



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:47 PM GMT

PDB ID : 1YNH  
Title : Crystal Structure of N-Succinylarginine Dihydrolase, AstB, bound to Substrate and Product, an Enzyme from the Arginine Catabolic Pathway of Escherichia coli  
Authors : Tocilj, A.; Schrag, J.D.; Li, Y.; Schneider, B.L.; Reitzer, L.; Matte, A.; Cygler, M.  
Deposited on : 2005-01-24  
Resolution : 1.95 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

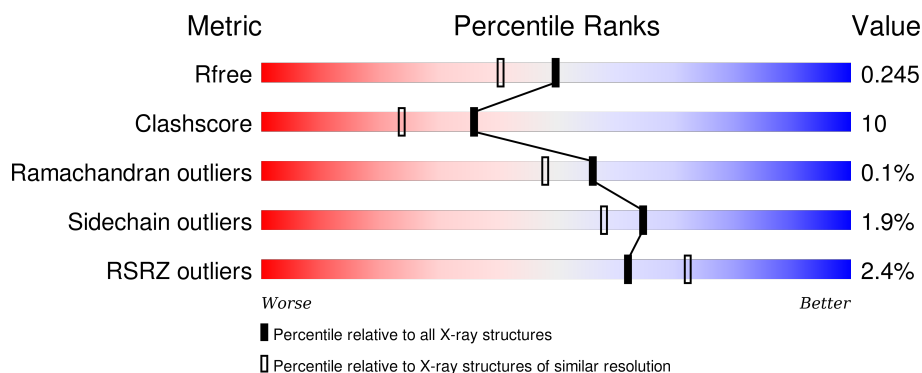
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	458	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	B	458	<div> <div>2%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
1	C	458	<div> <div>4%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	D	458	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>

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	SUO	A	1001	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14754 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 Succinylarginine Dihydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3424	2145	625	642	12			
1	B	440	Total	C	N	O	S	0	0	0
			3432	2149	627	644	12			
1	C	439	Total	C	N	O	S	0	0	0
			3424	2145	625	642	12			
1	D	439	Total	C	N	O	S	0	0	0
			3424	2145	625	642	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P76216
A	-9	GLY	-	EXPRESSION TAG	UNP P76216
A	-8	SER	-	EXPRESSION TAG	UNP P76216
A	-7	SER	-	EXPRESSION TAG	UNP P76216
A	-6	HIS	-	EXPRESSION TAG	UNP P76216
A	-5	HIS	-	EXPRESSION TAG	UNP P76216
A	-4	HIS	-	EXPRESSION TAG	UNP P76216
A	-3	HIS	-	EXPRESSION TAG	UNP P76216
A	-2	HIS	-	EXPRESSION TAG	UNP P76216
A	-1	HIS	-	EXPRESSION TAG	UNP P76216
A	0	GLY	-	EXPRESSION TAG	UNP P76216
A	1	SER	-	EXPRESSION TAG	UNP P76216
B	-10	MET	-	EXPRESSION TAG	UNP P76216
B	-9	GLY	-	EXPRESSION TAG	UNP P76216
B	-8	SER	-	EXPRESSION TAG	UNP P76216
B	-7	SER	-	EXPRESSION TAG	UNP P76216
B	-6	HIS	-	EXPRESSION TAG	UNP P76216
B	-5	HIS	-	EXPRESSION TAG	UNP P76216
B	-4	HIS	-	EXPRESSION TAG	UNP P76216
B	-3	HIS	-	EXPRESSION TAG	UNP P76216
B	-2	HIS	-	EXPRESSION TAG	UNP P76216

