Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 05:50 PM EDT

PDB ID	:	1GWZ
Title	:	CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF THE PROTEIN TYROSINE PHOSPHATASE SHP-1
Authors	:	Yang, J.; Liang, X.; Niu, T.; Meng, W.; Zhao, Z.; Zhou, G.W.
Deposited on	:	1998-08-22
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

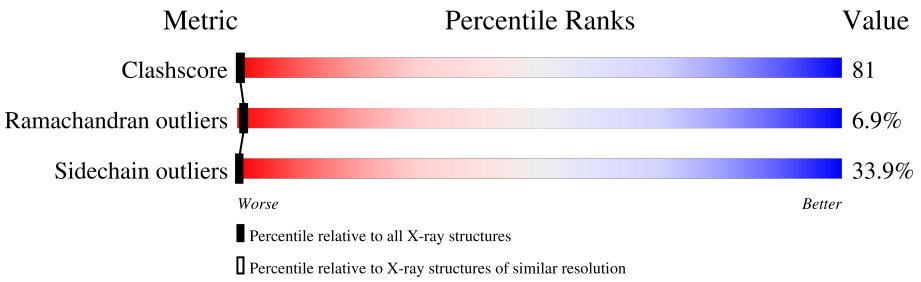
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 Å.

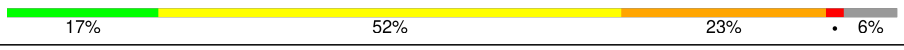
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	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	299	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2207 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 SHP-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2207	1385	396	414	12	0	0	0

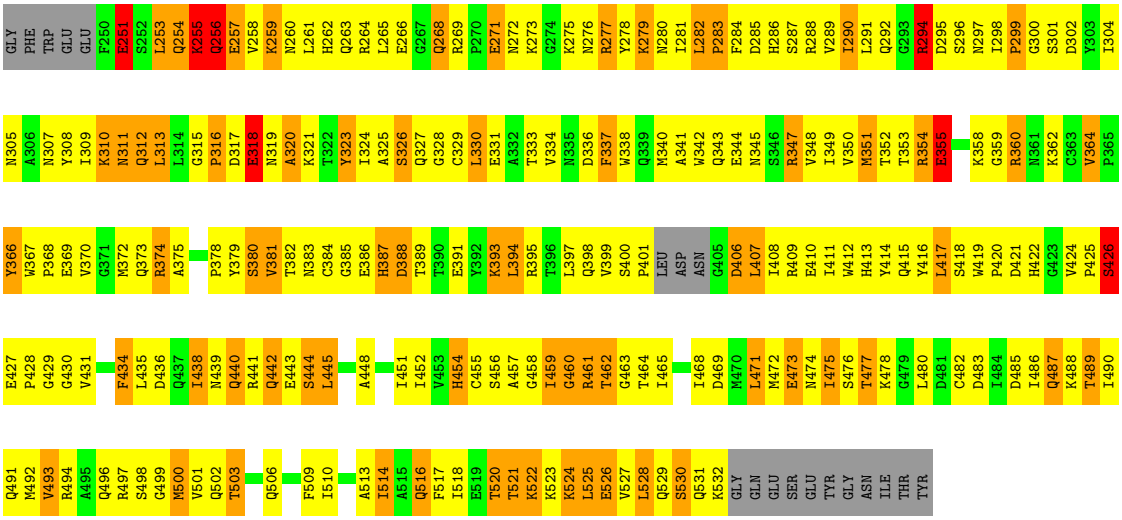
3 Residue-property plots (i)

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: SHP-1

Chain A: 17% 52% 23% • 6%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.82Å 87.78Å 43.00Å 90.00° 117.40° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.7 (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.209 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2207	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

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	0.57	0/2252	0.87	2/3050 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	GLU	N-CA-C	-5.62	95.82	111.00
1	A	318	GLU	N-CA-C	-5.59	95.89	111.00

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	2207	0	2149	351	0
All	All	2207	0	2149	351	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 81.

