



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 AM UTC

PDB ID : 2LIG / pdb_00002lig
Title : THREE-DIMENSIONAL STRUCTURES OF THE LIGAND-BINDING DOMAIN OF THE BACTERIAL ASPARTATE RECEPTOR WITH AND WITHOUT A LIGAND
Authors : Kim, S.-H.; Yeh, J.I.; Prive, G.G.; Milburn, M.; Scott, W.; Koshland Junior, D.E.
Deposited on : 1995-04-18
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

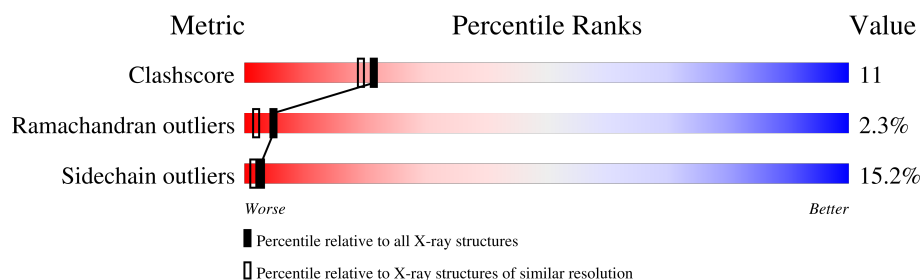
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	
1	B	164	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2622 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.

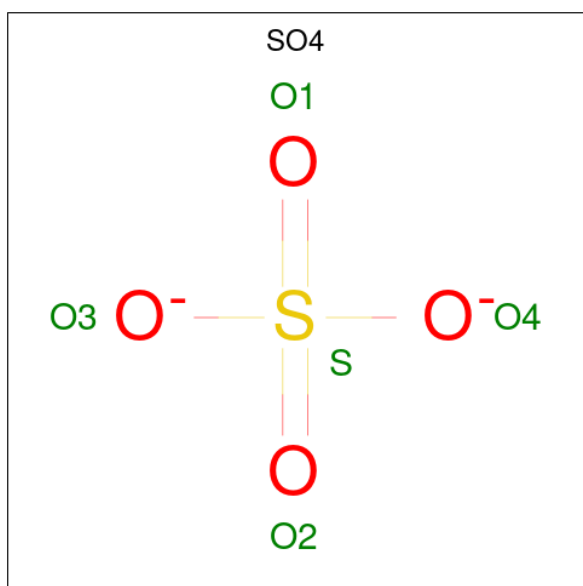
- Molecule 1 is a protein called ASPARTATE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1223	754	217	242	10			
1	B	157	Total	C	N	O	S	0	0	0
			1223	754	217	242	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	CYS	ASN	conflict	UNP P02941
B	36	CYS	ASN	conflict	UNP P02941

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



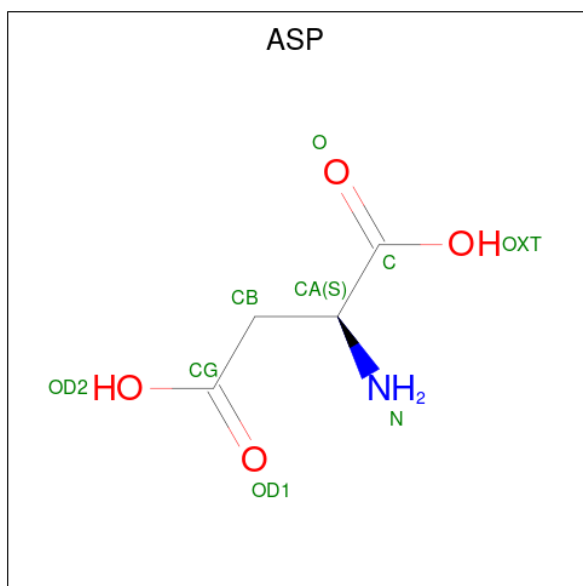
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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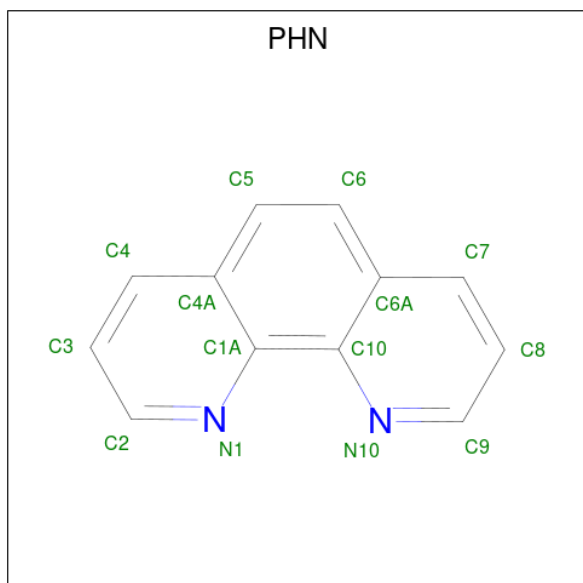
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is 1,10-PHENANTHROLINE (CCD ID: PHN) (formula: $C_{12}H_8N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			14	12	2		

- Molecule 5 is water.

