



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 2HRO / pdb_00002hro
Title : Structure of the full-lenght Enzyme I of the PTS system from *Staphylococcus carnosus*
Authors : Marquez, J.A.; Reinelt, S.; Koch, B.; Engelman, R.; Hengstenberg, W.; Schefzek, K.
Deposited on : 2006-07-20
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 ⓘ 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

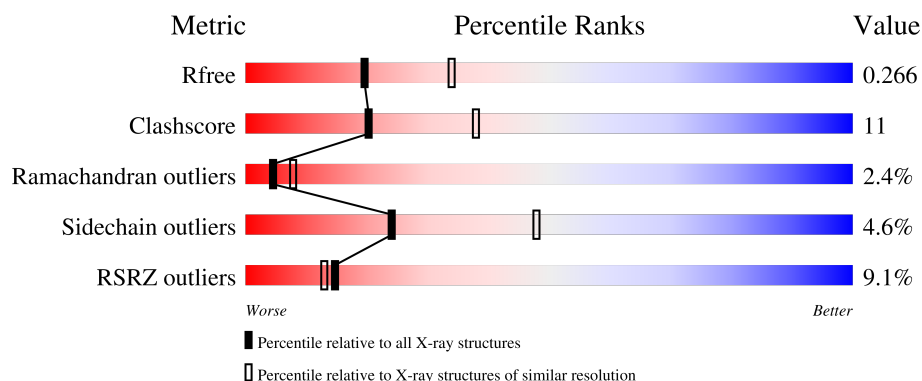
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	573	9% 68% 25% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4247 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.

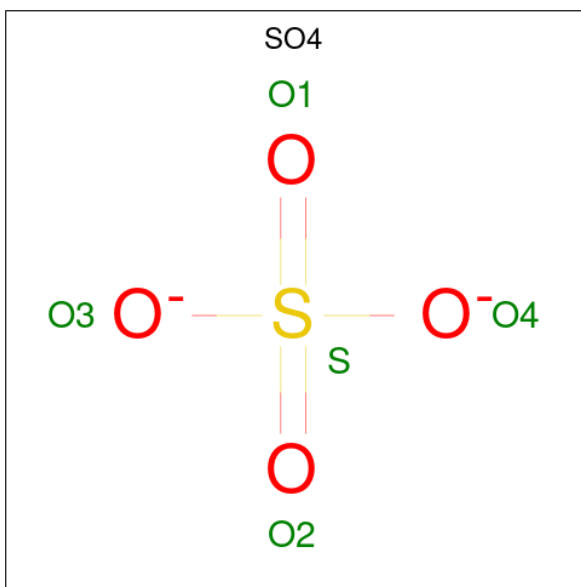
- Molecule 1 is a protein called Phosphoenolpyruvate-protein phosphotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4070	2551	697	803	19			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	ILE	SEE REMARK 999	UNP P23533
A	?	-	LYS	SEE REMARK 999	UNP P23533
A	406	LEU	PHE	SEE REMARK 999	UNP P23533
A	408	GLU	LYS	SEE REMARK 999	UNP P23533
A	409	GLU	LYS	SEE REMARK 999	UNP P23533
A	410	GLU	ASN	SEE REMARK 999	UNP P23533
A	411	ARG	VAL	SEE REMARK 999	UNP P23533
A	412	ALA	LEU	SEE REMARK 999	UNP P23533
A	413	ASN	THR	SEE REMARK 999	UNP P23533
A	416	ASN	MET	SEE REMARK 999	UNP P23533
A	417	GLU	LYS	SEE REMARK 999	UNP P23533
A	418	GLY	ALA	SEE REMARK 999	UNP P23533
A	419	TYR	MET	SEE REMARK 999	UNP P23533
A	420	GLU	LYS	SEE REMARK 999	UNP P23533
A	479	ASN	ILE	SEE REMARK 999	UNP P23533
A	480	PRO	SER	SEE REMARK 999	UNP P23533
A	481	ALA	ASN	SEE REMARK 999	UNP P23533
A	482	ILE	PHE	SEE REMARK 999	UNP P23533
A	483	LEU	SER	SEE REMARK 999	UNP P23533
A	484	ARG	PHE	SEE REMARK 999	UNP P23533
A	536	ARG	VAL	SEE REMARK 999	UNP P23533