All (351) 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:347:ARG:NH2	1:A:409:ARG:HG2	1.46	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HH11	1:A:277:ARG:HB2	1.05	1.16
1:A:425:PRO:HB2	1:A:428:PRO:HG3	1.18	1.16
1:A:277:ARG:HH11	1:A:277:ARG:CB	1.63	1.10
1:A:394:LEU:HD21	1:A:412:TRP:HE3	1.18	1.07
1:A:521:THR:HG22	1:A:524:LYS:HE3	1.09	1.05
1:A:251:GLU:CB	1:A:253:LEU:HG	1.86	1.05
1:A:353:THR:HG22	1:A:461:ARG:NH2	1.71	1.04
1:A:463:GLY:HA2	1:A:500:MET:CE	1.89	1.02
1:A:426:SER:O	1:A:428:PRO:HD3	1.60	1.01
1:A:277:ARG:HB2	1:A:277:ARG:NH1	1.74	1.01
1:A:294:ARG:NH2	1:A:336:ASP:HB3	1.76	1.01
1:A:426:SER:C	1:A:428:PRO:HD3	1.81	1.00
1:A:311:ASN:O	1:A:492:MET:SD	2.21	0.99
1:A:475:ILE:HD12	1:A:480:LEU:HG	1.43	0.98
1:A:524:LYS:HD3	1:A:525:LEU:CD1	1.93	0.98
1:A:347:ARG:HH21	1:A:409:ARG:HG2	1.16	0.97
1:A:251:GLU:HB3	1:A:253:LEU:HG	1.44	0.96
1:A:340:MET:HA	1:A:343:GLN:HG2	1.45	0.96
1:A:497:ARG:O	1:A:500:MET:HG2	1.66	0.96
1:A:521:THR:HG22	1:A:524:LYS:CE	1.95	0.96
1:A:524:LYS:HD3	1:A:525:LEU:HD13	1.47	0.95
1:A:353:THR:HG22	1:A:461:ARG:CZ	1.98	0.94
1:A:294:ARG:HG3	1:A:294:ARG:HH11	1.31	0.93
1:A:521:THR:CG2	1:A:524:LYS:HE3	1.99	0.93
1:A:463:GLY:HA2	1:A:500:MET:HE1	1.49	0.91
1:A:388:ASP:HB3	1:A:393:LYS:HZ2	1.33	0.91
1:A:255:LYS:HD3	1:A:255:LYS:N	1.87	0.89
1:A:351:MET:HE3	1:A:415:GLN:OE1	1.73	0.88
1:A:419:TRP:NE1	1:A:424:VAL:HA	1.89	0.88
1:A:521:THR:O	1:A:524:LYS:HD2	1.74	0.87
1:A:347:ARG:CZ	1:A:409:ARG:HG2	2.04	0.87
1:A:261:LEU:CB	1:A:286:HIS:ND1	2.38	0.86
1:A:384:CYS:SG	1:A:398:GLN:HG3	2.15	0.86
1:A:419:TRP:HE1	1:A:424:VAL:HA	1.41	0.86
1:A:342:TRP:CH2	1:A:401:PRO:HD3	2.12	0.85
1:A:281:ILE:HD13	1:A:459:ILE:HD11	1.57	0.84
1:A:251:GLU:HB2	1:A:253:LEU:HG	1.57	0.83
1:A:271:GLU:HG3	1:A:299:PRO:CB	2.08	0.83
1:A:387:HIS:HB2	1:A:394:LEU:HB3	1.61	0.83
1:A:348:VAL:HG12	1:A:451:ILE:HG23	1.62	0.81
1:A:394:LEU:HD21	1:A:412:TRP:CE3	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:GLU:HG2	1:A:443:GLU:O	1.81	0.80
1:A:463:GLY:HA2	1:A:500:MET:HE3	1.61	0.80
1:A:261:LEU:CB	1:A:286:HIS:CG	2.65	0.80
1:A:471:LEU:O	1:A:475:ILE:HG23	1.80	0.80
1:A:430:GLY:O	1:A:434:PHE:HB3	1.83	0.79
1:A:524:LYS:CD	1:A:525:LEU:HD13	2.11	0.79
1:A:271:GLU:HG3	1:A:299:PRO:HB3	1.65	0.78
1:A:310:LYS:HE3	1:A:313:LEU:HA	1.65	0.78
1:A:271:GLU:OE1	1:A:271:GLU:N	2.17	0.77
1:A:269:ARG:HB2	1:A:272:ASN:OD1	1.85	0.76
1:A:424:VAL:HG13	1:A:425:PRO:HD2	1.67	0.76
1:A:266:GLU:HA	1:A:266:GLU:OE1	1.84	0.76