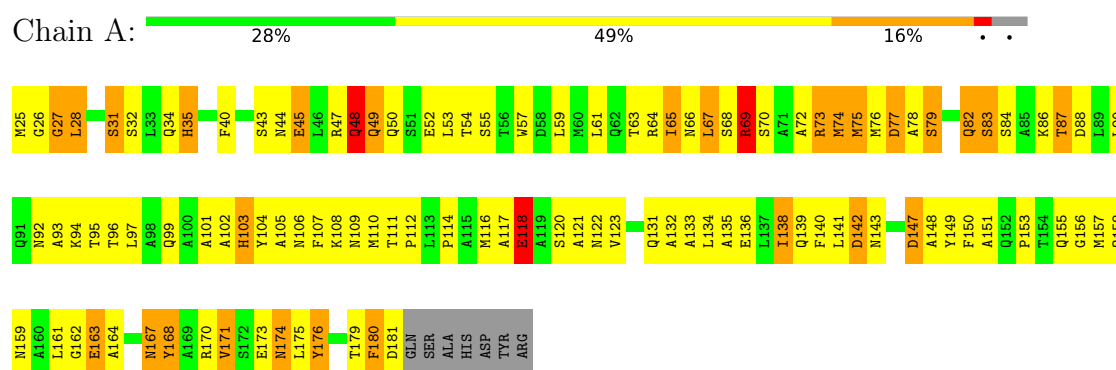
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	74	Total	O	0	0
			74	74		

3 Residue-property plots

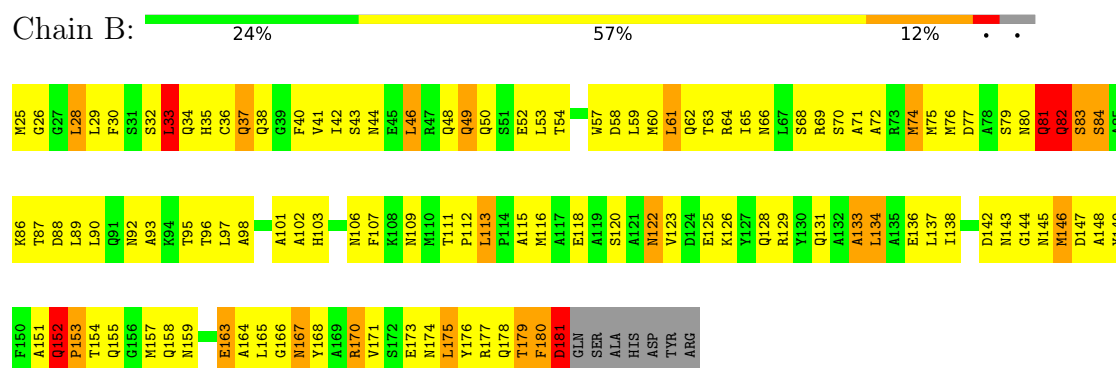
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ASPARTATE RECEPTOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.38Å 80.38Å 91.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2622	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: SO4, PHN

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	2.53	81/1241 (6.5%)	2.55	93/1675 (5.6%)
1	B	2.53	73/1241 (5.9%)	2.50	88/1675 (5.3%)
All	All	2.53	154/2482 (6.2%)	2.53	181/3350 (5.4%)