- 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		

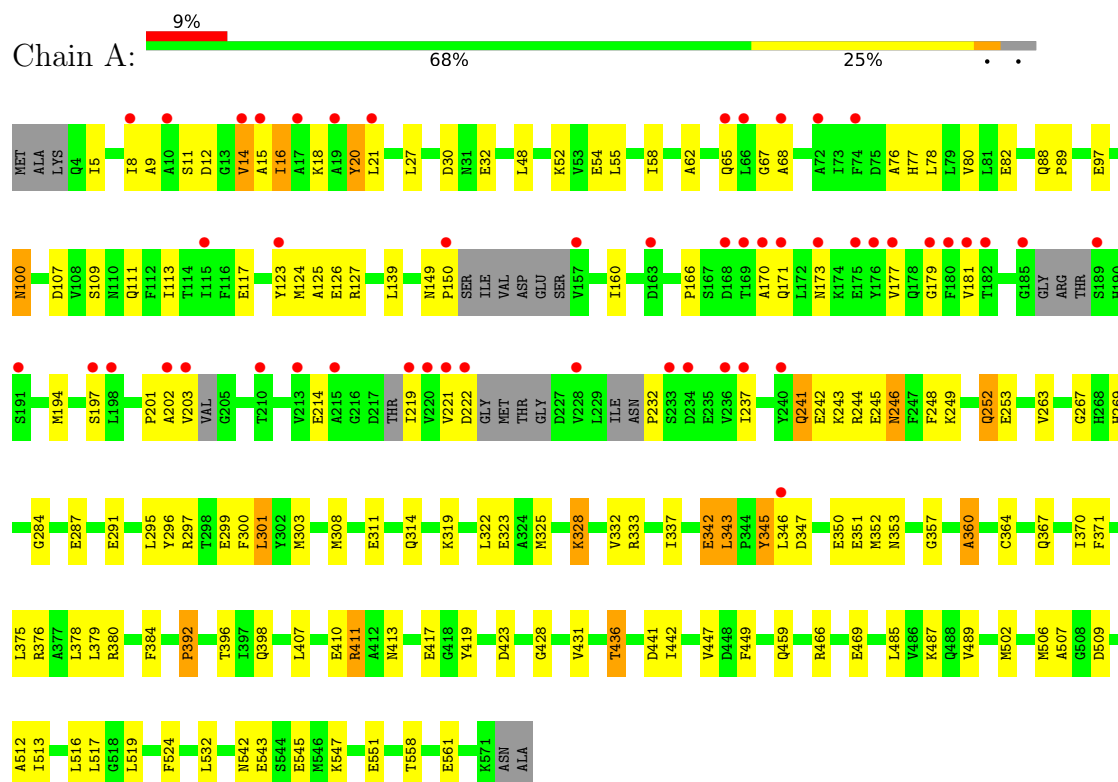
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total	O	0	0
			172	172		

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 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.

- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.36Å 46.85Å 85.30Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	34.86 – 2.50 34.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.86-2.50) 99.7 (34.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.267 0.216 , 0.266	Depositor DCC
R_{free} test set	1321 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.972	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4247	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.43	0/4119	0.92	15/5572 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	TYR	N-CA-C	-7.74	100.10	110.55
1	A	357	GLY	N-CA-C	7.25	121.28	111.20
1	A	350	GLU	N-CA-C	7.06	119.59	111.11
1	A	166	PRO	N-CA-CB	6.47	110.04	103.25
1	A	343	LEU	CA-C-N	6.45	125.95	119.24
1	A	343	LEU	C-N-CA	6.45	125.95	119.24
1	A	246	ASN	N-CA-C	-6.44	106.05	114.04
1	A	201	PRO	N-CA-CB	6.43	110.18	102.72
1	A	232	PRO	N-CA-CB	6.38	110.02	103.00
1	A	125	ALA	N-CA-C	-5.72	106.13	113.23
1	A	267	GLY	N-CA-C	5.41	122.82	115.30
1	A	243	LYS	N-CA-C	-5.40	106.64	113.18
1	A	62	ALA	N-CA-C	-5.39	106.64	113.43
1	A	360	ALA	CB-CA-C	-5.39	110.34	116.54
1	A	411	ARG	N-CA-C	-5.34	105.38	111.14

There are no chirality outliers.

There are no planarity outliers.