1:A:485:ASP:OD2	1:A:488:LYS:HB2	1.84	0.76
1:A:294:ARG:HG3	1:A:294:ARG:NH1	2.00	0.76
1:A:485:ASP:OD2	1:A:488:LYS:CB	2.35	0.75
1:A:381:VAL:HB	1:A:399:VAL:HG22	1.69	0.75
1:A:342:TRP:HH2	1:A:401:PRO:HD3	1.49	0.75
1:A:425:PRO:HB2	1:A:428:PRO:CG	2.10	0.74
1:A:421:ASP:HB2	1:A:461:ARG:CZ	2.18	0.74
1:A:524:LYS:HA	1:A:526:GLU:OE2	1.88	0.74
1:A:490:ILE:CD1	1:A:501:VAL:HG21	2.18	0.74
1:A:308:TYR:C	1:A:309:ILE:HG12	2.08	0.73
1:A:426:SER:O	1:A:428:PRO:CD	2.35	0.73
1:A:401:PRO:HG3	1:A:407:LEU:HB2	1.70	0.72
1:A:419:TRP:CD1	1:A:425:PRO:HD3	2.23	0.71
1:A:475:ILE:HG12	1:A:517:PHE:HE2	1.53	0.71
1:A:473:GLU:O	1:A:477:THR:HG23	1.90	0.71
1:A:256:GLN:O	1:A:256:GLN:CD	2.28	0.71
1:A:261:LEU:CB	1:A:263:GLN:OE1	2.39	0.71
1:A:351:MET:CE	1:A:415:GLN:OE1	2.38	0.71
1:A:531:GLN:O	1:A:532:LYS:O	2.09	0.70
1:A:294:ARG:HH22	1:A:336:ASP:HB3	1.55	0.70
1:A:388:ASP:HB3	1:A:393:LYS:NZ	2.05	0.70
1:A:290:ILE:HG23	1:A:302:ASP:OD2	1.91	0.70
1:A:310:LYS:CE	1:A:313:LEU:HA	2.21	0.70
1:A:362:LYS:O	1:A:456:SER:HB2	1.92	0.70
1:A:517:PHE:O	1:A:521:THR:OG1	2.10	0.69
1:A:418:SER:O	1:A:420:PRO:HD3	1.92	0.69
1:A:294:ARG:NH1	1:A:301:SER:O	2.27	0.68
1:A:271:GLU:HG3	1:A:299:PRO:HB2	1.75	0.68
1:A:277:ARG:CB	1:A:277:ARG:NH1	2.45	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HD13	1:A:336:ASP:HB2	1.76	0.67
1:A:524:LYS:HD3	1:A:525:LEU:HD11	1.74	0.67
1:A:367:TRP:CZ2	1:A:395:ARG:NH1	2.63	0.67
1:A:436:ASP:O	1:A:440:GLN:HG3	1.94	0.67
1:A:353:THR:HG22	1:A:461:ARG:HH22	1.58	0.67
1:A:421:ASP:HB2	1:A:461:ARG:NH1	2.10	0.67
1:A:424:VAL:CG1	1:A:509:PHE:CD1	2.78	0.67
1:A:266:GLU:HB2	1:A:285:ASP:OD1	1.95	0.67
1:A:493:VAL:HG13	1:A:500:MET:HG3	1.77	0.67
1:A:347:ARG:HH22	1:A:410:GLU:C	1.98	0.66
1:A:417:LEU:N	1:A:417:LEU:HD13	2.09	0.66
1:A:424:VAL:HG12	1:A:425:PRO:O	1.95	0.66
1:A:378:PRO:O	1:A:379:TYR:CD1	2.49	0.65
1:A:294:ARG:HH21	1:A:336:ASP:HB3	1.59	0.65
1:A:328:GLY:N	1:A:456:SER:O	2.30	0.65
1:A:490:ILE:HD11	1:A:501:VAL:HG21	1.79	0.65
1:A:294:ARG:HB3	1:A:301:SER:HB2	1.79	0.65
1:A:424:VAL:HG13	1:A:425:PRO:CD	2.26	0.65
1:A:394:LEU:CD2	1:A:412:TRP:HE3	2.04	0.64
1:A:310:LYS:HZ2	1:A:313:LEU:HD23	1.63	0.64
1:A:524:LYS:CA	1:A:526:GLU:OE2	2.45	0.64
1:A:328:GLY:HA3	1:A:456:SER:HA	1.79	0.64
1:A:424:VAL:HG11	1:A:509:PHE:CD1	2.33	0.64
1:A:253:LEU:HD23	1:A:253:LEU:N	2.12	0.63
1:A:323:TYR:CD1	1:A:323:TYR:N	2.66	0.63
1:A:463:GLY:CA	1:A:500:MET:CE	2.72	0.63
1:A:386:GLU:HG2	1:A:393:LYS:HE3	1.79	0.63