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	1
1	B	0	1
All	All	0	2

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	VAL	CA-C	10.21	1.65	1.52
1	A	156	GLY	CA-C	-10.11	1.40	1.52
1	A	162	GLY	CA-C	9.46	1.62	1.51
1	A	104	TYR	N-CA	-9.31	1.35	1.46
1	B	35	HIS	CD2-NE2	-8.90	1.28	1.37
1	A	95	THR	C-O	-8.72	1.14	1.24
1	A	55	SER	C-O	-8.14	1.14	1.24
1	A	135	ALA	N-CA	8.03	1.56	1.46
1	B	28	LEU	CA-C	-7.94	1.42	1.52
1	B	159	ASN	C-O	7.87	1.33	1.24
1	A	120	SER	N-CA	7.70	1.55	1.46
1	A	31	SER	CA-C	7.67	1.63	1.52
1	A	53	LEU	CA-C	-7.60	1.42	1.52
1	A	167	ASN	N-CA	7.52	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	ALA	C-O	7.51	1.32	1.24
1	B	168	TYR	C-O	-7.46	1.15	1.24
1	A	77	ASP	N-CA	7.44	1.55	1.46
1	B	64	ARG	C-O	7.37	1.32	1.24
1	B	103	HIS	CD2-NE2	-7.36	1.29	1.37
1	A	136	GLU	CA-CB	-7.22	1.42	1.53
1	B	122	ASN	CA-CB	-7.18	1.41	1.53
1	B	33	LEU	CA-CB	-7.09	1.42	1.53
1	A	167	ASN	C-N	7.08	1.42	1.33
1	B	120	SER	CA-CB	-6.93	1.42	1.53
1	B	115	ALA	C-O	-6.91	1.15	1.24
1	B	70	SER	N-CA	6.87	1.54	1.46
1	A	132	ALA	C-O	-6.83	1.15	1.24
1	A	170	ARG	NE-CZ	6.83	1.40	1.33
1	B	125	GLU	N-CA	-6.79	1.38	1.46
1	B	95	THR	CA-C	6.79	1.61	1.52
1	A	77	ASP	C-O	-6.68	1.15	1.24
1	B	48	GLN	N-CA	-6.67	1.38	1.46
1	A	64	ARG	CA-CB	6.64	1.64	1.53
1	B	181	ASP	CA-CB	6.59	1.66	1.53
1	B	129	ARG	N-CA	-6.58	1.38	1.46
1	B	165	LEU	CA-C	-6.54	1.44	1.52
1	B	175	LEU	CA-CB	6.53	1.63	1.53
1	A	150	PHE	CA-CB	-6.47	1.43	1.53
1	B	86	LYS	C-N	-6.46	1.23	1.33
1	A	43	SER	CA-C	-6.38	1.44	1.52
1	A	79	SER	CA-C	6.38	1.61	1.52
1	A	47	ARG	NE-CZ	6.36	1.40	1.33
1	A	53	LEU	C-O	6.30	1.32	1.24
1	A	141	LEU	CA-C	-6.29	1.44	1.52
1	B	36	CYS	C-N	6.28	1.42	1.33
1	B	66	ASN	C-O	-6.27	1.16	1.24
1	A	140	PHE	N-CA	6.26	1.53	1.46
1	B	77	ASP	CA-C	6.24	1.61	1.52
1	A	79	SER	N-CA	6.20	1.54	1.46
1	A	138	ILE	CA-CB	6.17	1.62	1.54
1	B	69	ARG	CA-CB	-6.16	1.43	1.53
1	A	164	ALA	C-N	-6.14	1.25	1.33
1	B	79	SER	CA-C	6.09	1.61	1.53
1	A	161	LEU	CA-CB	6.04	1.62	1.53
1	B	153	PRO	CA-C	-6.04	1.47	1.53
1	B	146	MET	C-N	5.99	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	SER	CA-CB	-5.98	1.44	1.53
1	B	163	GLU	C-N	5.97	1.41	1.33
1	A	74	MET	CA-CB	-5.97	1.44	1.53
1	A	35	HIS	CA-C	-5.97	1.45	1.52
1	A	83	SER	C-N	5.96	1.42	1.33
1	B	35	HIS	ND1-CE1	-5.94	1.26	1.32
1	A	102	ALA	N-CA	-5.94	1.39	1.46
1	A	121	ALA	C-O	-5.93	1.16	1.24
1	B	116	MET	CA-C	5.92	1.60	1.52
1	A	31	SER	N-CA	-5.91	1.38	1.46
1	B	138	ILE	N-CA	5.91	1.53	1.46
1	B	35	HIS	C-O	5.90	1.31	1.24
1	A	43	SER	C-O	5.88	1.31	1.24
1	B	82	GLN	C-O	5.87	1.31	1.24
1	A	158	GLN	C-O	-5.87	1.17	1.24
1	A	54	THR	C-N	-5.85	1.26	1.33
1	A	105	ALA	C-O	5.83	1.30	1.24
1	B	93	ALA	CA-CB	5.82	1.62	1.53
1	A	67	LEU	C-O	-5.79	1.16	1.24
1	A	75	MET	CA-C	5.78	1.62	1.52
1	B	112	PRO	N-CA	-5.78	1.40	1.47
1	B	148	ALA	CA-CB	-5.75	1.44	1.53
1	B	26	GLY	N-CA	5.72	1.53	1.45
1	A	147	ASP	CA-C	-5.71	1.45	1.52
1	A	151	ALA	N-CA	5.71	1.53	1.46
1	A	133	ALA	CA-C	-5.71	1.45	1.52
1	A	153	PRO	CA-CB	5.70	1.60	1.53
1	B	36	CYS	CA-CB	-5.65	1.44	1.53
1	A	35	HIS	CG-CD2	5.60	1.42	1.35
1	B	106	ASN	CA-CB	-5.59	1.44	1.53
1	A	122	ASN	C-N	5.56	1.41	1.33
1	A	101	ALA	C-N	5.56	1.41	1.33
1	A	96	THR	C-O	-5.55	1.17	1.24
1	B	76	MET	C-O	-5.55	1.17	1.23
1	B	173	GLU	CA-CB	-5.53	1.44	1.53
1	B	173	GLU	C-O	-5.52	1.17	1.24
1	B	35	HIS	CA-CB	-5.52	1.44	1.53
1	A	161	LEU	CA-C	5.52	1.59	1.52
1	A	54	THR	CB-OG1	-5.52	1.34	1.43
1	A	156	GLY	C-O	5.52	1.30	1.23
1	A	35	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	71	ALA	C-O	5.49	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	ASN	C-O	-5.48	1.16	1.24
1	A	61	LEU	C-O	5.48	1.30	1.24
1	A	75	MET	CA-CB	-5.46	1.44	1.53
1	A	149	TYR	CA-C	5.45	1.59	1.52
1	B	163	GLU	C-O	-5.45	1.17	1.24
1	B	174	ASN	C-O	-5.44	1.17	1.24
1	A	171	VAL	CA-C	5.44	1.59	1.52
1	B	153	PRO	CA-CB	-5.43	1.48	1.53
1	A	34	GLN	C-N	-5.42	1.26	1.33
1	A	94	LYS	CA-CB	-5.42	1.44	1.53
1	B	166	GLY	N-CA	5.42	1.52	1.45
1	A	123	VAL	CA-C	-5.42	1.46	1.52
1	A	61	LEU	C-N	-5.42	1.26	1.33
1	B	103	HIS	CG-ND1	-5.40	1.32	1.38
1	B	123	VAL	CA-C	5.40	1.59	1.52
1	B	38	GLN	CA-C	5.38	1.59	1.52
1	A	93	ALA	CA-C	-5.37	1.45	1.52
1	A	54	THR	C-O	-5.37	1.17	1.24
1	A	133	ALA	CA-CB	5.37	1.61	1.53
1	B	54	THR	C-O	5.36	1.30	1.24
1	A	68	SER	CA-CB	-5.36	1.44	1.53
1	A	94	LYS	C-N	-5.35	1.27	1.33
1	B	134	LEU	C-O	5.35	1.30	1.24
1	B	54	THR	CA-CB	5.34	1.61	1.53
1	B	143	ASN	C-O	-5.32	1.17	1.24
1	B	54	THR	CB-OG1	-5.30	1.35	1.43
1	A	103	HIS	CE1-NE2	-5.30	1.27	1.32
1	A	32	SER	CA-C	-5.28	1.46	1.52
1	A	142	ASP	N-CA	-5.28	1.39	1.46
1	B	178	GLN	C-O	5.27	1.30	1.24
1	B	40	PHE	C-O	-5.26	1.18	1.24
1	A	50	GLN	C-N	5.26	1.40	1.33
1	B	102	ALA	C-O	-5.23	1.17	1.24
1	A	96	THR	C-N	5.23	1.41	1.33
1	B	167	ASN	C-O	-5.22	1.17	1.24
1	A	47	ARG	CZ-NH2	5.22	1.40	1.33
1	B	106	ASN	N-CA	5.20	1.52	1.46
1	B	147	ASP	CA-CB	-5.19	1.45	1.53
1	B	61	LEU	C-N	5.18	1.41	1.34
1	B	136	GLU	CA-C	-5.17	1.46	1.52
1	A	55	SER	C-N	5.16	1.40	1.33
1	A	45	GLU	CA-C	5.16	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	ARG	CZ-NH1	5.14	1.40	1.32
1	A	48	GLN	CA-C	-5.13	1.46	1.52
1	B	60	MET	C-N	-5.12	1.26	1.34
1	A	88	ASP	CA-C	-5.11	1.43	1.52
1	A	49	GLN	C-O	5.11	1.30	1.24
1	B	32	SER	C-O	5.10	1.29	1.23
1	B	50	GLN	C-O	5.07	1.30	1.24
1	B	43	SER	N-CA	-5.06	1.40	1.46
1	A	70	SER	N-CA	5.06	1.52	1.46
1	A	69	ARG	CA-CB	-5.05	1.45	1.53
1	B	163	GLU	N-CA	-5.04	1.40	1.46
1	A	173	GLU	C-N	-5.04	1.27	1.33
1	B	164	ALA	N-CA	-5.02	1.40	1.46
1	A	116	MET	CA-CB	-5.00	1.44	1.53

