500:MET:O	1:A:501:VAL:HB	2.18	0.44
1:A:252:SER:O	1:A:256:GLN:CG	2.65	0.44
1:A:253:LEU:HA	1:A:256:GLN:NE2	2.32	0.44
1:A:466:ILE:HG22	1:A:470:MET:HG3	1.99	0.44
1:A:414:TYR:HB3	1:A:434:PHE:CE2	2.53	0.44
1:A:431:VAL:O	1:A:435:LEU:HG	2.18	0.44
1:A:281:ILE:CD1	1:A:459:ILE:CG2	2.93	0.44
1:A:335:ASN:N	1:A:335:ASN:OD1	2.50	0.44
1:A:347:ARG:HG2	1:A:347:ARG:NH1	2.32	0.44
2:B:1469:PTR:HB2	2:B:1470:ALA:H	1.39	0.44
1:A:269:ARG:C	1:A:271:GLU:N	2.71	0.43
1:A:368:PRO:HD2	1:A:383:ASN:HB2	1.99	0.43
1:A:374:ARG:HD2	1:A:376:TYR:OH	2.18	0.43
1:A:386:GLU:HA	1:A:395:ARG:HA	2.01	0.43
1:A:494:ARG:O	1:A:496:GLN:N	2.51	0.43
1:A:311:ASN:OD1	1:A:470:MET:SD	2.76	0.43
1:A:388:ASP:CG	1:A:393:LYS:HG3	2.37	0.43
1:A:278:TYR:HE2	2:B:1468:THR:O	1.97	0.43
1:A:356:VAL:N	1:A:363:CYS:HB3	2.33	0.43
1:A:396:THR:HG22	1:A:412:TRP:CZ3	2.53	0.43
1:A:498:SER:C	2:B:1472:LEU:HB3	2.38	0.43
1:A:283:PRO:HB3	1:A:307:ASN:OD1	2.18	0.43
1:A:349:ILE:HD12	1:A:411:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:HA	1:A:394:LEU:O	2.17	0.43
1:A:333:THR:HG23	1:A:336:ASP:OD1	2.19	0.43
1:A:382:THR:O	1:A:397:LEU:HA	2.18	0.43
1:A:395:ARG:CZ	1:A:415:GLN:NE2	2.82	0.43
1:A:480:LEU:HD12	1:A:518:ILE:HG12	2.00	0.43
1:A:281:ILE:HA	2:B:1472:LEU:CD2	2.49	0.43
1:A:445:LEU:HA	1:A:446:PRO:HD2	1.75	0.43
1:A:492:MET:O	1:A:496:GLN:HG3	2.19	0.43
1:A:368:PRO:HB2	1:A:372:MET:HB3	2.01	0.43
1:A:500:MET:HA	1:A:500:MET:HE2	2.00	0.43
1:A:342:TRP:CH2	1:A:401:PRO:HD3	2.53	0.42
1:A:507:TYR:O	1:A:511:TYR:HD1	2.02	0.42
1:A:357:GLU:CG	1:A:364:VAL:HG23	2.31	0.42
1:A:475:ILE:CG2	1:A:480:LEU:HD13	2.48	0.42
1:A:505:ALA:C	1:A:507:TYR:N	2.72	0.42
1:A:347:ARG:N	1:A:347:ARG:CD	2.82	0.42
1:A:385:GLY:O	1:A:395:ARG:HA	2.19	0.42
1:A:485:ASP:O	1:A:489:THR:N	2.47	0.42
1:A:420:PRO:HD2	1:A:425:PRO:CD	2.47	0.42
1:A:389:THR:CG2	1:A:390:THR:H	2.20	0.42
1:A:306:ALA:CA	1:A:497:ARG:HH12	2.32	0.42
1:A:291:LEU:HA	1:A:291:LEU:HD12	1.76	0.42
1:A:455:SER:OG	2:B:1469:PTR:P	2.77	0.42
1:A:408:ILE:HG13	1:A:409:ARG:N	2.35	0.41
1:A:394:LEU:HD23	1:A:395:ARG:N	2.35	0.41
1:A:398:GLN:HB3	1:A:408:ILE:CD1	2.27	0.41
1:A:441:ARG:O	1:A:442:GLN:C	2.57	0.41
1:A:285:ASP:HA	1:A:288:ARG:HD3	2.02	0.41
1:A:298:ILE:O	1:A:299:PRO:C	2.56	0.41
1:A:517:PHE:CD2	1:A:517:PHE:C	2.93	0.41
1:A:354:ARG:O	1:A:363:CYS:SG	2.79	0.41
1:A:386:GLU:HB2	1:A:393:LYS:HG2	2.02	0.41
1:A:425:PRO:HG2	1:A:509:PHE:CZ	2.49	0.41
1:A:492:MET:HE3	1:A:493:VAL:N	2.35	0.41
1:A:283:PRO:HB2	1:A:288:ARG:HB2	2.03	0.41
1:A:352:THR:HG22	1:A:352:THR:O	2.21	0.41
1:A:471:LEU:CD2	1:A:486:ILE:HD13	2.51	0.41
1:A:312:GLN:NE2	1:A:496:GLN:OE1	2.54	0.41
1:A:321:LYS:HD3	1:A:451:ILE:HD12	2.03	0.41
1:A:347:ARG:NH1	1:A:347:ARG:CG	2.83	0.41
1:A:434:PHE:O	1:A:438:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:GLY:HA2	1:A:462:THR:OG1	2.21	0.41
1:A:496:GLN:HE21	1:A:496:GLN:HB3	1.67	0.41
1:A:342:TRP:CG	1:A:379:TYR:CZ	3.09	0.41
1:A:270:PRO:HG2	1:A:271:GLU:OE2	2.21	0.40
1:A:351:MET:HG2	1:A:353:THR:O	2.21	0.40
1:A:278:TYR:CE2	2:B:1469:PTR:CB	2.90	0.40
1:A:370:VAL:CG1	1:A:385:GLY:HA2	2.51	0.40
1:A:473:GLU:HA	1:A:476:SER:HB2	2.03	0.40
1:A:377:GLY:HA3	1:A:378:PRO:HD3	1.92	0.40
1:A:412:TRP:CE3	1:A:441:ARG:NH2	2.89	0.40
1:A:498:SER:CB	2:B:1473:ASP:C	2.90	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	282/284 (99%)	228 (81%)	36 (13%)	18 (6%)	1	1
2	B	7/10 (70%)	1 (14%)	4 (57%)	2 (29%)	0	0
All	All	289/294 (98%)	229 (79%)	40 (14%)	20 (7%)	1	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	A	458	GLY
2	B	1470	ALA
1	A	299	PRO
1	A	319	ASN
1	A	368	PRO
1	A	388	ASP

