



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:57 AM GMT

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.
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Deposited on : 2000-08-31
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

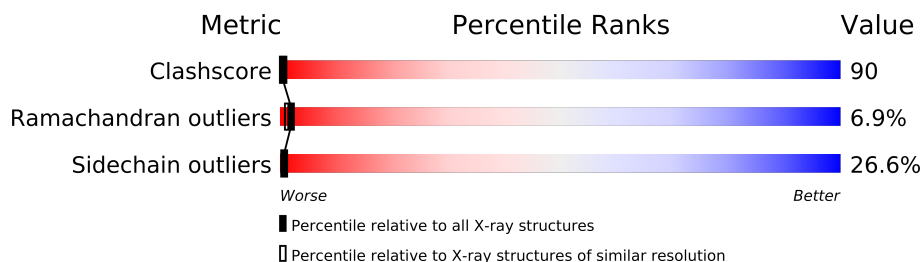
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	284	
2	B	10	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2374 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 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	UNP P29350

- Molecule 2 is a protein called PEPTIDE PY469.

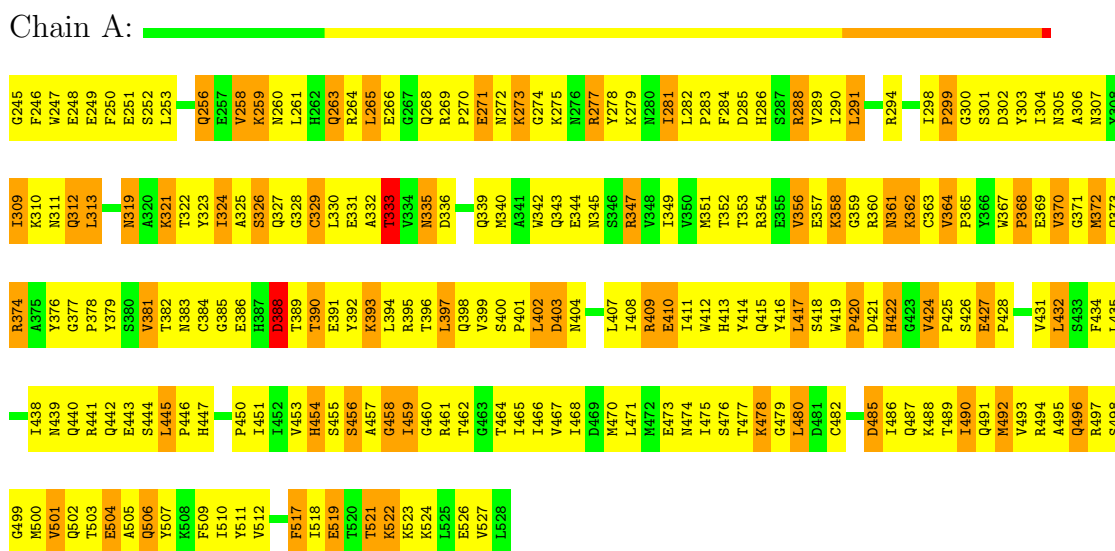
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			85	49	10	25	1			

3 Residue-property plots

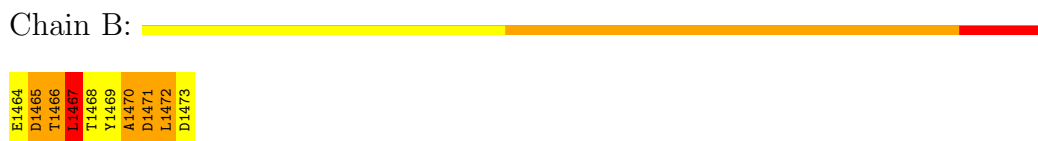
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: PROTEIN-TYROSINE PHOSPHATASE 1C



• Molecule 2: PEPTIDE PY469



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

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	0.38	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 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	2289	0	2243	412	0
2	B	85	0	65	59	0
All	All	2374	0	2308	422	0

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 90.

