



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 09:02 AM EDT

PDB ID : 3BRH  
Title : Protein Tyrosine Phosphatase PTPN-22 (Lyp) bound to the mono-Phosphorylated Lck active site peptide  
Authors : Seidel, R.D.; Love, J.; Piserchio, A.; Cowburn, D.  
Deposited on : 2007-12-21  
Resolution : 2.20 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](mailto: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 ⓘ symbol.

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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)  
Xtrriage (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

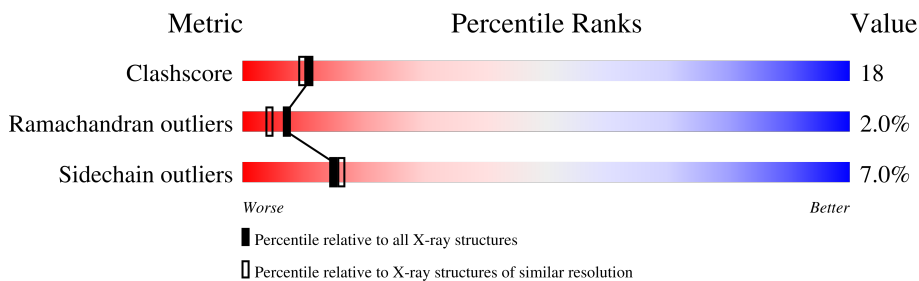
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	65% 27% 5%
1	B	310	67% 23% 5%
2	C	7	14% 29% 57%
2	D	7	29% 29% 43%

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
3	PO4	A	400	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5335 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 phosphatase non-receptor type 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2442	1575	397	454	16	0	4	0
1	B	296	2475	1594	406	457	18	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	ASP	engineered mutation	UNP Q9Y2R2
A	227	SER	CYS	engineered mutation	UNP Q9Y2R2
B	195	ALA	ASP	engineered mutation	UNP Q9Y2R2
B	227	SER	CYS	engineered mutation	UNP Q9Y2R2

- Molecule 2 is a protein called Lck Active Site Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	7	68	40	12	16	0	1	0
2	D	4	45	27	6	12	0	1	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

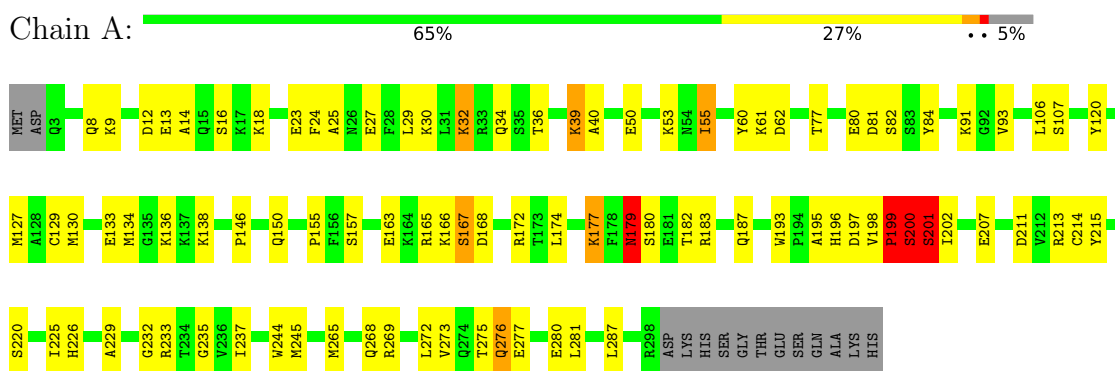
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	149	Total	O	0	1
			150	150		
4	C	5	Total	O	0	0
			5	5		
4	D	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