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Mol	Chain	Res	Type
1	A	495	ALA
1	A	333	THR
1	A	421	ASP
1	A	332	ALA
2	B	1467	LEU
1	A	329	CYS
1	A	361	ASN
1	A	501	VAL
1	A	359	GLY
1	A	420	PRO
1	A	459	ILE
1	A	356	VAL
1	A	324	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	251/251 (100%)	188 (75%)	63 (25%)	0	1
2	B	8/8 (100%)	2 (25%)	6 (75%)	0	0
All	All	259/259 (100%)	190 (73%)	69 (27%)	0	0

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	GLU
1	A	256	GLN
1	A	258	VAL
1	A	259	LYS
1	A	260	ASN
1	A	263	GLN
1	A	265	LEU
1	A	271	GLU
1	A	273	LYS
1	A	277	ARG

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Mol	Chain	Res	Type
1	A	279	LYS
1	A	281	ILE
1	A	288	ARG
1	A	291	LEU
1	A	309	ILE
1	A	312	GLN
1	A	313	LEU
1	A	319	ASN
1	A	321	LYS
1	A	326	SER
1	A	333	THR
1	A	335	ASN
1	A	347	ARG
1	A	362	LYS
1	A	364	VAL
1	A	370	VAL
1	A	372	MET
1	A	374	ARG
1	A	381	VAL
1	A	388	ASP
1	A	390	THR
1	A	393	LYS
1	A	397	LEU
1	A	400	SER
1	A	402	LEU
1	A	403	ASP
1	A	409	ARG
1	A	410	GLU
1	A	417	LEU
1	A	418	SER
1	A	422	HIS
1	A	424	VAL
1	A	427	GLU
1	A	432	LEU
1	A	440	GLN
1	A	445	LEU
1	A	447	HIS
1	A	454	HIS
1	A	456	SER
1	A	478	LYS
1	A	480	LEU
1	A	485	ASP

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Mol	Chain	Res	Type
1	A	490	ILE
1	A	492	MET
1	A	496	GLN
1	A	504	GLU
1	A	506	GLN
1	A	517	PHE
1	A	519	GLU
1	A	521	THR
1	A	522	LYS
1	A	524	LYS
1	A	526	GLU
2	B	1464	GLU
2	B	1465	ASP
2	B	1466	THR
2	B	1467	LEU
2	B	1471	ASP
2	B	1472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	260	ASN
1	A	272	ASN
1	A	286	HIS
1	A	311	ASN
1	A	312	GLN
1	A	339	GLN
1	A	404	ASN
1	A	415	GLN
1	A	447	HIS
1	A	487	GLN
1	A	496	GLN
1	A	516	GLN

5.3.3 RNA (i)

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	#$|Z| > 2$
2	PTR	B	1469	1,2	15,16,17	1.85	1 (6%)	19,22,24	0.94	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
2	PTR	B	1469	1,2	-	3/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1469	PTR	P-OH	-6.45	1.49	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1469	PTR	CB-CA-C	-2.68	106.44	111.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1469	PTR	O-C-CA-CB
2	B	1469	PTR	N-CA-CB-CG
2	B	1469	PTR	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1469	PTR	23	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.