1:A:520:THR:HG22	1:A:521:THR:N	2.13	0.63
1:A:329:CYS:HB3	1:A:364:VAL:HG12	1.81	0.62
1:A:337:PHE:HD1	1:A:338:TRP:N	1.96	0.62
1:A:528:LEU:HD23	1:A:530:SER:N	2.14	0.62
1:A:259:LYS:HD3	1:A:259:LYS:O	1.99	0.62
1:A:350:VAL:HG22	1:A:438:ILE:HD13	1.82	0.62
1:A:294:ARG:HG3	1:A:301:SER:O	1.99	0.62
1:A:373:GLN:HG2	1:A:374:ARG:N	2.13	0.62
1:A:288:ARG:NH2	1:A:302:ASP:OD2	2.30	0.61
1:A:408:ILE:O	1:A:408:ILE:HG22	2.00	0.61
1:A:337:PHE:HZ	1:A:349:ILE:HD13	1.65	0.61
1:A:347:ARG:NH2	1:A:410:GLU:O	2.34	0.61
1:A:419:TRP:NE1	1:A:425:PRO:HD3	2.16	0.61
1:A:347:ARG:HH22	1:A:410:GLU:N	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HG2	1:A:360:ARG:HH11	1.66	0.60
1:A:490:ILE:O	1:A:493:VAL:HG12	2.01	0.60
1:A:310:LYS:O	1:A:311:ASN:C	2.40	0.60
1:A:350:VAL:HG13	1:A:434:PHE:HZ	1.66	0.60
1:A:401:PRO:CG	1:A:407:LEU:HB2	2.32	0.60
1:A:310:LYS:NZ	1:A:313:LEU:HD23	2.17	0.60
1:A:524:LYS:C	1:A:526:GLU:OE2	2.40	0.60
1:A:353:THR:CG2	1:A:461:ARG:CZ	2.77	0.59
1:A:255:LYS:N	1:A:255:LYS:CD	2.65	0.59
1:A:319:ASN:O	1:A:320:ALA:O	2.19	0.59
1:A:291:LEU:CD1	1:A:336:ASP:HB2	2.32	0.59
1:A:480:LEU:HD23	1:A:518:ILE:HG23	1.83	0.59
1:A:255:LYS:HD3	1:A:255:LYS:H	1.63	0.59
1:A:492:MET:O	1:A:496:GLN:NE2	2.35	0.59
1:A:518:ILE:O	1:A:522:LYS:HB2	2.02	0.59
1:A:337:PHE:CD1	1:A:338:TRP:N	2.70	0.59
1:A:475:ILE:CD1	1:A:480:LEU:HG	2.26	0.59
1:A:350:VAL:HG22	1:A:438:ILE:CD1	2.33	0.58
1:A:521:THR:O	1:A:524:LYS:CD	2.48	0.58
1:A:353:THR:CG2	1:A:461:ARG:NH1	2.66	0.58
1:A:463:GLY:CA	1:A:500:MET:HE3	2.33	0.58
1:A:325:ALA:HB3	1:A:497:ARG:HD3	1.84	0.58
1:A:347:ARG:NH1	1:A:410:GLU:O	2.38	0.57
1:A:485:ASP:CG	1:A:488:LYS:HB3	2.25	0.57
1:A:524:LYS:CD	1:A:525:LEU:CD1	2.73	0.57
1:A:526:GLU:H	1:A:526:GLU:CD	2.08	0.57
1:A:354:ARG:NH2	1:A:417:LEU:HB2	2.20	0.57
1:A:292:GLN:HE21	1:A:343:GLN:CD	2.08	0.57
1:A:524:LYS:HG2	1:A:525:LEU:CD1	2.35	0.57
1:A:284:PHE:HB3	1:A:286:HIS:CE1	2.40	0.56
1:A:475:ILE:HD13	1:A:518:ILE:HD13	1.87	0.56
1:A:277:ARG:HH11	1:A:277:ARG:CG	2.17	0.56
1:A:460:GLY:O	1:A:464:THR:OG1	2.18	0.56
1:A:307:ASN:OD1	1:A:497:ARG:HD2	2.05	0.56
1:A:251:GLU:HB3	1:A:253:LEU:CG	2.28	0.56
1:A:521:THR:C	1:A:524:LYS:HD2	2.26	0.56
1:A:358:LYS:C	1:A:360:ARG:H	2.10	0.56
1:A:456:SER:OG	1:A:457:ALA:N	2.39	0.56
1:A:391:GLU:HG2	1:A:416:TYR:OH	2.05	0.55
1:A:266:GLU:HG3	1:A:288:ARG:CZ	2.37	0.55
1:A:317:ASP:C	1:A:318:GLU:O	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CD1	1:A:337:PHE:C	2.80	0.55
1:A:406:ASP:OD1	1:A:408:ILE:HD12	2.06	0.55