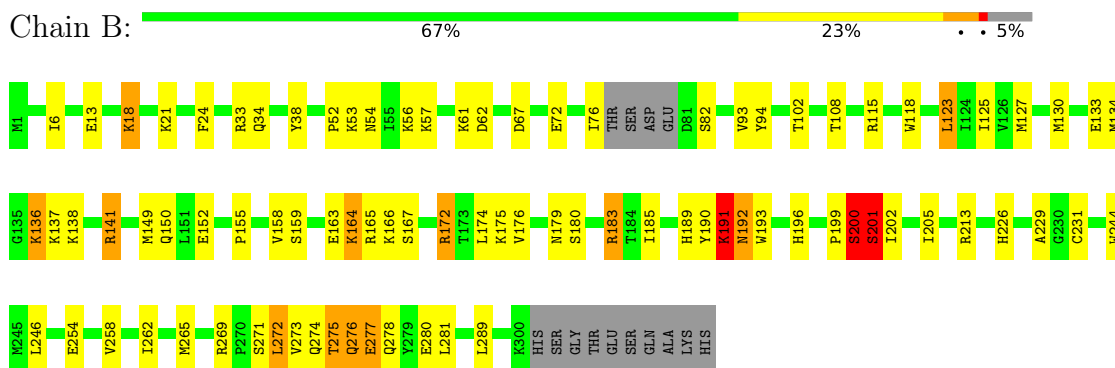
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Tyrosine-protein phosphatase non-receptor type 22



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 22



- Molecule 2: Lck Active Site Peptide



- Molecule 2: Lck Active Site Peptide



D891
M392
E393
Y394
THR
ALA
ARG

## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	60.85Å 48.51Å 119.97Å 90.00° 103.49° 90.00°	Depositor
Resolution (Å)	29.59 – 2.20	Depositor
% Data completeness (in resolution range)	98.6 (29.59-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.188 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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: PO4

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	0.94	5/2507 (0.2%)	1.29	14/3387 (0.4%)
1	B	0.89	0/2542	1.34	20/3429 (0.6%)
2	C	1.06	0/68	2.13	2/90 (2.2%)
2	D	1.28	1/45 (2.2%)	1.12	0/59
All	All	0.92	6/5162 (0.1%)	1.33	36/6965 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
2	C	3	5
2	D	0	1
All	All	3	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	TYR	CD1-CE1	-6.04	1.30	1.39
1	A	120	TYR	CD1-CE1	-5.68	1.30	1.39
1	A	84	TYR	CZ-OH	-5.45	1.28	1.37
1	A	84	TYR	CD2-CE2	-5.32	1.31	1.39
2	D	394	TYR	CB-CG	-5.12	1.44	1.51
1	A	129	CYS	CB-SG	-5.01	1.73	1.81

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	394	TYR	N-CA-CB	15.35	138.23	110.60
2	C	394	TYR	CA-CB-CG	8.94	130.38	113.40
1	B	123	LEU	CA-CB-CG	8.78	135.49	115.30
1	B	201	SER	N-CA-C	8.40	133.69	111.00
1	B	165	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	B	115	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	B	137	LYS	CD-CE-NZ	-7.70	93.98	111.70
1	B	213	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	B	115	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	200	SER	N-CA-C	-7.50	90.75	111.00
1	A	269	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	A	166	LYS	CD-CE-NZ	7.31	128.52	111.70
1	B	141	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	B	67	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	165	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	B	213	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	172	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	179	ASN	CB-CA-C	6.42	123.25	110.40
1	B	183	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	B	33	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	174	LEU	CB-CG-CD2	-6.18	100.50	111.00
1	B	246	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	200[A]	SER	N-CA-C	6.07	127.39	111.00
1	A	200[B]	SER	N-CA-C	6.07	127.39	111.00
1	B	165	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	199	PRO	CA-C-N	5.92	130.22	117.20
1	B	191	LYS	O-C-N	-5.52	113.86	122.70
1	A	183	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	106	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	A	81	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	174	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	67	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	193	TRP	N-CA-C	-5.06	97.33	111.00
1	A	82	SER	CB-CA-C	5.04	119.67	110.10
1	A	215	TYR	CB-CG-CD1	5.04	124.02	121.00
1	A	29	LEU	CB-CG-CD1	5.02	119.54	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	394	TYR	CA
2	C	395	THR	CA
2	C	396	ALA	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	PRO	Mainchain,Peptide
1	B	191	LYS	Peptide
1	B	199	PRO	Peptide
1	B	200	SER	Peptide
2	C	391	ASP	Peptide
2	C	393[A]	GLU	Peptide
2	C	393[B]	GLU	Mainchain,Peptide
2	C	396	ALA	Peptide
2	D	391	ASP	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2442	0	2422	90	0
1	B	2475	0	2469	71	0
2	C	68	0	53	47	0
2	D	45	0	28	15	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	139	0	0	12	0
4	B	150	0	0	10	0
4	C	5	0	0	7	0
4	D	1	0	0	0	0
All	All	5335	0	4972	181	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 18.