All (422) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:H	1:A:445:LEU:HD22	1.40	0.85
1:A:428:PRO:O	1:A:432:LEU:HB2	1.76	0.85
1:A:369:GLU:O	1:A:372:MET: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
1:A:498:SER:HB3	2:B:1473:ASP:O	1.76	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:ARG:NH1	2:B:1465:ASP:HB3	1.92	0.84
1:A:522:LYS:HB2	1:A:522:LYS:HZ3	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:278:TYR:CZ	2:B:1469:PTR:CB	2.63	0.82
1:A:273:LYS:HE3	1:A:274:GLY:H	1.44	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:N	1:A:445:LEU:HD22	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:467:VAL:HG12	1:A:471:LEU:HD12	1.75	0.69
1:A:291:LEU:HD23	1:A:294:ARG:NH2	2.08	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:N	1:A:417:LEU:HD23	2.06	0.68
1:A:389:THR:HG22	1:A:390:THR:N	2.08	0.68
1:A:498:SER:HB2	2:B:1473:ASP:H	1.59	0.67
1:A:386:GLU:HB3	1:A:395:ARG:HG2	1.75	0.67
1:A:522:LYS:HZ3	1:A:522:LYS:CB	2.07	0.67
1:A:324:ILE:HG22	1:A:324:ILE:O	1.92	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:428:PRO:HG3	1:A:512:VAL:HG12	1.75	0.67
1:A:309:ILE:HD11	1:A:325:ALA:CB	2.25	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:455:SER:HB2	2:B:1469:PTR:O2P	1.95	0.67
1:A:395:ARG:NH1	1:A:415:GLN:NE2	2.39	0.67
1:A:392:TYR:HA	1:A:417:LEU:HD23	1.75	0.66
1:A:311:ASN:ND2	1:A:313:LEU:HB2	2.11	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:HH11	1:A:347:ARG:HG2	1.61	0.65
1:A:420:PRO:HD2	1:A:425:PRO:HD3	1.78	0.65
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:ARG:HE	1:A:330:LEU:HD13	1.61	0.64
1:A:431:VAL:HA	1:A:434:PHE:HB3	1.79	0.64
1:A:372:MET:HE2	1:A:372:MET:HA	1.78	0.64
1:A:322:THR:OG1	1:A:450:PRO:HA	1.96	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:498:SER:HB2	2:B:1473:ASP:N	2.14	0.62
1:A:404:ASN:ND2	1:A:407:LEU:HB2	2.13	0.62
1:A:424:VAL:HG22	1:A:425:PRO:HD2	1.81	0.62
1:A:339:GLN:HA	1:A:379:TYR:HE1	1.63	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:O	1:A:281:ILE:HG22	2.00	0.62
1:A:347:ARG:O	1:A:411:ILE:HG23	2.00	0.62
1:A:467:VAL:HG12	1:A:471:LEU:HD11	1.82	0.61
1:A:335:ASN:HD22	1:A:377:GLY:N	1.99	0.61
1:A:356:VAL:HB	1:A:362:LYS:HG2	1.82	0.61
1:A:277:ARG:NH1	1:A:456:SER:HB3	2.15	0.61
1:A:322:THR:O	1:A:451:ILE:N	2.32	0.61
1:A:417:LEU:CD2	1:A:417:LEU:N	2.63	0.60
2:B:1471:ASP:OD1	2:B:1471:ASP:C	2.39	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:LYS:HB2	1:A:259:LYS:HZ3	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:461:ARG:HG3	2:B:1469:PTR:O1P	2.02	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: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:278:TYR:OH	2:B:1469:PTR:CG	2.52	0.58
1:A:259:LYS:HZ1	2:B:1472:LEU:HD13	1.69	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
2:B:1466:THR:OG1	2:B:1467:LEU:N	2.37	0.57
1:A:374:ARG:HG2	1:A:376:TYR:CE1	2.38	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:358:LYS:O	1:A:360:ARG:N	2.33	0.57
1:A:321:LYS:HD3	1:A:451:ILE:HD11	1.87	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:457:ALA:O	1:A:459:ILE:CG1	2.53	0.56
1:A:398:GLN:CD	1:A:410:GLU:HG3	2.26	0.56
1:A:284:PHE:CB	1:A:286:HIS:HE1	2.18	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:442:GLN:HA	1:A:445:LEU:HD23	1.88	0.56
1:A:266:GLU:HG3	1:A:288:ARG:CZ	2.36	0.56
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:331:GLU:HG3	1:A:364:VAL:HG11	1.88	0.55
1:A:252:SER:O	1:A:256:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:ARG:HG3	1:A:302:ASP:HA	1.89	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:502:GLN:NE2	2:B:1471:ASP:O	2.39	0.54