1:A:287:SER:C	1:A:307:ASN:HD22	2.10	0.55
1:A:326:SER:O	1:A:454:HIS:HB2	2.07	0.55
1:A:360:ARG:HG2	1:A:360:ARG:NH1	2.21	0.55
1:A:445:LEU:HB2	1:A:448:ALA:HB2	1.89	0.54
1:A:440:GLN:HA	1:A:443:GLU:HB3	1.89	0.54
1:A:338:TRP:CZ3	1:A:399:VAL:HG21	2.43	0.53
1:A:384:CYS:SG	1:A:398:GLN:CG	2.94	0.53
1:A:266:GLU:O	1:A:269:ARG:HG3	2.09	0.53
1:A:278:TYR:HE2	1:A:457:ALA:HB2	1.73	0.53
1:A:353:THR:HG22	1:A:461:ARG:NH1	2.20	0.53
1:A:386:GLU:HG2	1:A:393:LYS:CE	2.39	0.53
1:A:475:ILE:HG13	1:A:476:SER:N	2.17	0.53
1:A:259:LYS:O	1:A:259:LYS:CG	2.55	0.53
1:A:347:ARG:HE	1:A:409:ARG:HD3	1.73	0.53
1:A:468:ILE:HD13	1:A:513:ALA:CB	2.39	0.53
1:A:366:TYR:CD1	1:A:366:TYR:N	2.77	0.53
1:A:334:VAL:CG1	1:A:364:VAL:CG1	2.87	0.52
1:A:430:GLY:O	1:A:434:PHE:CB	2.56	0.52
1:A:485:ASP:OD2	1:A:488:LYS:HB3	2.07	0.52
1:A:347:ARG:NH2	1:A:409:ARG:CG	2.42	0.52
1:A:385:GLY:O	1:A:387:HIS:CE1	2.62	0.52
1:A:471:LEU:HD21	1:A:486:ILE:HG12	1.92	0.52
1:A:424:VAL:CG1	1:A:425:PRO:N	2.72	0.52
1:A:442:GLN:C	1:A:444:SER:H	2.14	0.52
1:A:255:LYS:CD	1:A:255:LYS:H	2.23	0.51
1:A:284:PHE:HB3	1:A:286:HIS:ND1	2.25	0.51
1:A:486:ILE:HA	1:A:489:THR:OG1	2.09	0.51
1:A:435:LEU:O	1:A:439:ASN:ND2	2.43	0.51
1:A:463:GLY:CA	1:A:500:MET:HE1	2.33	0.51
1:A:259:LYS:NZ	1:A:262:HIS:HB3	2.26	0.51
1:A:424:VAL:HG13	1:A:509:PHE:CD1	2.46	0.51
1:A:426:SER:C	1:A:428:PRO:CD	2.68	0.51
1:A:386:GLU:CG	1:A:393:LYS:HE3	2.41	0.51
1:A:275:LYS:NZ	1:A:300:GLY:O	2.44	0.51
1:A:340:MET:CA	1:A:343:GLN:HG2	2.30	0.51
1:A:347:ARG:HH21	1:A:409:ARG:CG	2.05	0.51
1:A:474:ASN:OD1	1:A:478:LYS:HE2	2.11	0.51
1:A:373:GLN:CG	1:A:374:ARG:N	2.74	0.50
1:A:258:VAL:O	1:A:259:LYS:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TYR:CE2	1:A:457:ALA:HB2	2.46	0.50
1:A:354:ARG:NH2	1:A:417:LEU:CB	2.74	0.50
1:A:280:ASN:OD1	1:A:280:ASN:N	2.34	0.50
1:A:355:GLU:O	1:A:362:LYS:N	2.43	0.49
1:A:487:GLN:O	1:A:491:GLN:HG2	2.12	0.49
1:A:266:GLU:HG3	1:A:288:ARG:NH1	2.27	0.49
1:A:351:MET:HE1	1:A:367:TRP:HH2	1.77	0.49
1:A:378:PRO:O	1:A:401:PRO:O	2.30	0.49
1:A:294:ARG:HD3	1:A:294:ARG:N	2.27	0.49
1:A:308:TYR:O	1:A:309:ILE:HG12	2.11	0.49
1:A:387:HIS:CD2	1:A:394:LEU:HD13	2.47	0.49
1:A:490:ILE:HD13	1:A:501:VAL:CG2	2.43	0.49
1:A:263:GLN:O	1:A:284:PHE:HA	2.12	0.49
1:A:268:GLN:O	1:A:269:ARG:C	2.51	0.49
1:A:292:GLN:NE2	1:A:343:GLN:HB2	2.28	0.49
1:A:388:ASP:OD1	1:A:388:ASP:N	2.45	0.49
1:A:276:ASN:HA	1:A:327:GLN:HE22	1.76	0.49
1:A:386:GLU:HB3	1:A:393:LYS:HE3	1.94	0.49