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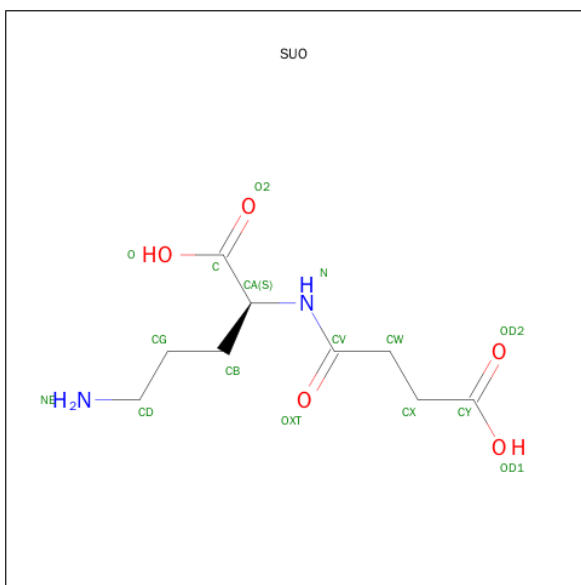
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	EXPRESSION TAG	UNP P76216
B	0	GLY	-	EXPRESSION TAG	UNP P76216
B	1	SER	-	EXPRESSION TAG	UNP P76216
C	-10	MET	-	EXPRESSION TAG	UNP P76216
C	-9	GLY	-	EXPRESSION TAG	UNP P76216
C	-8	SER	-	EXPRESSION TAG	UNP P76216
C	-7	SER	-	EXPRESSION TAG	UNP P76216
C	-6	HIS	-	EXPRESSION TAG	UNP P76216
C	-5	HIS	-	EXPRESSION TAG	UNP P76216
C	-4	HIS	-	EXPRESSION TAG	UNP P76216
C	-3	HIS	-	EXPRESSION TAG	UNP P76216
C	-2	HIS	-	EXPRESSION TAG	UNP P76216
C	-1	HIS	-	EXPRESSION TAG	UNP P76216
C	0	GLY	-	EXPRESSION TAG	UNP P76216
C	1	SER	-	EXPRESSION TAG	UNP P76216
D	-10	MET	-	EXPRESSION TAG	UNP P76216
D	-9	GLY	-	EXPRESSION TAG	UNP P76216
D	-8	SER	-	EXPRESSION TAG	UNP P76216
D	-7	SER	-	EXPRESSION TAG	UNP P76216
D	-6	HIS	-	EXPRESSION TAG	UNP P76216
D	-5	HIS	-	EXPRESSION TAG	UNP P76216
D	-4	HIS	-	EXPRESSION TAG	UNP P76216
D	-3	HIS	-	EXPRESSION TAG	UNP P76216
D	-2	HIS	-	EXPRESSION TAG	UNP P76216
D	-1	HIS	-	EXPRESSION TAG	UNP P76216
D	0	GLY	-	EXPRESSION TAG	UNP P76216
D	1	SER	-	EXPRESSION TAG	UNP P76216

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0

- Molecule 3 is N 2 -(3-CARBOXYPROPANOYL)-L-ORNITHINE (three-letter code: SUO) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	9	2	5		
3	B	1	Total	C	N	O	0	0
			16	9	2	5		
3	C	1	Total	C	N	O	0	0
			16	9	2	5		
3	D	1	Total	C	N	O	0	0
			16	9	2	5		

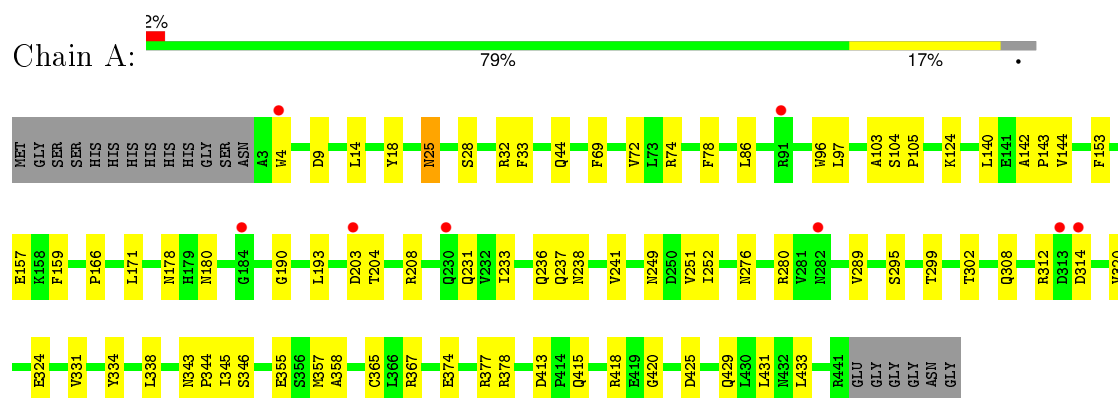
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	251	Total	O	0	0
			251	251		
4	B	304	Total	O	0	0
			304	304		
4	C	185	Total	O	0	0
			185	185		
4	D	242	Total	O	0	0
			242	242		

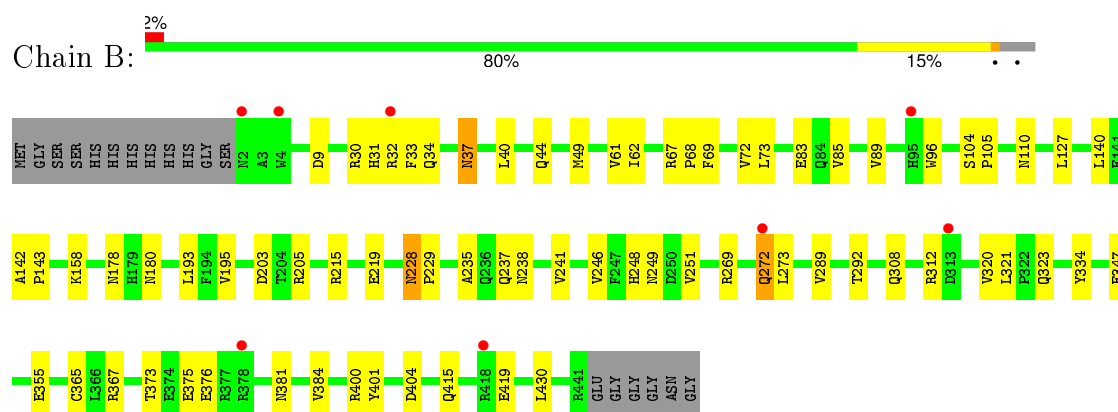
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