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	4070	0	3828	89	0
2	A	5	0	0	0	0
3	A	172	0	0	0	0
All	All	4247	0	3828	89	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 (89) 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:396:THR:HG22	1:A:398:GLN:H	1.42	0.85
1:A:345:TYR:O	1:A:346:LEU:HB2	1.80	0.79
1:A:558:THR:OG1	1:A:561:GLU:HG3	1.81	0.78
1:A:428:GLY:HA2	1:A:447:VAL:HG13	1.68	0.76
1:A:54:GLU:O	1:A:58:ILE:HG12	1.92	0.69
1:A:547:LYS:O	1:A:551:GLU:HG3	1.94	0.68
1:A:411:ARG:NH2	1:A:423:ASP:HA	2.08	0.68
1:A:65:GLN:HE22	1:A:173:ASN:HA	1.60	0.66
1:A:431:VAL:HG13	1:A:436:THR:CG2	2.26	0.66
1:A:411:ARG:HH21	1:A:423:ASP:HA	1.60	0.65
1:A:299:GLU:HB3	1:A:303:MET:HE2	1.79	0.64
1:A:100:ASN:C	1:A:100:ASN:HD22	2.04	0.64
1:A:246:ASN:HA	1:A:249:LYS:HE3	1.79	0.64
1:A:367:GLN:O	1:A:370:ILE:HG22	1.99	0.62
1:A:149:ASN:HB2	1:A:150:PRO:HD2	1.86	0.58
1:A:352:MET:HE2	1:A:353:ASN:HD21	1.67	0.58
1:A:8:ILE:HA	1:A:203:VAL:HA	1.85	0.58
1:A:447:VAL:HG12	1:A:449:PHE:H	1.69	0.58
1:A:345:TYR:HD1	1:A:346:LEU:HD13	1.69	0.57
1:A:506:MET:HE2	1:A:516:LEU:HD21	1.88	0.56
1:A:428:GLY:HA2	1:A:447:VAL:CG1	2.36	0.56
1:A:308:MET:SD	1:A:370:ILE:HD12	2.46	0.56
1:A:396:THR:HG22	1:A:398:GLN:N	2.16	0.55
1:A:14:VAL:H	1:A:222:ASP:HA	1.72	0.55
1:A:509:ASP:O	1:A:513:ILE:HG13	2.07	0.54
1:A:297:ARG:HG2	1:A:333:ARG:NH2	2.23	0.53
1:A:487:LYS:HB2	1:A:519:LEU:HD22	1.90	0.53
1:A:325:MET:O	1:A:328:LYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:C	1:A:100:ASN:ND2	2.68	0.51
1:A:380:ARG:HD3	1:A:419:TYR:CD2	2.45	0.51
1:A:78:LEU:O	1:A:82:GLU:HG2	2.11	0.50
1:A:300:PHE:CE2	1:A:301:LEU:HD22	2.46	0.50
1:A:345:TYR:CD1	1:A:346:LEU:HD13	2.46	0.50
1:A:150:PRO:HB3	1:A:171:GLN:O	2.10	0.50
1:A:30:ASP:O	1:A:32:GLU:HG3	2.13	0.49
1:A:21:LEU:HA	1:A:160:ILE:O	2.12	0.49
1:A:301:LEU:HG	1:A:314:GLN:HG2	1.94	0.49
1:A:337:ILE:HD13	1:A:343:LEU:HD11	1.93	0.49
1:A:332:VAL:HG11	1:A:378:LEU:HD21	1.95	0.49
1:A:244:ARG:C	1:A:246:ASN:H	2.21	0.49
1:A:67:GLY:O	1:A:68:ALA:HB3	2.13	0.48
1:A:113:ILE:O	1:A:117:GLU:HG2	2.13	0.48
1:A:237:ILE:O	1:A:241:GLN:HB2	2.14	0.47
1:A:14:VAL:H	1:A:222:ASP:CA	2.26	0.47
1:A:109:SER:O	1:A:113:ILE:HG13	2.14	0.47
1:A:76:ALA:O	1:A:80:VAL:HG23	2.14	0.46
1:A:245:GLU:O	1:A:249:LYS:HB2	2.15	0.46
1:A:88:GLN:HB2	1:A:89:PRO:HD3	1.97	0.46
1:A:319:LYS:HE2	1:A:384:PHE:CE2	2.51	0.46
1:A:542:ASN:HB3	1:A:545:GLU:HB2	1.97	0.46
1:A:20:TYR:H	1:A:21:LEU:HD12	1.82	0.45
1:A:431:VAL:HG13	1:A:436:THR:HG22	1.97	0.45
1:A:328:LYS:HA	1:A:328:LYS:HE2	1.99	0.45
1:A:459:GLN:OE1	1:A:466:ARG:HG2	2.16	0.45
1:A:248:PHE:O	1:A:252:GLN:HB2	2.17	0.45
1:A:65:GLN:NE2	1:A:173:ASN:HA	2.31	0.45
1:A:15:ALA:HB1	1:A:179:GLY:HA2	1.99	0.44
1:A:55:LEU:HB2	1:A:78:LEU:HD21	1.99	0.44
1:A:124:MET:SD	1:A:127:ARG:HD3	2.57	0.44
1:A:194:MET:HA	1:A:197:SER:CB	2.48	0.44
1:A:364:CYS:HB3	1:A:371:PHE:CG	2.52	0.44
1:A:502:MET:HG2	1:A:507:ALA:HB2	1.99	0.44
1:A:360:ALA:HB1	1:A:392:PRO:HG2	2.00	0.44
1:A:48:LEU:CD1	1:A:52:LYS:HE3	2.48	0.43
1:A:48:LEU:HD11	1:A:52:LYS:HE3	2.00	0.43
1:A:263:VAL:HG22	1:A:269:HIS:CD2	2.53	0.43
1:A:16:ILE:HA	1:A:219:ILE:O	2.17	0.43
1:A:323:GLU:HG3	1:A:384:PHE:HB3	2.00	0.43
1:A:27:LEU:HB3	1:A:139:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG12	1:A:449:PHE:N	2.32	0.42
1:A:123:TYR:O	1:A:126:GLU:HB3	2.19	0.42
1:A:311:GLU:OE1	1:A:376:ARG:HD3	2.20	0.42
1:A:512:ALA:O	1:A:516:LEU:HG	2.19	0.42
1:A:21:LEU:HD12	1:A:21:LEU:N	2.35	0.42
1:A:107:ASP:O	1:A:111:GLN:HG2	2.20	0.41
1:A:547:LYS:HE3	1:A:547:LYS:HB2	1.87	0.41
1:A:9:ALA:C	1:A:11:SER:H	2.29	0.41
1:A:524:PHE:CD1	1:A:524:PHE:N	2.88	0.41
1:A:296:TYR:HB3	1:A:332:VAL:HA	2.01	0.41
1:A:469:GLU:OE1	1:A:469:GLU:HA	2.20	0.41
1:A:249:LYS:O	1:A:253:GLU:HG3	2.20	0.41
1:A:485:LEU:O	1:A:489:VAL:HG23	2.21	0.41
1:A:9:ALA:O	1:A:202:ALA:HB3	2.21	0.41
1:A:291:GLU:O	1:A:328:LYS:HG3	2.20	0.41
1:A:413:ASN:O	1:A:417:GLU:HG3	2.20	0.41
1:A:284:GLY:HA2	1:A:287:GLU:HG2	2.03	0.40
1:A:375:LEU:HD22	1:A:407:LEU:CD1	2.51	0.40
1:A:410:GLU:HA	1:A:410:GLU:OE1	2.21	0.40
1:A:441:ASP:OD2	1:A:442:ILE:N	2.54	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	537/573 (94%)	460 (86%)	64 (12%)	13 (2%)	4 8