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	CA-CB-CG	13.41	126.01	112.60
1	B	154	THR	N-CA-C	10.44	123.63	111.11
1	B	81	GLN	N-CA-C	10.10	132.32	110.80
1	A	171	VAL	CA-C-O	-9.64	110.63	120.85
1	A	112	PRO	N-CA-CB	9.63	111.88	103.31
1	B	143	ASN	OD1-CG-ND2	-9.45	113.15	122.60
1	A	99	GLN	OE1-CD-NE2	-9.23	113.36	122.60
1	A	78	ALA	N-CA-C	9.02	122.08	111.71
1	A	167	ASN	OD1-CG-ND2	-8.92	113.68	122.60
1	A	77	ASP	N-CA-C	8.33	128.54	110.80
1	B	83	SER	N-CA-C	8.08	128.00	110.80
1	A	108	LYS	CB-CG-CD	-8.05	92.79	111.30
1	A	163	GLU	CA-CB-CG	7.87	129.83	114.10
1	A	64	ARG	NE-CZ-NH2	7.82	126.23	119.20
1	A	69	ARG	CD-NE-CZ	7.80	135.32	124.40
1	A	88	ASP	CA-CB-CG	7.75	120.36	112.60
1	A	180	PHE	CA-CB-CG	7.71	121.51	113.80
1	B	82	GLN	N-CA-C	7.68	127.16	110.80
1	A	123	VAL	CB-CA-C	-7.58	101.91	112.14
1	A	68	SER	N-CA-C	-7.57	103.11	111.36
1	A	123	VAL	CA-C-O	-7.57	113.08	120.95
1	B	34	GLN	CB-CG-CD	7.56	125.45	112.60
1	B	42	ILE	CB-CA-C	-7.55	102.31	111.97
1	A	122	ASN	OD1-CG-ND2	-7.52	115.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	GLY	O-C-N	-7.42	115.00	122.19
1	B	30	PHE	CA-CB-CG	-7.31	106.49	113.80
1	B	48	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	B	54	THR	O-C-N	-7.24	114.44	122.12
1	A	82	GLN	CA-CB-CG	7.14	128.38	114.10
1	A	50	GLN	CG-CD-NE2	7.11	127.06	116.40
1	A	65	ILE	O-C-N	-7.09	114.97	121.91
1	B	152	GLN	OE1-CD-NE2	-7.08	115.52	122.60
1	A	157	MET	CG-SD-CE	-7.07	85.36	100.90
1	B	103	HIS	CA-CB-CG	-7.05	106.75	113.80
1	A	159	ASN	OD1-CG-ND2	-7.00	115.59	122.60
1	A	155	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	A	176	TYR	N-CA-C	-6.91	103.67	111.07
1	A	112	PRO	CA-N-CD	-6.89	102.36	112.00
1	B	125	GLU	CA-CB-CG	6.70	127.50	114.10
1	B	35	HIS	CB-CG-ND1	6.69	132.73	122.70
1	A	57	TRP	CB-CG-CD1	-6.68	116.87	126.90
1	B	155	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	A	87	THR	N-CA-C	6.61	120.19	108.24
1	A	35	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	131	GLN	N-CA-CB	-6.58	100.53	110.07
1	B	52	GLU	O-C-N	6.54	131.10	122.33
1	A	143	ASN	CA-CB-CG	6.52	119.12	112.60
1	A	111	THR	CA-C-N	6.51	126.47	119.76
1	A	111	THR	C-N-CA	6.51	126.47	119.76
1	B	123	VAL	CB-CA-C	-6.49	103.38	112.14
1	B	97	LEU	CA-C-O	-6.49	113.54	120.42
1	B	37	GLN	CB-CA-C	-6.49	99.65	110.68
1	B	92	ASN	CA-C-O	-6.46	112.54	119.97
1	A	76	MET	O-C-N	6.45	130.95	123.02
1	A	63	THR	CA-C-O	-6.44	113.60	120.42
1	A	135	ALA	CA-C-N	6.41	128.78	120.44
1	A	135	ALA	C-N-CA	6.41	128.78	120.44
1	A	164	ALA	CA-C-O	-6.40	112.61	119.97
1	A	57	TRP	CG-CD1-NE1	-6.37	101.92	110.20
1	A	174	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	B	152	GLN	CG-CD-NE2	6.29	125.84	116.40
1	B	44	ASN	CB-CG-ND2	6.29	125.83	116.40
1	A	53	LEU	O-C-N	-6.27	114.56	122.27
1	B	63	THR	O-C-N	6.26	128.76	122.12
1	B	96	THR	CA-C-O	-6.26	112.77	119.97
1	B	129	ARG	N-CA-CB	-6.24	100.92	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	GLN	CA-C-N	6.23	133.44	121.54
1	B	81	GLN	C-N-CA	6.23	133.44	121.54
1	A	134	LEU	O-C-N	6.21	129.23	122.15
1	B	76	MET	CA-C-N	6.19	133.37	121.54
1	B	76	MET	C-N-CA	6.19	133.37	121.54
1	A	35	HIS	CB-CG-ND1	6.18	131.97	122.70
1	A	69	ARG	CG-CD-NE	6.18	125.59	112.00
1	A	25	MET	CA-C-N	6.18	133.52	121.41
1	A	25	MET	C-N-CA	6.18	133.52	121.41
1	B	50	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	B	57	TRP	CE2-CD2-CG	-6.17	99.80	107.20
1	A	82	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	92	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	A	50	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	B	49	GLN	CB-CG-CD	6.14	123.04	112.60
1	A	133	ALA	O-C-N	-6.13	115.17	122.15
1	B	170	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	A	161	LEU	CA-C-N	6.11	126.89	119.99
1	A	161	LEU	C-N-CA	6.11	126.89	119.99
1	A	117	ALA	O-C-N	6.11	128.44	122.09
1	B	57	TRP	CB-CG-CD1	-6.10	117.74	126.90
1	B	148	ALA	O-C-N	-6.10	115.79	122.07
1	B	107	PHE	CA-CB-CG	-6.10	107.70	113.80
1	B	58	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	103	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	A	163	GLU	CB-CA-C	6.06	120.85	110.79