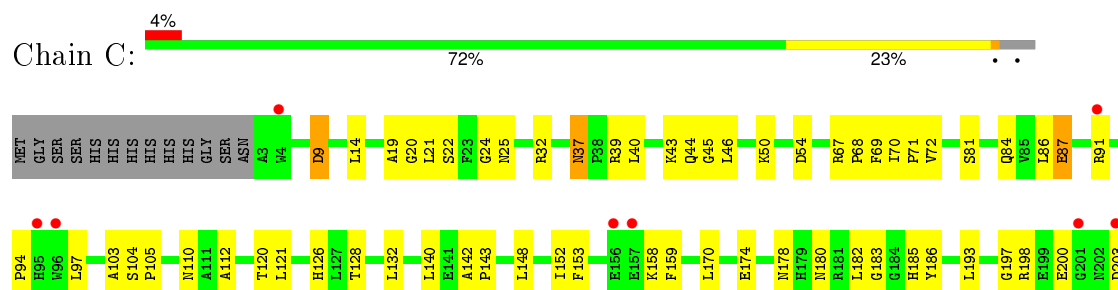
#### • Molecule 1: Succinylarginine Dihydrolase

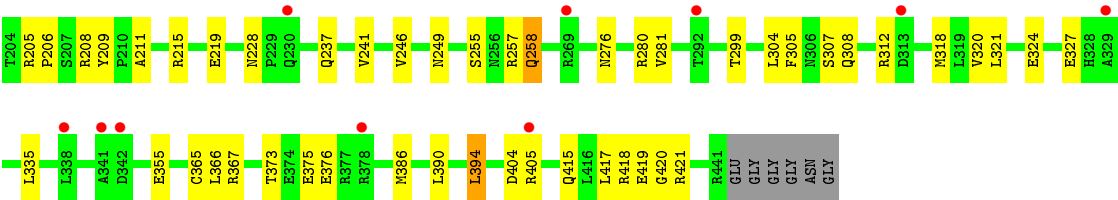


#### • Molecule 1: Succinylarginine Dihydrolase

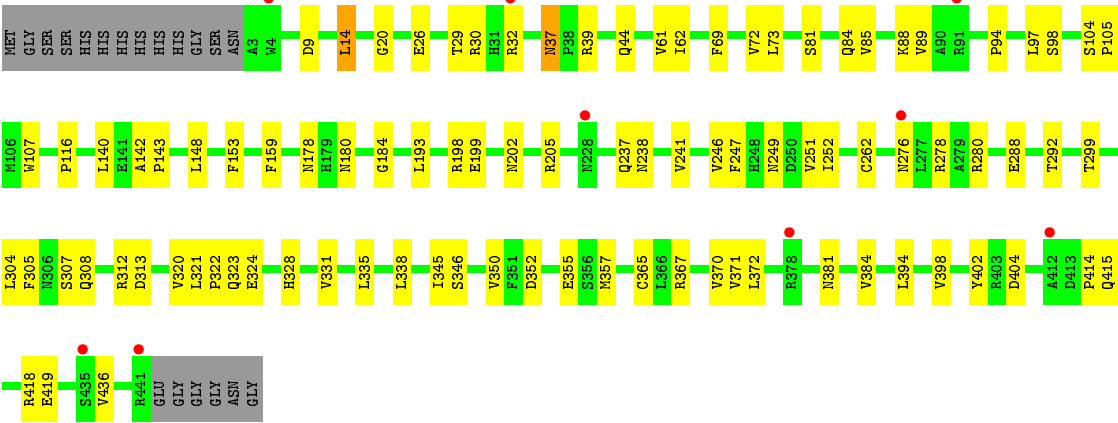
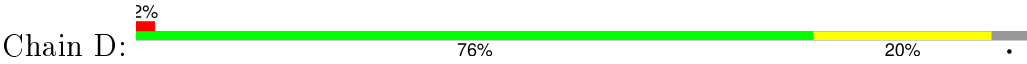


#### • Molecule 1: Succinylarginine Dihydrolase





● Molecule 1: Succinylarginine Dihydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.86Å 166.91Å 185.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.30 – 1.95 53.30 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.6 (53.30-1.95) 96.6 (53.30-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.219 , 0.246 0.218 , 0.245	Depositor DCC
$R_{free}$ test set	4850 reflections (4.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 121063 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6068e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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: SUO, K

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	0.33	0/3497	0.58	0/4753
1	B	0.34	0/3505	0.59	0/4764
1	C	0.32	0/3497	0.57	0/4753
1	D	0.33	0/3497	0.58	0/4753
All	All	0.33	0/13996	0.58	0/19023

There are no bond length outliers.