1:A:445:LEU:CD2	1:A:445:LEU:H	2.15	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: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:384:CYS:N	1:A:396:THR:O	2.28	0.54
1:A:490:ILE:HG23	1:A:501:VAL:HG21	1.90	0.53
1:A:386:GLU:OE2	1:A:393:LYS:HE2	2.08	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:386:GLU:HB2	1:A:393:LYS:CG	2.39	0.53
1:A:378:PRO:O	1:A:402:LEU:HD12	2.08	0.53
1:A:278:TYR:CE1	2:B:1469:PTR:CB	2.92	0.53
1:A:388:ASP:N	1:A:388:ASP:OD1	2.41	0.53
1:A:504:GLU:OE2	1:A:504:GLU:HA	2.05	0.53
1:A:328:GLY:HA3	1:A:455:SER:O	2.09	0.53
2:B:1466:THR:O	2:B:1467:LEU:HD22	2.09	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
1:A:272:ASN:ND2	1:A:275:LYS:HD2	2.24	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:471:LEU:O	1:A:475:ILE:HD12	2.09	0.52
1:A:305:ASN:OD1	1:A:497:ARG:NH2	2.37	0.52
1:A:306:ALA:HB2	1:A:326:SER:HB3	1.91	0.52
1:A:394:LEU:HD11	1:A:441:ARG:HH21	1.75	0.52
1:A:371:GLY:O	1:A:372:MET:CE	2.58	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:428:PRO:HG3	1:A:512:VAL:CG1	2.40	0.51
1:A:278:TYR:CE1	2:B:1469:PTR:CD1	2.94	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:468:ILE:HG13	1:A:510:ILE:HG12	1.92	0.51
1:A:349:ILE:CD1	1:A:411:ILE:HG21	2.41	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:466:ILE:O	1:A:470:MET:HG3	2.12	0.50
1:A:426:SER:C	1:A:427:GLU:HG3	2.30	0.50
1:A:419:TRP:CD1	1:A:420:PRO:HD2	2.46	0.50
1:A:269:ARG:C	1:A:271:GLU:H	2.13	0.50
1:A:416:TYR:CZ	1:A:431:VAL:HG12	2.46	0.50
1:A:258:VAL:HA	1:A:261:LEU:HG	1.92	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
2:B:1468:THR:HG22	2:B:1469:PTR:N	2.26	0.50
1:A:454:HIS:C	1:A:454:HIS:ND1	2.64	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:324:ILE:HG22	1:A:326:SER:OG	2.12	0.49
1:A:275:LYS:HD3	1:A:303:TYR:HD2	1.76	0.49
1:A:281:ILE:HA	2:B:1472:LEU:HD21	1.94	0.49
1:A:364:VAL:HG22	1:A:365:PRO:CD	2.27	0.49
1:A:245:GLY:O	1:A:249:GLU:HG2	2.12	0.49
1:A:329:CYS:HB2	1:A:364:VAL:N	2.28	0.49
1:A:259:LYS:CE	2:B:1472:LEU:HD13	2.42	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
1:A:480:LEU:HD21	1:A:521:THR:HG22	1.88	0.48
1:A:475:ILE:HG21	1:A:517:PHE:HE2	1.78	0.48
1:A:459:ILE:HG13	1:A:460:GLY:H	1.78	0.48
1:A:333:THR:HG22	1:A:336:ASP:CB	2.41	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:357:GLU:CA	1:A:361:ASN:HA	2.37	0.48
1:A:269:ARG:HB2	1:A:271:GLU:HG2	1.96	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: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:278:TYR:CD1	1:A:457:ALA:CB	2.96	0.47
1:A:263:GLN:CD	1:A:265:LEU:HD13	2.33	0.47
1:A:321:LYS:HG2	1:A:323:TYR:CZ	2.50	0.47
1:A:349:ILE:HD12	1:A:411:ILE:HG21	1.96	0.47
1:A:306:ALA:CA	1:A:497:ARG:NH1	2.78	0.47
1:A:486:ILE:O	1:A:490:ILE:CG1	2.58	0.47
1:A:360:ARG:CD	2:B:1465:ASP:HA	2.45	0.47
1:A:345:ASN:ND2	1:A:347:ARG:NH1	2.63	0.47
1:A:259:LYS:HE3	2:B:1472:LEU:HD13	1.95	0.46
1:A:490:ILE:H	1:A:490:ILE:HG13	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:357:GLU:O	1:A:360:ARG:N	2.49	0.46
1:A:321:LYS:HG3	1:A:322:THR:N	2.31	0.46
1:A:471:LEU:HD21	1:A:486:ILE:HD13	1.97	0.46
1:A:386:GLU:OE2	1:A:393:LYS:CD	2.60	0.46
1:A:457:ALA:O	1:A:459:ILE:N	2.49	0.46
1:A:347:ARG:HH11	1:A:347:ARG:CG	2.29	0.46
1:A:419:TRP:CZ3	1:A:465:ILE:HD11	2.44	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
2:B:1467:LEU:O	2:B:1468:THR:OG1	2.30	0.45
1:A:441:ARG:O	1:A:444:SER:N	2.32	0.45
1:A:304:ILE:HD13	1:A:340:MET:HB2	1.98	0.45
1:A:519:GLU:O	1:A:519:GLU:HG2	2.17	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:459:ILE:HB	1:A:502:GLN:HE21	1.82	0.45
1:A:283:PRO:CB	1:A:307:ASN:OD1	2.64	0.45
1:A:474:ASN:O	1:A:478:LYS:HB2	2.17	0.45
1:A:356:VAL:O	1:A:358:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:412:TRP:CE3	1:A:441:ARG:CZ	3.00	0.45