1	B	62	GLN	CG-CD-NE2	6.05	125.47	116.40
1	A	40	PHE	CA-CB-CG	-6.03	107.77	113.80
1	A	27	GLY	N-CA-C	-6.01	101.58	111.38
1	A	106	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	107	PHE	CA-CB-CG	6.00	119.80	113.80
1	A	73	ARG	CA-C-N	5.99	128.62	120.54
1	A	73	ARG	C-N-CA	5.99	128.62	120.54
1	A	168	TYR	CA-C-N	5.98	128.29	120.28
1	A	168	TYR	C-N-CA	5.98	128.29	120.28
1	B	33	LEU	N-CA-C	-5.97	104.68	111.07
1	B	177	ARG	O-C-N	-5.92	115.85	122.12
1	B	174	ASN	CB-CA-C	-5.88	101.04	110.79
1	A	163	GLU	N-CA-CB	-5.86	101.51	110.12
1	A	26	GLY	CA-C-N	5.85	126.11	121.61
1	A	26	GLY	C-N-CA	5.85	126.11	121.61
1	B	181	ASP	CA-CB-CG	5.84	118.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ALA	CA-C-O	5.81	126.67	120.10
1	A	34	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	106	ASN	O-C-N	5.76	128.01	122.07
1	B	84	SER	N-CA-C	5.76	123.06	110.80
1	B	143	ASN	CB-CG-ND2	5.76	125.04	116.40
1	B	86	LYS	CA-C-O	-5.75	112.53	119.49
1	B	62	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	A	50	GLN	O-C-N	-5.71	116.07	122.12
1	B	33	LEU	CA-C-O	-5.67	114.86	120.82
1	B	77	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	88	ASP	N-CA-C	-5.66	105.02	111.14
1	B	37	GLN	N-CA-CB	5.66	118.55	110.06
1	B	76	MET	CB-CG-SD	-5.65	95.74	112.70
1	B	75	MET	CA-C-O	5.64	126.10	119.28
1	B	109	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	B	54	THR	N-CA-CB	-5.60	101.66	110.06
1	A	162	GLY	CA-C-O	-5.59	115.29	121.05
1	B	131	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	55	SER	CA-CB-OG	-5.57	99.97	111.10
1	B	118	GLU	N-CA-CB	-5.57	102.00	110.07
1	B	34	GLN	CA-C-O	-5.56	114.65	120.55
1	B	96	THR	N-CA-C	-5.56	105.38	111.82
1	B	171	VAL	CA-C-N	5.54	127.65	120.44
1	B	171	VAL	C-N-CA	5.54	127.65	120.44
1	A	111	THR	CA-C-O	-5.54	115.06	119.71
1	B	151	ALA	N-CA-CB	-5.53	101.38	110.40
1	A	111	THR	CA-CB-CG2	5.53	119.89	110.50
1	B	92	ASN	CA-CB-CG	5.49	118.09	112.60
1	B	157	MET	CA-CB-CG	-5.49	103.12	114.10
1	B	101	ALA	CA-C-O	-5.47	114.62	120.42
1	B	174	ASN	N-CA-CB	5.46	118.15	110.12
1	A	44	ASN	CA-CB-CG	-5.46	107.14	112.60
1	B	65	ILE	CB-CA-C	-5.45	104.88	112.02
1	A	48	GLN	CB-CA-C	-5.45	102.30	110.90
1	B	133	ALA	CA-C-N	5.43	127.50	120.44
1	B	133	ALA	C-N-CA	5.43	127.50	120.44
1	B	158	GLN	CG-CD-NE2	5.42	124.53	116.40
1	B	50	GLN	CG-CD-NE2	5.42	124.52	116.40
1	A	69	ARG	CA-CB-CG	-5.39	103.32	114.10
1	B	113	LEU	CB-CA-C	5.37	117.15	109.26
1	A	99	GLN	CG-CD-NE2	5.36	124.44	116.40
1	B	109	ASN	CA-CB-CG	-5.35	107.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LEU	N-CA-CB	-5.35	101.45	110.49
1	B	145	ASN	CA-C-N	5.34	127.44	120.28
1	B	145	ASN	C-N-CA	5.34	127.44	120.28
1	B	57	TRP	CG-CD1-NE1	-5.34	103.26	110.20
1	A	136	GLU	O-C-N	-5.32	116.59	122.07
1	A	76	MET	CA-C-N	5.30	131.66	121.54
1	A	76	MET	C-N-CA	5.30	131.66	121.54
1	A	75	MET	N-CA-C	5.29	119.48	113.19
1	B	57	TRP	O-C-N	5.27	128.16	122.15
1	A	148	ALA	CA-C-O	5.27	126.00	120.42
1	A	90	LEU	N-CA-C	-5.24	105.64	111.36
1	B	80	ASN	N-CA-C	-5.24	101.31	108.38
1	A	118	GLU	CB-CG-CD	5.22	121.47	112.60
1	B	64	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	B	35	HIS	CA-CB-CG	5.21	119.01	113.80
1	B	146	MET	N-CA-C	5.21	116.95	111.28
1	B	50	GLN	CA-C-O	-5.16	114.95	120.42
1	A	162	GLY	CA-C-N	5.15	127.18	120.28
1	A	162	GLY	C-N-CA	5.15	127.18	120.28
1	B	70	SER	O-C-N	-5.14	116.53	122.09
1	A	44	ASN	CA-C-O	-5.10	114.10	119.97
1	A	88	ASP	CA-C-O	5.10	127.07	118.91
1	A	94	LYS	CA-C-N	5.10	127.07	120.44
1	A	94	LYS	C-N-CA	5.10	127.07	120.44
1	A	139	GLN	CB-CG-CD	5.09	121.25	112.60
1	B	118	GLU	CA-CB-CG	5.07	124.24	114.10
1	B	163	GLU	N-CA-C	5.07	116.49	111.07
1	A	66	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	30	PHE	CA-C-O	5.01	126.43	120.66
1	B	68	SER	N-CA-C	5.01	116.82	111.36
1	A	55	SER	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	TYR	Sidechain
1	B	180	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1223	0	1178	19	0
1	B	1223	0	1178	38	0
2	A	10	0	0	0	0
3	A	9	0	3	0	0
4	A	14	0	8	5	0
5	A	69	0	0	2	0
5	B	74	0	0	0	0
All	All	2622	0	2367	53	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 11.