There are no bond angle outliers.

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	3424	0	3353	59	0
1	B	3432	0	3359	50	0
1	C	3424	0	3353	85	0
1	D	3424	0	3353	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	14	1	0
3	C	16	0	14	1	0
3	D	16	0	14	2	0
4	A	251	0	0	2	0
4	B	304	0	0	1	0
4	C	185	0	0	2	0
4	D	242	0	0	3	0
All	All	14754	0	13474	262	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 10.

All (262) 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:415:GLN:HE21	1:A:418:ARG:HH11	1.18	0.91
1:D:328:HIS:HD2	1:D:331:VAL:H	1.24	0.85
1:C:258:GLN:H	1:C:258:GLN:HE21	1.25	0.82
1:D:14:LEU:H	1:D:14:LEU:HD12	1.48	0.79
1:D:323:GLN:HG3	1:D:352:ASP:HA	1.66	0.78
1:A:312:ARG:NH2	1:A:346:SER:HB2	1.98	0.78
1:D:198:ARG:HB2	1:D:205:ARG:HH12	1.48	0.76
1:A:415:GLN:NE2	1:A:418:ARG:HH11	1.84	0.76
1:D:237:GLN:HE22	1:D:249:ASN:HD22	1.33	0.76
1:A:415:GLN:HE21	1:A:418:ARG:NH1	1.85	0.75
1:C:81:SER:OG	1:C:84:GLN:HG3	1.87	0.75
1:D:29:THR:O	1:D:32:ARG:HG3	1.88	0.73
1:A:178:ASN:ND2	1:A:249:ASN:H	1.86	0.73
1:A:276:ASN:HD21	1:A:280:ARG:HH11	1.37	0.70
1:D:26:GLU:O	1:D:30:ARG:HG3	1.91	0.69
1:D:198:ARG:HB2	1:D:205:ARG:NH1	2.07	0.69
1:C:72:VAL:HG21	1:C:140:LEU:HD22	1.74	0.69
1:C:237:GLN:HE22	1:C:249:ASN:HD22	1.40	0.69
1:A:237:GLN:HE22	1:A:249:ASN:HD22	1.41	0.69
1:D:292:THR:HG23	4:D:2115:HOH:O	1.94	0.67
1:B:312:ARG:NH2	1:B:347:GLU:HB2	2.08	0.67
1:A:312:ARG:HH22	1:A:346:SER:HB2	1.60	0.67
1:B:178:ASN:ND2	1:B:249:ASN:H	1.93	0.67
1:C:185:HIS:HD2	1:C:257:ARG:HH21	1.41	0.67
1:C:241:VAL:HG13	1:C:246:VAL:HG21	1.76	0.66
1:C:258:GLN:NE2	1:C:258:GLN:H	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ARG:HD3	1:D:404:ASP:OD2	1.94	0.66
1:A:144:VAL:HG23	4:A:2161:HOH:O	1.96	0.66
1:A:276:ASN:HD21	1:A:280:ARG:NH1	1.93	0.66
1:D:73:LEU:HD13	1:D:89:VAL:HG21	1.78	0.66
1:C:307:SER:HB3	1:C:321:LEU:HD23	1.76	0.66
1:B:237:GLN:HE22	1:B:249:ASN:HD22	1.44	0.66
1:D:81:SER:OG	1:D:84:GLN:HG3	1.96	0.65
1:B:272:GLN:HG3	1:B:273:LEU:N	2.11	0.65
1:D:178:ASN:ND2	1:D:249:ASN:H	1.94	0.65
1:B:72:VAL:HG21	1:B:140:LEU:HD22	1.79	0.64
1:A:204:THR:HG22	1:A:236:GLN:HE22	1.62	0.64
1:D:308:GLN:HB2	1:D:320:VAL:HB	1.80	0.64
1:C:304:LEU:CD1	1:C:335:LEU:HD21	2.28	0.63
1:B:312:ARG:HH21	1:B:347:GLU:HB2	1.61	0.63
1:D:324:GLU:H	1:D:324:GLU:CD	2.01	0.63
1:A:72:VAL:HG21	1:A:140:LEU:HD22	1.80	0.63
1:A:308:GLN:HB2	1:A:320:VAL:HB	1.81	0.62
1:C:70:ILE:HD11	1:C:86:LEU:HD13	1.81	0.62