1:A:246:PHE:HD2	1:A:247:TRP:CD1	2.35	0.45
1:A:250:PHE:C	1:A:252:SER:H	2.20	0.45
1:A:361:ASN:O	1:A:362:LYS:C	2.52	0.45
1:A:272:ASN:HD21	1:A:300:GLY:HA3	1.82	0.45
1:A:425:PRO:HG2	1:A:509:PHE:HE1	1.70	0.44
1:A:367:TRP:CZ3	1:A:413:HIS:NE2	2.85	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:500:MET:O	1:A:501:VAL:HB	2.18	0.44
1:A:498:SER:CB	2:B:1473:ASP:H	2.28	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
2:B:1469:PTR:HB2	2:B:1470:ALA:H	1.39	0.44
1:A:347:ARG:NH1	1:A:347:ARG:HG2	2.32	0.44
1:A:335:ASN:OD1	1:A:335:ASN:N	2.50	0.44
1:A:494:ARG:O	1:A:496:GLN:N	2.51	0.43
1:A:386:GLU:HA	1:A:395:ARG:HA	2.01	0.43
1:A:374:ARG:HD2	1:A:376:TYR:OH	2.18	0.43
1:A:368:PRO:HD2	1:A:383:ASN:HB2	1.99	0.43
1:A:269:ARG:C	1:A:271:GLU:N	2.71	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:356:VAL:N	1:A:363:CYS:HB3	2.33	0.43
1:A:278:TYR:HE2	2:B:1468:THR:O	1.97	0.43
1:A:498:SER:C	2:B:1472:LEU:HB3	2.38	0.43
1:A:396:THR:HG22	1:A:412:TRP:CZ3	2.53	0.43
1:A:349:ILE:HD12	1:A:411:ILE:CG2	2.48	0.43
1:A:386:GLU:HA	1:A:394:LEU:O	2.17	0.43
1:A:283:PRO:HB3	1:A:307:ASN:OD1	2.18	0.43
1:A:395:ARG:CZ	1:A:415:GLN:NE2	2.82	0.43
1:A:382:THR:O	1:A:397:LEU:HA	2.18	0.43
1:A:333:THR:HG23	1:A:336:ASP:OD1	2.19	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:492:MET:O	1:A:496:GLN:HG3	2.19	0.43
1:A:445:LEU:HA	1:A:446:PRO:HD2	1.75	0.43
1:A:500:MET:HE2	1:A:500:MET:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:PRO:HB2	1:A:372:MET:HB3	2.01	0.43
1:A:507:TYR:O	1:A:511:TYR:HD1	2.02	0.42
1:A:342:TRP:CH2	1:A:401:PRO:HD3	2.53	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:CD	1:A:347:ARG:N	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:455:SER:OG	2:B:1469:PTR:P	2.77	0.42
1:A:291:LEU:HD12	1:A:291:LEU:HA	1.76	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:517:PHE:C	1:A:517:PHE:CD2	2.93	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:354:ARG:O	1:A:363:CYS:SG	2.79	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:386:GLU:HB2	1:A:393:LYS:HG2	2.02	0.41
1:A:471:LEU:CD2	1:A:486:ILE:HD13	2.51	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:312:GLN:NE2	1:A:496:GLN:OE1	2.54	0.41
1:A:496:GLN:HE21	1:A:496:GLN:HB3	1.67	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
1:A:458:GLY:HA2	1:A:462:THR:OG1	2.21	0.41
1:A:321:LYS:HD3	1:A:451:ILE:HD12	2.03	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:498:SER:CB	2:B:1473:ASP:C	2.90	0.40
1:A:412:TRP:CE3	1:A:441:ARG:NH2	2.89	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:377:GLY:HA3	1:A:378:PRO:HD3	1.92	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%)	2	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%)	2	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
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

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Mol	Chain	Res	Type
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%)	1	1
2	B	8/8 (100%)	2 (25%)	6 (75%)	0	0
All	All	259/259 (100%)	190 (73%)	69 (27%)	1	1

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	B	1467	LEU
2	B	1471	ASP
2	B	1472	LEU

Some 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 ⓘ

There are no RNA chains 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	16,16,17	5.08	3 (18%)	20,22,24	1.38	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	-	0/9/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1469	PTR	O-C	18.56	1.24	1.11
2	B	1469	PTR	P-OH	-7.10	1.49	1.60
2	B	1469	PTR	CA-C	3.21	1.54	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1469	PTR	C-CA-N	5.44	119.26	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.