1:A:510:ILE:O	1:A:514:ILE:HG12	2.12	0.49
1:A:310:LYS:O	1:A:311:ASN:O	2.31	0.49
1:A:475:ILE:HG12	1:A:517:PHE:CE2	2.43	0.49
1:A:279:LYS:O	1:A:282:LEU:HD21	2.12	0.48
1:A:459:ILE:O	1:A:500:MET:O	2.30	0.48
1:A:375:ALA:HA	1:A:380:SER:HA	1.95	0.48
1:A:516:GLN:O	1:A:517:PHE:C	2.50	0.48
1:A:358:LYS:O	1:A:360:ARG:N	2.46	0.48
1:A:255:LYS:O	1:A:257:GLU:N	2.47	0.48
1:A:330:LEU:HB2	1:A:333:THR:HG23	1.95	0.48
1:A:309:ILE:HD13	1:A:496:GLN:HB3	1.96	0.48
1:A:340:MET:HA	1:A:343:GLN:CG	2.32	0.48
1:A:329:CYS:HB3	1:A:334:VAL:HG12	1.94	0.48
1:A:347:ARG:CZ	1:A:410:GLU:O	2.62	0.48
1:A:441:ARG:O	1:A:445:LEU:HD12	2.14	0.48
1:A:524:LYS:CG	1:A:525:LEU:HD13	2.43	0.48
1:A:524:LYS:HG2	1:A:525:LEU:HD13	1.96	0.47
1:A:529:GLN:O	1:A:530:SER:HB2	2.14	0.47
1:A:264:ARG:HG2	1:A:284:PHE:HA	1.96	0.47
1:A:290:ILE:CG2	1:A:302:ASP:OD2	2.61	0.47
1:A:328:GLY:H	1:A:456:SER:C	2.18	0.47
1:A:366:TYR:OH	1:A:413:HIS:HE1	1.98	0.47
1:A:474:ASN:CG	1:A:478:LYS:HE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH1	1:A:277:ARG:CG	2.74	0.47
1:A:351:MET:CE	1:A:367:TRP:HH2	2.27	0.47
1:A:419:TRP:CE2	1:A:425:PRO:HD3	2.49	0.47
1:A:441:ARG:O	1:A:445:LEU:CD1	2.63	0.47
1:A:493:VAL:O	1:A:496:GLN:HB2	2.15	0.47
1:A:323:TYR:HA	1:A:451:ILE:O	2.14	0.47
1:A:424:VAL:HG11	1:A:509:PHE:HB2	1.96	0.47
1:A:490:ILE:HD13	1:A:501:VAL:HG21	1.92	0.47
1:A:340:MET:HG3	1:A:341:ALA:N	2.30	0.47
1:A:347:ARG:NH2	1:A:411:ILE:HG13	2.29	0.47
1:A:395:ARG:HB2	1:A:413:HIS:HB3	1.96	0.47
1:A:289:VAL:O	1:A:304:ILE:HG22	2.15	0.46
1:A:516:GLN:O	1:A:520:THR:HB	2.15	0.46
1:A:524:LYS:O	1:A:526:GLU:OE1	2.34	0.46
1:A:328:GLY:H	1:A:456:SER:CA	2.28	0.46
1:A:316:PRO:O	1:A:318:GLU:O	2.34	0.46
1:A:337:PHE:CZ	1:A:366:TYR:CE2	3.03	0.46
1:A:259:LYS:O	1:A:259:LYS:CD	2.63	0.46
1:A:354:ARG:O	1:A:355:GLU:C	2.54	0.46
1:A:412:TRP:CD1	1:A:441:ARG:HD2	2.51	0.46
1:A:525:LEU:HA	1:A:527:VAL:HG22	1.96	0.46
1:A:406:ASP:OD1	1:A:408:ILE:CD1	2.63	0.46
1:A:328:GLY:CA	1:A:456:SER:HA	2.46	0.46
1:A:251:GLU:C	1:A:253:LEU:N	2.69	0.45
1:A:347:ARG:CZ	1:A:409:ARG:CG	2.87	0.45
1:A:387:HIS:ND1	1:A:387:HIS:N	2.64	0.45
1:A:312:GLN:HG3	1:A:313:LEU:N	2.30	0.45
1:A:494:ARG:NH2	1:A:501:VAL:O	2.49	0.45
1:A:387:HIS:CB	1:A:394:LEU:HB3	2.41	0.45
1:A:455:CYS:SG	1:A:458:GLY:HA2	2.57	0.45
1:A:351:MET:HG2	1:A:415:GLN:HG3	1.98	0.45
1:A:503:THR:O	1:A:506:GLN:HB2	2.16	0.45
1:A:337:PHE:CZ	1:A:366:TYR:HE2	2.35	0.45
1:A:421:ASP:CB	1:A:461:ARG:CZ	2.91	0.45
1:A:285:ASP:HA	1:A:288:ARG:HD2	1.98	0.45