1:C:20:GLY:HA3	1:C:32:ARG:HG2	1.81	0.62
1:B:142:ALA:HB3	1:B:143:PRO:HD3	1.82	0.62
1:C:365:CYS:SG	3:C:1003:SUO:NE	2.73	0.61
1:C:405:ARG:HB3	1:C:405:ARG:NH1	2.16	0.61
1:B:37:ASN:HD22	1:B:37:ASN:C	2.02	0.61
1:A:324:GLU:HG3	1:A:357:MET:CE	2.31	0.60
1:B:158:LYS:NZ	1:B:375:GLU:OE2	2.34	0.60
1:B:44:GLN:HE22	1:B:355:GLU:H	1.48	0.59
1:A:365:CYS:SG	3:A:1001:SUO:NE	2.75	0.59
1:C:44:GLN:HE22	1:C:355:GLU:H	1.48	0.59
1:D:394:LEU:O	1:D:398:VAL:HG23	2.03	0.58
1:B:32:ARG:HG2	1:B:33:PHE:CD1	2.39	0.58
1:C:405:ARG:HH11	1:C:405:ARG:HB3	1.68	0.58
1:B:365:CYS:SG	3:B:1002:SUO:NE	2.75	0.58
1:C:120:THR:HG21	1:C:126:HIS:HD2	1.68	0.58
1:B:228:ASN:HD22	1:B:229:PRO:CD	2.16	0.58
1:D:69:PHE:CD2	1:D:72:VAL:HG23	2.39	0.58
1:A:233:ILE:CD1	1:A:276:ASN:HD22	2.17	0.57
1:A:324:GLU:HG3	1:A:357:MET:HE3	1.86	0.57
1:C:81:SER:H	1:C:84:GLN:NE2	2.02	0.57
1:A:233:ILE:HD12	1:A:276:ASN:ND2	2.19	0.57
1:B:269:ARG:O	1:B:272:GLN:HG2	2.04	0.57
1:D:328:HIS:CD2	1:D:331:VAL:H	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:HG23	1:C:305:PHE:HD1	1.70	0.56
1:A:14:LEU:HD21	1:A:420:GLY:HA2	1.86	0.56
1:C:37:ASN:C	1:C:37:ASN:HD22	2.09	0.56
1:D:307:SER:HB3	1:D:321:LEU:HD23	1.88	0.56
1:B:228:ASN:HD22	1:B:229:PRO:HD2	1.71	0.56
1:D:328:HIS:CD2	1:D:331:VAL:HG23	2.41	0.56
1:B:31:HIS:O	1:B:34:GLN:HG3	2.06	0.55
1:C:215:ARG:O	1:C:219:GLU:HG3	2.07	0.55
1:C:304:LEU:HD11	1:C:335:LEU:HD21	1.87	0.55
1:C:373:THR:OG1	1:C:376:GLU:HG3	2.07	0.55
1:D:44:GLN:HE22	1:D:355:GLU:H	1.55	0.55
1:C:415:GLN:NE2	1:C:419:GLU:HG3	2.22	0.55
1:C:308:GLN:HB2	1:C:320:VAL:HB	1.89	0.54
1:C:104:SER:N	1:C:105:PRO:HD2	2.22	0.54
1:B:49:MET:SD	1:B:61:VAL:HG22	2.48	0.54
1:C:37:ASN:ND2	1:C:404:ASP:HA	2.23	0.54
1:B:415:GLN:O	1:B:419:GLU:HG3	2.08	0.54
1:D:324:GLU:HG3	1:D:357:MET:CE	2.38	0.54
1:B:238:ASN:O	1:B:241:VAL:HG22	2.08	0.54
1:C:39:ARG:O	1:C:43:LYS:HG2	2.07	0.54
1:A:178:ASN:HD22	1:A:249:ASN:H	1.55	0.53
1:C:312:ARG:NH2	1:C:318:MET:HE1	2.23	0.53
1:A:180:ASN:HB2	1:A:193:LEU:HB3	1.90	0.53
1:C:258:GLN:HE21	1:C:258:GLN:N	1.99	0.53
1:A:144:VAL:HG21	4:A:2198:HOH:O	2.09	0.53
1:D:142:ALA:HB3	1:D:143:PRO:HD3	1.91	0.53
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.91	0.53
1:C:69:PHE:CD2	1:C:72:VAL:HG23	2.44	0.52
1:A:276:ASN:ND2	1:A:280:ARG:HH11	2.06	0.52
1:C:415:GLN:OE1	1:C:418:ARG:NH2	2.34	0.52
1:A:238:ASN:HB3	1:A:241:VAL:HG22	1.92	0.52
1:D:304:LEU:CD1	1:D:335:LEU:HD21	2.39	0.52