All (53) 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:B:29:LEU:CB	1:B:181:ASP:O	1.68	1.38
1:B:29:LEU:CD1	1:B:181:ASP:O	1.75	1.32
1:B:29:LEU:CG	1:B:181:ASP:O	1.92	1.17
1:B:29:LEU:HB3	1:B:181:ASP:O	1.47	1.11
1:B:29:LEU:HD12	1:B:181:ASP:O	1.43	1.09
1:B:29:LEU:CA	1:B:181:ASP:C	2.37	0.98
1:B:29:LEU:HA	1:B:181:ASP:C	1.91	0.96
1:B:29:LEU:CA	1:B:181:ASP:O	2.16	0.92
1:B:29:LEU:CB	1:B:181:ASP:C	2.52	0.82
4:A:390:PHN:H8	1:B:179:THR:CG2	2.13	0.79
1:B:29:LEU:HB3	1:B:181:ASP:C	2.10	0.77
1:B:167:ASN:HD21	1:B:170:ARG:HH21	1.34	0.75
1:B:74:MET:HE1	1:B:144:GLY:HA2	1.70	0.72
1:A:147:ASP:HA	1:B:81:GLN:HE22	1.58	0.69
1:B:122:ASN:HD21	1:B:126:LYS:HZ3	1.41	0.68
4:A:390:PHN:H8	1:B:179:THR:HG23	1.80	0.63
1:B:167:ASN:ND2	1:B:170:ARG:HH21	1.95	0.62
1:A:74:MET:O	1:A:83:SER:HA	1.99	0.62
1:A:49:GLN:HG2	1:A:110:MET:SD	2.41	0.60
1:B:29:LEU:HA	1:B:181:ASP:O	1.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:HG2	5:A:476:HOH:O	2.05	0.56
1:A:67:LEU:HD21	1:A:138:ILE:HG12	1.89	0.55
1:B:122:ASN:ND2	1:B:126:LYS:NZ	2.56	0.55
1:B:29:LEU:HD13	1:B:181:ASP:O	1.94	0.53
1:B:122:ASN:HD21	1:B:126:LYS:NZ	2.05	0.53
1:B:176:TYR:O	1:B:179:THR:HB	2.09	0.52
1:B:133:ALA:HB1	1:B:152:GLN:HE22	1.75	0.51
1:B:29:LEU:C	1:B:181:ASP:C	2.79	0.51
4:A:390:PHN:H8	1:B:179:THR:HG21	1.91	0.50
1:B:74:MET:HE2	1:B:146:MET:SD	2.52	0.49
1:A:75:MET:HE1	1:B:72:ALA:HB1	1.94	0.49
1:B:29:LEU:O	1:B:181:ASP:C	2.55	0.49
1:B:179:THR:HG22	1:B:180:PHE:HD1	1.78	0.48
1:A:167:ASN:O	1:A:171:VAL:HG23	2.14	0.47
1:A:147:ASP:HA	1:B:81:GLN:NE2	2.27	0.47
1:B:74:MET:CE	1:B:146:MET:SD	3.03	0.47
1:B:29:LEU:HD12	1:B:181:ASP:C	2.33	0.46
1:A:176:TYR:CE1	4:A:390:PHN:H2	2.51	0.46
1:B:49:GLN:NE2	1:B:111:THR:O	2.49	0.46
1:A:45:GLU:HA	1:A:48:GLN:HG2	1.98	0.45
1:B:167:ASN:HD22	1:B:170:ARG:HE	1.64	0.45
1:A:31:SER:H	1:A:35:HIS:CD2	2.36	0.44
1:A:27:GLY:HA3	1:B:33:LEU:HD13	2.00	0.43
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.91	0.43
1:A:72:ALA:HB2	5:A:463:HOH:O	2.20	0.42
1:A:31:SER:N	1:A:35:HIS:HD2	2.17	0.42
1:A:31:SER:H	1:A:35:HIS:HD2	1.67	0.41
1:A:65:ILE:HG22	1:A:69:ARG:HD3	2.02	0.41
1:A:73:ARG:HG3	1:A:73:ARG:HH11	1.84	0.41
1:B:137:LEU:HD22	1:B:149:TYR:CD2	2.55	0.41
1:A:52:GLU:OE1	1:A:103:HIS:HD2	2.04	0.41
1:B:137:LEU:HG	1:B:152:GLN:HE21	1.86	0.40
1:A:179:THR:OG1	4:A:390:PHN:H3	2.21	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	155/164 (94%)	147 (95%)	4 (3%)	4 (3%)	4	1
1	B	155/164 (94%)	146 (94%)	6 (4%)	3 (2%)	6	3
All	All	310/328 (94%)	293 (94%)	10 (3%)	7 (2%)	5	2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	79	SER
1	A	86	LYS
1	B	82	GLN
1	B	83	SER
1	B	84	SER
1	A	84	SER