All (181) 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:196:HIS:CE1	2:C:394:TYR:CE2	2.13	1.34
4:A:570:HOH:O	1:B:149:MET:HG3	1.32	1.27
1:B:196:HIS:HE1	2:D:394:TYR:CE1	1.53	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:HIS:NE2	2:C:394:TYR:HE2	1.37	1.22
1:A:280:GLU:HB3	4:A:329:HOH:O	1.47	1.13
2:C:395:THR:HA	2:C:396:ALA:CB	1.71	1.13
1:B:196:HIS:CE1	2:D:394:TYR:CE1	2.36	1.12
1:A:196:HIS:CD2	2:C:397:ARG:H	1.71	1.09
1:A:196:HIS:NE2	2:C:394:TYR:CE2	2.17	1.08
2:C:395:THR:CA	2:C:396:ALA:HB3	1.85	1.05
2:C:396:ALA:O	2:C:397:ARG:HG2	1.59	1.02
2:C:393[A]:GLU:HG3	2:C:394:TYR:N	1.71	1.01
1:A:196:HIS:CE1	2:C:394:TYR:HE2	1.65	1.00
1:A:18:LYS:HB2	4:A:483:HOH:O	1.61	0.99
1:B:61[B]:LYS:HE3	1:B:62:ASP:HB3	1.44	0.99
2:C:396:ALA:CB	4:C:593:HOH:O	2.13	0.96
1:A:134:MET:CE	4:A:570:HOH:O	2.16	0.93
2:C:391:ASP:CB	4:C:594:HOH:O	2.17	0.93
1:B:200:SER:HB3	4:B:440:HOH:O	1.68	0.92
2:C:391:ASP:HB2	4:C:594:HOH:O	1.68	0.92
1:A:200[B]:SER:HB3	1:A:201:SER:HA	1.51	0.92
1:B:61[B]:LYS:HE2	2:D:393[B]:GLU:OE2	1.69	0.91
1:A:196:HIS:CD2	2:C:397:ARG:HA	2.05	0.90
1:A:196:HIS:CD2	2:C:397:ARG:N	2.39	0.89
2:C:395:THR:HA	2:C:396:ALA:HB3	0.89	0.85
1:A:91:LYS:H	1:A:268:GLN:HE22	1.25	0.85
1:A:200[B]:SER:CB	1:A:201:SER:HA	2.06	0.85
1:A:244:TRP:CH2	4:A:578:HOH:O	2.28	0.85
1:A:244:TRP:CZ2	4:A:578:HOH:O	2.29	0.85
1:A:276:GLN:O	1:A:280:GLU:HG3	1.77	0.83
2:C:394:TYR:HD2	2:C:394:TYR:O	1.62	0.83
1:B:196:HIS:CE1	2:D:394:TYR:HE1	1.94	0.83
2:C:394:TYR:O	2:C:396:ALA:HA	1.78	0.82
2:C:396:ALA:O	2:C:397:ARG:CG	2.30	0.80
1:A:61:LYS:HD2	2:C:391:ASP:N	1.97	0.79
1:A:133:GLU:HB2	1:A:138:LYS:HG3	1.63	0.79
1:A:280:GLU:OE1	4:A:329:HOH:O	2.01	0.79
1:B:150:GLN:HB2	4:B:456:HOH:O	1.81	0.79
1:A:196:HIS:CD2	2:C:397:ARG:CA	2.67	0.78
1:A:8:GLN:NE2	1:A:12:ASP:OD1	2.17	0.77
1:B:202:ILE:HG22	1:B:281:LEU:HD12	1.68	0.76
1:A:200[B]:SER:HB3	1:A:201:SER:CA	2.14	0.76
1:A:60:TYR:CE2	2:C:394:TYR:HD1	2.07	0.72
1:B:276:GLN:O	1:B:280:GLU:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:MET:O	1:B:136:LYS:HD3	1.90	0.71