1:A:394:LEU:HD11	1:A:412:TRP:CZ3	2.51	0.44
1:A:264:ARG:O	1:A:268:GLN:HG3	2.17	0.44
1:A:292:GLN:NE2	1:A:343:GLN:CD	2.70	0.44
1:A:259:LYS:HZ2	1:A:262:HIS:HB3	1.81	0.44
1:A:334:VAL:HG11	1:A:364:VAL:CG1	2.47	0.44
1:A:524:LYS:CG	1:A:525:LEU:CD1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ILE:O	1:A:472:MET:HG3	2.17	0.44
1:A:277:ARG:NH1	1:A:330:LEU:HD21	2.33	0.44
1:A:298:ILE:HA	1:A:299:PRO:HD2	1.69	0.44
1:A:368:PRO:HD3	1:A:381:VAL:HG22	1.99	0.44
1:A:310:LYS:NZ	1:A:313:LEU:CD2	2.81	0.44
1:A:345:ASN:OD1	1:A:347:ARG:HD2	2.17	0.44
1:A:374:ARG:CG	1:A:374:ARG:HH11	2.30	0.44
1:A:345:ASN:O	1:A:347:ARG:HG2	2.18	0.43
1:A:386:GLU:HG3	1:A:395:ARG:HG3	1.99	0.43
1:A:455:CYS:SG	1:A:458:GLY:N	2.91	0.43
1:A:524:LYS:HG2	1:A:525:LEU:HD12	2.00	0.43
1:A:445:LEU:O	1:A:448:ALA:HB3	2.18	0.43
1:A:518:ILE:O	1:A:518:ILE:HG22	2.18	0.43
1:A:514:ILE:N	1:A:514:ILE:HD13	2.32	0.43
1:A:261:LEU:CB	1:A:286:HIS:CE1	3.02	0.43
1:A:285:ASP:HA	1:A:288:ARG:CD	2.48	0.43
1:A:520:THR:CG2	1:A:521:THR:N	2.80	0.43
1:A:337:PHE:O	1:A:340:MET:HG2	2.19	0.43
1:A:271:GLU:CD	1:A:271:GLU:H	2.18	0.42
1:A:272:ASN:O	1:A:273:LYS:C	2.57	0.42
1:A:318:GLU:OE1	1:A:319:ASN:OD1	2.36	0.42
1:A:524:LYS:O	1:A:526:GLU:CD	2.58	0.42
1:A:294:ARG:NH1	1:A:294:ARG:CG	2.73	0.42
1:A:254:GLN:CG	1:A:254:GLN:O	2.67	0.42
1:A:324:ILE:HD11	1:A:344:GLU:HG3	2.01	0.42
1:A:386:GLU:C	1:A:387:HIS:ND1	2.73	0.42
1:A:350:VAL:CG1	1:A:434:PHE:HZ	2.32	0.42
1:A:340:MET:O	1:A:344:GLU:HB2	2.20	0.42
1:A:334:VAL:CG1	1:A:364:VAL:HG11	2.50	0.42
1:A:421:ASP:CB	1:A:461:ARG:NH1	2.81	0.42
1:A:259:LYS:O	1:A:259:LYS:HG2	2.19	0.42
1:A:385:GLY:O	1:A:387:HIS:HE1	2.03	0.42
1:A:431:VAL:O	1:A:435:LEU:HD12	2.19	0.42
1:A:319:ASN:O	1:A:320:ALA:C	2.58	0.42
1:A:315:GLY:HA3	1:A:316:PRO:HD2	1.86	0.41
1:A:251:GLU:HB3	1:A:253:LEU:H	1.84	0.41
1:A:435:LEU:HD22	1:A:469:ASP:OD1	2.19	0.41
1:A:451:ILE:HG22	1:A:452:ILE:N	2.34	0.41
1:A:422:HIS:O	1:A:422:HIS:CD2	2.74	0.41
1:A:257:GLU:HB3	1:A:260:ASN:HB3	2.02	0.41
1:A:462:THR:HG22	1:A:463:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:HB2	1:A:461:ARG:NH2	2.35	0.41
1:A:386:GLU:CB	1:A:393:LYS:HE3	2.51	0.41
1:A:494:ARG:HG2	1:A:499:GLY:H	1.86	0.41
1:A:256:GLN:O	1:A:256:GLN:OE1	2.37	0.41
1:A:258:VAL:O	1:A:259:LYS:O	2.39	0.41
1:A:276:ASN:OD1	1:A:305:ASN:ND2	2.53	0.41
1:A:383:ASN:C	1:A:383:ASN:OD1	2.59	0.41
1:A:422:HIS:O	1:A:422:HIS:CG	2.74	0.41
1:A:282:LEU:CB	1:A:283:PRO:CD	2.99	0.41
1:A:368:PRO:HG2	1:A:381:VAL:O	2.21	0.41