1:A:44:GLN:HE22	1:A:355:GLU:H	1.57	0.52
1:D:20:GLY:HA3	1:D:32:ARG:HG2	1.92	0.52
1:A:103:ALA:C	1:A:105:PRO:HD2	2.30	0.52
1:A:18:TYR:CE2	1:A:358:ALA:HB3	2.44	0.52
1:B:228:ASN:HD22	1:B:229:PRO:N	2.07	0.52
1:A:4:TRP:CZ3	1:A:377:ARG:NH1	2.77	0.52
1:C:183:GLY:HA2	1:C:281:VAL:HG13	1.91	0.52
1:C:91:ARG:HB2	1:C:91:ARG:NH1	2.25	0.51
1:D:14:LEU:HG	1:D:402:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLU:OE1	1:C:91:ARG:NE	2.43	0.51
1:D:37:ASN:C	1:D:37:ASN:HD22	2.14	0.51
1:A:413:ASP:OD1	1:A:415:GLN:HB2	2.12	0.50
1:B:430:LEU:HD23	1:B:430:LEU:C	2.32	0.50
1:C:37:ASN:ND2	1:C:40:LEU:H	2.09	0.50
1:C:91:ARG:HH11	1:C:91:ARG:CB	2.25	0.50
1:C:241:VAL:HG13	1:C:246:VAL:CG2	2.41	0.50
1:A:142:ALA:HB3	1:A:143:PRO:HD3	1.92	0.50
1:C:81:SER:HB3	1:C:84:GLN:HE21	1.77	0.49
1:B:69:PHE:CD2	1:B:72:VAL:HG23	2.47	0.49
1:A:343:ASN:HB2	1:A:344:PRO:CD	2.42	0.49
1:D:14:LEU:H	1:D:14:LEU:CD1	2.22	0.49
1:B:400:ARG:HD3	1:B:401:TYR:CE1	2.47	0.49
1:B:158:LYS:NZ	1:B:375:GLU:HG2	2.27	0.49
1:D:415:GLN:O	1:D:419:GLU:HG3	2.13	0.49
1:D:180:ASN:HB2	1:D:193:LEU:HB3	1.95	0.49
1:C:205:ARG:HB2	1:C:206:PRO:HD2	1.94	0.49
1:A:124:LYS:HE2	1:A:157:GLU:O	2.13	0.49
1:A:25:ASN:HD22	1:A:25:ASN:C	2.15	0.49
1:C:91:ARG:CB	1:C:91:ARG:NH1	2.76	0.48
1:C:22:SER:O	1:C:25:ASN:HB3	2.12	0.48
1:C:70:ILE:CD1	1:C:86:LEU:HD13	2.43	0.48
1:C:50:LYS:HE3	1:C:54:ASP:OD2	2.14	0.48
1:D:381:ASN:O	1:D:384:VAL:HG22	2.13	0.48
1:A:237:GLN:NE2	1:A:249:ASN:HD22	2.11	0.48
1:D:251:VAL:O	1:D:251:VAL:HG12	2.13	0.48
1:C:9:ASP:HA	1:C:366:LEU:O	2.13	0.48
1:B:104:SER:N	1:B:105:PRO:HD2	2.28	0.48
1:D:84:GLN:O	1:D:88:LYS:HG3	2.14	0.48
1:A:233:ILE:HD12	1:A:276:ASN:HD22	1.77	0.47
1:D:322:PRO:HB2	1:D:324:GLU:OE2	2.15	0.47
1:B:67:ARG:HA	1:B:68:PRO:C	2.35	0.47
1:D:39:ARG:HG3	1:D:398:VAL:HG12	1.95	0.47
1:D:241:VAL:HG22	1:D:246:VAL:HG21	1.96	0.47
1:C:91:ARG:HH11	1:C:91:ARG:HB3	1.80	0.47
1:D:238:ASN:O	1:D:241:VAL:HG12	2.14	0.47
1:D:323:GLN:HA	1:D:350:VAL:CG1	2.45	0.47
1:C:299:THR:HG23	1:C:305:PHE:CD1	2.50	0.47
1:A:104:SER:N	1:A:105:PRO:HD2	2.30	0.47
1:B:308:GLN:HB2	1:B:320:VAL:HB	1.97	0.47
1:B:215:ARG:O	1:B:219:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:HG13	1:B:251:VAL:HB	1.96	0.47
1:C:46:LEU:HD21	1:C:394:LEU:HD23	1.97	0.47
1:D:365:CYS:SG	3:D:1004:SUA:NE	2.87	0.47
1:C:178:ASN:ND2	1:C:249:ASN:H	2.13	0.47
1:D:85:VAL:O	1:D:89:VAL:HG23	2.15	0.47
1:B:37:ASN:ND2	1:B:404:ASP:HA	2.30	0.47