1:B:265:MET:HB3	1:B:272:LEU:HD23	1.72	0.71
1:B:275:THR:HG22	1:B:278:GLN:H	1.55	0.71
1:B:196:HIS:HE1	2:D:394:TYR:CD1	2.04	0.70
1:B:275:THR:CG2	1:B:278:GLN:H	2.03	0.70
1:A:8:GLN:HE21	1:A:12:ASP:CG	1.94	0.70
1:B:61[C]:LYS:HG2	2:D:391:ASP:OD1	1.92	0.70
1:B:202:ILE:HG22	1:B:281:LEU:CD1	2.22	0.70
1:A:36:THR:HG23	1:A:39:LYS:HE2	1.76	0.68
1:A:196:HIS:HE1	2:C:394:TYR:CE2	2.05	0.67
1:B:127:MET:HG3	1:B:226:HIS:CE1	2.30	0.66
1:A:197[A]:ASP:O	4:A:573:HOH:O	2.14	0.66
1:A:265:MET:HB3	1:A:272:LEU:CD1	2.25	0.66
1:B:61[A]:LYS:HE3	2:D:393[A]:GLU:OE2	1.96	0.66
2:C:394:TYR:O	2:C:394:TYR:CD2	2.47	0.66
1:A:62:ASP:OD1	2:C:393[A]:GLU:HA	1.95	0.66
2:C:391:ASP:HB3	4:C:594:HOH:O	1.87	0.66
1:B:133:GLU:HB2	1:B:138:LYS:HG3	1.78	0.65
1:B:164:LYS:HE2	1:B:166:LYS:HG2	1.78	0.65
1:A:196:HIS:CG	2:C:397:ARG:HA	2.32	0.65
1:A:280:GLU:CB	4:A:329:HOH:O	2.21	0.65
1:B:269:ARG:HG2	1:B:272:LEU:HD13	1.78	0.64
1:B:277:GLU:HB2	4:B:339:HOH:O	1.97	0.64
1:B:6:ILE:HD11	1:B:254:GLU:HG2	1.80	0.64
1:A:193:TRP:CD1	1:A:199:PRO:HD3	2.33	0.63
1:A:200[A]:SER:CB	1:A:201:SER:HA	2.28	0.63
2:D:392:ASN:HD22	2:D:393[A]:GLU:HG2	1.64	0.63
1:A:200[B]:SER:CB	1:A:201:SER:CA	2.73	0.63
1:A:127:MET:HG3	1:A:226:HIS:CE1	2.33	0.63
1:A:39:LYS:HD2	1:A:40:ALA:H	1.64	0.62
1:A:195:ALA:HB1	2:C:394:TYR:CZ	2.34	0.62
2:C:396:ALA:C	2:C:397:ARG:HG2	2.19	0.62
3:A:400:PO4:O2	2:C:394:TYR:CZ	2.54	0.61
1:B:192:ASN:H	1:B:192:ASN:ND2	1.97	0.61
1:B:72:GLU:OE2	4:B:402:HOH:O	2.16	0.61
1:B:258:VAL:O	1:B:262:ILE:HG12	2.01	0.61
1:B:61[C]:LYS:CG	2:D:391:ASP:OD1	2.49	0.61
1:A:196:HIS:CE1	2:C:394:TYR:CD2	2.85	0.60
1:A:62:ASP:OD2	2:C:395:THR:HB	2.03	0.59
1:A:62:ASP:OD1	2:C:393[B]:GLU:HA	2.03	0.59
1:B:54:ASN:HA	1:B:57:LYS:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG12	1:A:281:LEU:HD22	1.85	0.59
1:A:275:THR:HG22	2:C:397:ARG:HB3	1.85	0.58
1:B:275:THR:HG23	1:B:277:GLU:N	2.18	0.58
1:B:21[B]:LYS:HE2	4:B:377:HOH:O	2.04	0.57
1:A:196:HIS:NE2	2:C:397:ARG:N	2.46	0.57
1:B:275:THR:HG23	1:B:277:GLU:H	1.68	0.57