1:A:414:TYR:HB2	1:A:438:ILE:HD11	2.02	0.41
1:A:428:PRO:CG	1:A:509:PHE:HE1	2.34	0.41
1:A:309:ILE:HA	1:A:496:GLN:OE1	2.21	0.40
1:A:428:PRO:HG2	1:A:509:PHE:HE1	1.86	0.40
1:A:295:ASP:C	1:A:297:ASN:N	2.74	0.40
1:A:354:ARG:HE	1:A:354:ARG:HB3	1.65	0.40
1:A:474:ASN:O	1:A:478:LYS:HB2	2.21	0.40
1:A:499:GLY:O	1:A:500:MET:C	2.60	0.40
1:A:265:LEU:H	1:A:265:LEU:HD22	1.86	0.40
1:A:330:LEU:O	1:A:331:GLU:C	2.58	0.40
1:A:354:ARG:CZ	1:A:417:LEU:HB2	2.52	0.40
1:A:415:GLN:HG2	1:A:417:LEU:HD12	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	276/299 (92%)	217 (79%)	40 (14%)	19 (7%)	1 1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	PRO
1	A	320	ALA
1	A	500	MET
1	A	255	LYS
1	A	256	GLN
1	A	311	ASN
1	A	316	PRO
1	A	406	ASP
1	A	426	SER
1	A	251	GLU
1	A	294	ARG
1	A	313	LEU
1	A	355	GLU
1	A	359	GLY
1	A	459	ILE
1	A	427	GLU
1	A	462	THR
1	A	460	GLY
1	A	429	GLY

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	236/264 (89%)	156 (66%)	80 (34%)	0 0

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	GLU
1	A	253	LEU
1	A	254	GLN
1	A	255	LYS
1	A	256	GLN
1	A	257	GLU
1	A	259	LYS
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	271	GLU
1	A	277	ARG
1	A	279	LYS
1	A	282	LEU
1	A	283	PRO
1	A	290	ILE
1	A	294	ARG
1	A	296	SER
1	A	310	LYS
1	A	312	GLN
1	A	318	GLU
1	A	321	LYS
1	A	323	TYR
1	A	326	SER
1	A	330	LEU
1	A	337	PHE
1	A	347	ARG
1	A	351	MET
1	A	352	THR
1	A	354	ARG
1	A	355	GLU
1	A	360	ARG
1	A	364	VAL
1	A	366	TYR
1	A	369	GLU
1	A	370	VAL
1	A	372	MET
1	A	374	ARG
1	A	380	SER
1	A	381	VAL
1	A	382	THR
1	A	387	HIS
1	A	388	ASP
1	A	389	THR
1	A	393	LYS
1	A	394	LEU
1	A	397	LEU
1	A	400	SER
1	A	407	LEU
1	A	417	LEU
1	A	426	SER
1	A	434	PHE

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Mol	Chain	Res	Type
1	A	438	ILE
1	A	440	GLN
1	A	442	GLN
1	A	444	SER
1	A	445	LEU
1	A	454	HIS
1	A	461	ARG
1	A	465	ILE
1	A	471	LEU
1	A	473	GLU
1	A	475	ILE
1	A	477	THR
1	A	482	CYS
1	A	483	ASP
1	A	487	GLN
1	A	489	THR
1	A	493	VAL
1	A	498	SER
1	A	502	GLN
1	A	503	THR
1	A	514	ILE
1	A	516	GLN
1	A	520	THR
1	A	521	THR
1	A	522	LYS
1	A	523	LYS
1	A	524	LYS
1	A	525	LEU
1	A	528	LEU
1	A	530	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	262	HIS
1	A	272	ASN
1	A	292	GLN
1	A	327	GLN
1	A	339	GLN
1	A	413	HIS
1	A	487	GLN

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Mol	Chain	Res	Type
1	A	502	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 (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.