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	128/134 (96%)	113 (88%)	15 (12%)	5	3
1	B	128/134 (96%)	104 (81%)	24 (19%)	1	1
All	All	256/268 (96%)	217 (85%)	39 (15%)	3	1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	48	GLN
1	A	59	LEU
1	A	69	ARG
1	A	82	GLN
1	A	87	THR
1	A	97	LEU
1	A	109	ASN
1	A	114	PRO
1	A	118	GLU
1	A	142	ASP
1	A	163	GLU
1	A	174	ASN
1	A	175	LEU
1	A	180	PHE
1	B	25	MET
1	B	28	LEU
1	B	33	LEU
1	B	37	GLN
1	B	46	LEU
1	B	53	LEU
1	B	59	LEU
1	B	61	LEU
1	B	74	MET
1	B	81	GLN
1	B	82	GLN
1	B	87	THR
1	B	89	LEU
1	B	90	LEU
1	B	113	LEU
1	B	128	GLN
1	B	134	LEU
1	B	142	ASP
1	B	152	GLN
1	B	153	PRO
1	B	163	GLU
1	B	175	LEU
1	B	179	THR
1	B	181	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	44	ASN
1	A	49	GLN
1	A	50	GLN
1	A	99	GLN
1	A	103	HIS
1	A	106	ASN
1	A	131	GLN
1	A	143	ASN
1	B	81	GLN
1	B	103	HIS
1	B	122	ASN
1	B	131	GLN
1	B	152	GLN
1	B	167	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	SO4	A	900	-	4,4,4	0.70	0	6,6,6	0.54	0
2	SO4	A	901	-	4,4,4	0.97	0	6,6,6	0.82	0
4	PHN	A	390	-	16,16,16	2.64	9 (56%)	22,22,22	1.81	5 (22%)
3	ASP	A	189	-	7,8,8	2.06	3 (42%)	6,10,10	1.73	2 (33%)