1:A:39:LYS:HD2	1:A:40:ALA:N	2.20	0.57
1:B:163:GLU:HG2	1:B:172:ARG:HG2	1.86	0.57
4:A:570:HOH:O	1:B:149:MET:CG	2.13	0.56
1:A:198:VAL:CG1	1:A:281:LEU:HD22	2.36	0.56
1:A:50:GLU:HA	1:A:55:ILE:HD13	1.87	0.56
1:A:172:ARG:HD2	1:A:187:GLN:OE1	2.04	0.56
1:A:91:LYS:H	1:A:268:GLN:NE2	1.98	0.55
1:B:125:ILE:HD12	1:B:185:ILE:HG21	1.88	0.55
1:B:200:SER:H	1:B:201:SER:CA	2.18	0.54
2:C:396:ALA:HB3	4:C:593:HOH:O	1.94	0.54
1:A:225:ILE:HD13	1:A:237:ILE:HG22	1.89	0.53
1:A:265:MET:HB3	1:A:272:LEU:HD13	1.90	0.53
1:B:61[C]:LYS:HG2	2:D:391:ASP:CG	2.29	0.53
1:A:134:MET:HE3	4:A:570:HOH:O	1.92	0.53
1:A:61:LYS:CD	2:C:391:ASP:N	2.70	0.53
1:A:235:GLY:HA2	1:A:272:LEU:HD22	1.91	0.53
1:A:150:GLN:HB3	1:A:157[A]:SER:OG	2.08	0.52
1:A:32:LYS:NZ	2:C:397:ARG:HH22	2.07	0.52
1:A:53:LYS:O	1:A:53:LYS:HG2	2.11	0.50
2:C:395:THR:HG23	4:C:581:HOH:O	2.10	0.50
1:B:231[B]:CYS:HB2	1:B:271:SER:O	2.11	0.50
1:A:30:LYS:O	1:A:34:GLN:HG3	2.12	0.50
1:A:179:ASN:OD1	1:A:180:SER:N	2.41	0.50
1:A:195:ALA:HB2	1:A:233:ARG:NH2	2.27	0.50
1:B:130:MET:SD	1:B:192:ASN:HA	2.52	0.50
2:C:395:THR:HG22	4:C:593:HOH:O	2.12	0.49
1:A:14:ALA:CB	1:A:287:LEU:HD11	2.41	0.49
1:A:62:ASP:OD1	1:A:62:ASP:N	2.33	0.49
1:A:60:TYR:CZ	2:C:394:TYR:HD1	2.30	0.49
1:A:211:ASP:O	1:A:214:CYS:HB2	2.13	0.49
1:A:163:GLU:HG2	1:A:172:ARG:HG2	1.95	0.49
1:B:102:THR:O	1:B:226:HIS:HB2	2.12	0.49
1:B:76:ILE:HD11	1:B:155:PRO:HG3	1.95	0.48
1:A:196:HIS:CA	1:A:197[B]:ASP:N	2.76	0.48
1:B:192:ASN:H	1:B:192:ASN:HD22	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:TRP:NE1	1:A:199:PRO:HD3	2.30	0.47
1:A:277:GLU:HB2	4:A:565:HOH:O	2.14	0.47
1:A:177:LYS:HG2	1:A:182:THR:OG1	2.14	0.47
2:C:391:ASP:O	2:C:392:ASN:HB2	2.14	0.47
1:A:167:SER:HB3	1:A:168:ASP:OD2	2.14	0.47
1:A:229:ALA:HB2	2:C:394:TYR:CD1	2.50	0.47
1:A:200[A]:SER:CB	1:A:201:SER:CA	2.93	0.46
1:B:53:LYS:HG2	4:B:555:HOH:O	2.15	0.46
1:B:269:ARG:HB3	1:B:272:LEU:HD22	1.97	0.46
1:A:136:LYS:HB2	1:A:138:LYS:HE2	1.95	0.46
1:A:133:GLU:HB2	1:A:138:LYS:CG	2.39	0.46
1:B:18:LYS:HD3	4:B:387:HOH:O	2.14	0.46