1:D:94:PRO:O	1:D:97:LEU:HB2	2.15	0.46
1:A:166:PRO:HD2	1:A:171:LEU:HD13	1.97	0.46
1:D:323:GLN:HG3	1:D:352:ASP:CA	2.43	0.46
1:D:104:SER:N	1:D:105:PRO:HD2	2.30	0.46
1:C:103:ALA:C	1:C:105:PRO:HD2	2.36	0.46
1:C:417:LEU:O	1:C:421:ARG:HG2	2.15	0.46
1:B:289:VAL:HG22	1:B:334:TYR:OH	2.14	0.46
1:A:295:SER:O	1:A:299:THR:HG23	2.15	0.46
1:B:180:ASN:HB2	1:B:193:LEU:HB3	1.97	0.46
1:D:14:LEU:N	1:D:14:LEU:HD12	2.24	0.46
1:A:96:TRP:HA	1:A:96:TRP:CE3	2.50	0.46
1:C:170:LEU:HD11	1:C:200:GLU:CD	2.36	0.46
1:B:430:LEU:O	1:B:430:LEU:HD23	2.16	0.46
1:A:190:GLY:O	1:A:231:GLN:HB3	2.16	0.46
1:B:30:ARG:HH21	1:B:31:HIS:CE1	2.34	0.46
1:C:386:MET:HA	1:C:390:LEU:HD23	1.96	0.45
1:D:89:VAL:CG1	1:D:97:LEU:HG	2.47	0.45
1:A:74:ARG:HA	1:A:78:PHE:O	2.15	0.45
1:A:69:PHE:CD2	1:A:72:VAL:HG23	2.51	0.45
1:D:304:LEU:HD11	1:D:335:LEU:HD21	1.98	0.45
1:C:110:ASN:HB3	1:C:132:LEU:HD21	1.98	0.45
1:D:178:ASN:HD22	1:D:249:ASN:H	1.64	0.45
1:B:195:VAL:HA	1:B:235:ALA:O	2.17	0.45
1:A:324:GLU:HG3	1:A:357:MET:HE2	1.99	0.45
1:C:44:GLN:NE2	4:C:2083:HOH:O	2.49	0.45
1:C:81:SER:CB	1:C:84:GLN:HE21	2.29	0.45
1:A:32:ARG:O	1:A:33:PHE:HB2	2.17	0.45
1:C:182:LEU:HD21	1:C:255:SER:HB2	1.98	0.45
1:C:70:ILE:N	1:C:71:PRO:CD	2.79	0.44
1:A:302:THR:HG21	1:A:331:VAL:HG21	1.99	0.44
1:D:276:ASN:HD21	1:D:280:ARG:HD2	1.82	0.44
1:B:228:ASN:C	1:B:228:ASN:HD22	2.20	0.44
1:C:197:GLY:HA3	1:C:211:ALA:HB1	1.98	0.44
1:D:199:GLU:HG3	1:D:202:ASN:HB2	2.00	0.44
1:B:37:ASN:ND2	1:B:40:LEU:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:VAL:HG22	1:B:334:TYR:CZ	2.53	0.44
1:A:237:GLN:HE22	1:A:249:ASN:ND2	2.13	0.44
1:C:180:ASN:HB2	1:C:193:LEU:HB3	1.99	0.44
1:B:292:THR:HG23	4:B:2144:HOH:O	2.18	0.44
1:B:203:ASP:O	1:B:205:ARG:HG2	2.18	0.44
1:A:431:LEU:HB2	1:A:433:LEU:HG	2.00	0.44
1:C:45:GLY:HA3	4:C:2134:HOH:O	2.17	0.43
1:B:373:THR:OG1	1:B:376:GLU:HG3	2.18	0.43
1:D:252:ILE:HD12	1:D:299:THR:HG21	2.01	0.43
1:D:324:GLU:HG3	1:D:357:MET:HE3	2.01	0.43
1:A:289:VAL:HG22	1:A:334:TYR:OH	2.19	0.43
1:A:374:GLU:HG2	1:A:378:ARG:NH1	2.34	0.43
1:C:67:ARG:HA	1:C:68:PRO:C	2.39	0.43
1:A:153:PHE:HB3	1:A:159:PHE:CG	2.53	0.43
1:A:338:LEU:HD21	1:A:345:ILE:CD1	2.49	0.43
1:D:247:PHE:CE1	3:D:1004:SUO:HD1A	2.54	0.43
1:B:381:ASN:O	1:B:384:VAL:HG22	2.19	0.43
1:B:85:VAL:O	1:B:89:VAL:HG23	2.18	0.43
1:D:414:PRO:O	1:D:418:ARG:HG3	2.19	0.43
1:D:370:VAL:HG12	1:D:372:LEU:HG	2.01	0.43
1:B:37:ASN:ND2	1:B:37:ASN:C	2.71	0.42