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	VAL

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Mol	Chain	Res	Type
1	A	342	GLU
1	A	12	ASP
1	A	18	LYS
1	A	20	TYR
1	A	170	ALA
1	A	351	GLU
1	A	14	VAL
1	A	177	VAL
1	A	181	VAL
1	A	16	ILE
1	A	214	GLU
1	A	5	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	391/481 (81%)	373 (95%)	18 (5%)	24	48

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	97	GLU
1	A	100	ASN
1	A	241	GLN
1	A	242	GLU
1	A	252	GLN
1	A	295	LEU
1	A	301	LEU
1	A	322	LEU
1	A	328	LYS
1	A	342	GLU
1	A	347	ASP
1	A	379	LEU
1	A	392	PRO

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Mol	Chain	Res	Type
1	A	436	THR
1	A	517	LEU
1	A	532	LEU
1	A	543	GLU

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	65	GLN
1	A	100	ASN
1	A	103	GLN
1	A	121	ASN
1	A	246	ASN
1	A	252	GLN
1	A	255	GLN
1	A	353	ASN
1	A	416	ASN
1	A	488	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	SO4	A	900	-	4,4,4	0.33	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/573 (96%)	0.42	50 (9%) 15 13	29, 58, 132, 139	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	ALA	6.1
1	A	181	VAL	4.6
1	A	202	ALA	4.6
1	A	180	PHE	4.1
1	A	176	TYR	3.9
1	A	189	SER	3.6
1	A	222	ASP	3.6
1	A	234	ASP	3.3
1	A	150	PRO	3.2
1	A	169	THR	3.1
1	A	74	PHE	3.1
1	A	236	VAL	3.0
1	A	14	VAL	3.0
1	A	220	VAL	2.8
1	A	170	ALA	2.8
1	A	215	ALA	2.7
1	A	171	GLN	2.7
1	A	175	GLU	2.6
1	A	123	TYR	2.6
1	A	240	TYR	2.6
1	A	237	ILE	2.6
1	A	203	VAL	2.5
1	A	168	ASP	2.5
1	A	219	ILE	2.5
1	A	68	ALA	2.5
1	A	191	SER	2.5
1	A	233	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	8	ILE	2.4
1	A	66	LEU	2.4
1	A	221	VAL	2.4
1	A	210	THR	2.3
1	A	65	GLN	2.3
1	A	17	ALA	2.3
1	A	197	SER	2.3
1	A	157	VAL	2.3
1	A	173	ASN	2.2
1	A	19	ALA	2.2
1	A	177	VAL	2.2
1	A	213	VAL	2.2
1	A	72	ALA	2.2
1	A	21	LEU	2.2
1	A	179	GLY	2.1
1	A	182	THR	2.1
1	A	228	VAL	2.1
1	A	198	LEU	2.1
1	A	163	ASP	2.1
1	A	185	GLY	2.1
1	A	10	ALA	2.1
1	A	115	ILE	2.1
1	A	346	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	900	5/5	0.95	0.09	63,64,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.