1:B:158:VAL:HG22	1:B:176:VAL:HG22	1.97	0.46
1:A:36:THR:HG23	1:A:39:LYS:CE	2.46	0.46
1:B:136:LYS:HE3	1:B:136:LYS:HB2	1.63	0.46
1:B:274:GLN:OE1	3:B:400:PO4:O2	2.34	0.46
1:A:39:LYS:O	1:A:40:ALA:C	2.54	0.45
1:A:55:ILE:HD12	1:A:55:ILE:HA	1.75	0.45
1:B:24:PHE:CG	1:B:280:GLU:HG2	2.51	0.45
1:A:146:PRO:O	1:B:130:MET:CE	2.64	0.45
1:B:175:LYS:HD3	1:B:175:LYS:HA	1.74	0.45
1:A:61:LYS:HG3	2:C:391:ASP:N	2.31	0.45
1:B:189:HIS:CE1	1:B:191:LYS:HE2	2.52	0.45
1:A:61:LYS:CG	2:C:391:ASP:N	2.80	0.45
1:B:118:TRP:O	1:B:183:ARG:NH1	2.42	0.44
1:B:275:THR:HG23	1:B:278:GLN:H	1.83	0.44
1:A:196:HIS:NE2	2:C:394:TYR:CD2	2.77	0.44
1:B:21[B]:LYS:HE2	1:B:280:GLU:OE1	2.18	0.43
1:B:275:THR:HG22	1:B:278:GLN:N	2.27	0.43
1:A:32:LYS:HZ1	2:C:397:ARG:HH22	1.65	0.43
1:B:53:LYS:CG	4:B:555:HOH:O	2.66	0.43
1:B:275:THR:HG22	1:B:278:GLN:CB	2.49	0.43
1:A:213:ARG:HD3	1:A:213:ARG:HA	1.76	0.43
1:A:146:PRO:O	1:B:130:MET:HE1	2.19	0.43
1:B:244:TRP:HB2	1:B:289:LEU:HD13	2.01	0.42
1:A:25:ALA:HB2	1:A:276:GLN:NE2	2.34	0.42
1:A:93:VAL:HG21	1:A:245[B]:MET:HG2	2.01	0.42
2:D:392:ASN:ND2	2:D:393[A]:GLU:HG2	2.32	0.42
1:A:9:LYS:O	1:A:13:GLU:HG3	2.19	0.42
1:A:23:GLU:O	1:A:27:GLU:HB2	2.20	0.42
1:B:229:ALA:HB2	2:D:394:TYR:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ASN:O	1:B:180:SER:HB2	2.20	0.41
1:A:130:MET:CE	4:B:567:HOH:O	2.68	0.41
1:B:93:VAL:HG23	1:B:94:TYR:CD2	2.56	0.41
1:A:24:PHE:CG	1:A:280:GLU:HG2	2.56	0.41
1:B:275:THR:HG22	1:B:278:GLN:CG	2.51	0.41
1:B:34:GLN:HG3	1:B:38:TYR:CZ	2.55	0.41
1:B:52:PRO:HD2	4:B:555:HOH:O	2.21	0.41
1:B:62:ASP:OD1	2:D:393[B]:GLU:HA	2.21	0.41
1:B:62:ASP:OD1	2:D:393[A]:GLU:HA	2.20	0.40
1:B:205:ILE:HG21	1:B:205:ILE:HD13	1.68	0.40
1:B:61[A]:LYS:CE	2:D:393[A]:GLU:OE2	2.67	0.40
1:A:77:THR:HB	1:A:155:PRO:HG3	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	295/310 (95%)	273 (92%)	17 (6%)	5 (2%)	9	6
1	B	298/310 (96%)	276 (93%)	19 (6%)	3 (1%)	15	14
2	C	6/7 (86%)	2 (33%)	1 (17%)	3 (50%)	0	0
2	D	3/7 (43%)	2 (67%)	0	1 (33%)	0	0
All	All	602/634 (95%)	553 (92%)	37 (6%)	12 (2%)	7	4