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
4	PHN	A	390	-	-	-	0/3/3/3
3	ASP	A	189	-	-	0/8/8/8	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	390	PHN	C6-C6A	-5.79	1.29	1.42
4	A	390	PHN	C7-C6A	-3.89	1.33	1.42
3	A	189	ASP	OD2-CG	-3.26	1.20	1.30
4	A	390	PHN	C5-C4A	-3.25	1.34	1.42
3	A	189	ASP	CB-CA	-2.99	1.39	1.53
4	A	390	PHN	C9-N10	2.93	1.38	1.32
4	A	390	PHN	C2-N1	2.93	1.38	1.32
4	A	390	PHN	C10-N10	2.72	1.40	1.36
3	A	189	ASP	OXT-C	-2.54	1.22	1.30
4	A	390	PHN	C3-C2	2.32	1.44	1.37
4	A	390	PHN	C8-C7	-2.20	1.32	1.36
4	A	390	PHN	C6-C5	2.13	1.40	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	390	PHN	C8-C9-N10	-4.86	116.83	123.97
4	A	390	PHN	C7-C8-C9	3.76	123.62	118.92
4	A	390	PHN	C6-C5-C4A	-3.00	116.90	121.34
3	A	189	ASP	OD2-CG-OD1	-2.75	116.26	123.33
3	A	189	ASP	OD2-CG-CB	2.55	121.93	114.00
4	A	390	PHN	C3-C2-N1	-2.47	120.35	123.97
4	A	390	PHN	C5-C6-C6A	2.11	124.46	121.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	390	PHN	5	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

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.