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	199	PRO
1	B	201	SER

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Mol	Chain	Res	Type
2	C	396	ALA
2	C	392	ASN
2	C	395	THR
1	B	82	SER
2	D	392	ASN
1	A	201	SER
1	A	273	VAL
1	B	273	VAL
1	A	232	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	269/284 (95%)	254 (94%)	15 (6%)	21	25
1	B	274/284 (96%)	256 (93%)	18 (7%)	16	19
2	C	7/6 (117%)	3 (43%)	4 (57%)	0	0
2	D	5/6 (83%)	1 (20%)	4 (80%)	0	0
All	All	555/580 (96%)	514 (93%)	41 (7%)	15	14

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	32	LYS
1	A	39	LYS
1	A	55	ILE
1	A	80	GLU
1	A	107	SER
1	A	167	SER
1	A	177	LYS
1	A	200[A]	SER
1	A	200[B]	SER
1	A	201	SER
1	A	202	ILE

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Mol	Chain	Res	Type
1	A	207	GLU
1	A	220	SER
1	A	276	GLN
1	B	13	GLU
1	B	18	LYS
1	B	56	LYS
1	B	108	THR
1	B	123	LEU
1	B	136	LYS
1	B	141	ARG
1	B	152	GLU
1	B	159	SER
1	B	164	LYS
1	B	167	SER
1	B	190	TYR
1	B	192	ASN
1	B	201	SER
1	B	272	LEU
1	B	275	THR
1	B	276	GLN
1	B	277	GLU
2	C	393[A]	GLU
2	C	393[B]	GLU
2	C	394	TYR
2	C	395	THR
2	D	392	ASN
2	D	393[A]	GLU
2	D	393[B]	GLU
2	D	394	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	196	HIS
1	A	268	GLN
1	A	276	GLN
1	B	192	ASN
1	B	196	HIS
2	D	392	ASN

### 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](#)

2 ligands are 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
3	PO4	B	400	-	4,4,4	1.27	0	6,6,6	1.48	1 (16%)
3	PO4	A	400	-	4,4,4	5.29	4 (100%)	6,6,6	1.20	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	PO4	P-O3	-5.97	1.36	1.54
3	A	400	PO4	P-O2	-5.97	1.36	1.54
3	A	400	PO4	P-O4	-4.62	1.40	1.54
3	A	400	PO4	P-O1	-4.36	1.40	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	PO4	O3-P-O2	2.84	117.08	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	PO4	1	0
3	A	400	PO4	1	0

## 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.