1:A:203:ASP:HB3	1:C:405:ARG:HD3	2.00	0.42
1:A:86:LEU:HD12	1:A:97:LEU:HD21	2.01	0.42
1:C:415:GLN:HE21	1:C:419:GLU:CG	2.32	0.42
1:C:324:GLU:HA	1:C:327:GLU:OE1	2.19	0.42
1:D:89:VAL:HG12	1:D:97:LEU:HG	2.00	0.42
1:D:104:SER:HA	1:D:107:TRP:CZ3	2.55	0.42
1:D:153:PHE:HB3	1:D:159:PHE:CG	2.53	0.42
1:C:405:ARG:CB	1:C:405:ARG:HH11	2.30	0.42
1:D:312:ARG:NH2	1:D:346:SER:HB2	2.34	0.42
1:D:44:GLN:NE2	4:D:2036:HOH:O	2.52	0.42
1:C:87:GLU:OE1	1:C:87:GLU:C	2.57	0.42
1:B:83:GLU:CD	1:B:83:GLU:H	2.23	0.42
1:D:116:PRO:HB3	1:D:371:VAL:HB	2.01	0.42
1:A:251:VAL:HG12	1:A:251:VAL:O	2.20	0.42
1:B:61:VAL:HG12	1:B:62:ILE:N	2.35	0.42
1:C:415:GLN:HE21	1:C:419:GLU:HG3	1.85	0.42
1:C:14:LEU:HD21	1:C:420:GLY:HA2	2.02	0.42
1:B:127:LEU:HD12	1:B:127:LEU:N	2.35	0.42
1:C:24:GLY:HA2	1:C:209:TYR:CD2	2.56	0.41
1:C:321:LEU:HD13	1:C:335:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:H	1:A:324:GLU:CD	2.24	0.41
1:A:238:ASN:O	1:A:241:VAL:HG22	2.20	0.41
1:C:153:PHE:HB3	1:C:159:PHE:CG	2.55	0.41
1:C:112:ALA:HB1	1:C:128:THR:O	2.20	0.41
1:D:61:VAL:HG22	1:D:62:ILE:N	2.36	0.41
1:C:312:ARG:HG2	1:C:312:ARG:HH11	1.85	0.41
1:B:73:LEU:HD13	1:B:89:VAL:HG21	2.03	0.41
1:B:110:ASN:HD21	1:B:248:HIS:CE1	2.39	0.41
1:D:324:GLU:HG3	1:D:357:MET:HE2	2.01	0.41
1:C:158:LYS:HE2	1:C:375:GLU:HG2	2.01	0.41
1:D:237:GLN:HE22	1:D:249:ASN:ND2	2.10	0.41
1:C:186:TYR:CE2	1:C:257:ARG:HD3	2.56	0.41
1:A:203:ASP:O	1:C:405:ARG:NE	2.54	0.41
1:D:69:PHE:HD2	1:D:72:VAL:HG23	1.82	0.41
1:A:25:ASN:ND2	1:A:28:SER:H	2.19	0.41
1:C:208:ARG:NH1	1:C:209:TYR:CE2	2.89	0.41
1:C:19:ALA:HB3	1:C:21:LEU:HG	2.02	0.41
1:C:94:PRO:O	1:C:97:LEU:HB2	2.21	0.41
1:D:305:PHE:C	1:D:307:SER:H	2.24	0.41
1:B:96:TRP:HA	1:B:96:TRP:CE3	2.56	0.41
1:D:262:CYS:O	1:D:288:GLU:HA	2.21	0.41
1:C:276:ASN:O	1:C:280:ARG:HG3	2.21	0.41
1:D:72:VAL:HG21	1:D:140:LEU:HD22	2.03	0.40
1:A:252:ILE:HG13	1:A:252:ILE:O	2.21	0.40
1:D:278:ARG:NH2	4:D:2195:HOH:O	2.55	0.40
1:C:121:LEU:HD23	1:C:228:ASN:OD1	2.21	0.40
1:C:132:LEU:HD23	1:C:174:GLU:HA	2.03	0.40
1:C:148:LEU:O	1:C:152:ILE:HG13	2.22	0.40
1:C:182:LEU:CD2	1:C:255:SER:HB2	2.52	0.40
1:D:148:LEU:HD23	1:D:436:VAL:HG21	2.02	0.40
1:D:338:LEU:HD21	1:D:345:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/458 (95%)	425 (97%)	12 (3%)	0	100	100
1	B	438/458 (96%)	422 (96%)	16 (4%)	0	100	100
1	C	437/458 (95%)	419 (96%)	18 (4%)	0	100	100
1	D	437/458 (95%)	423 (97%)	13 (3%)	1 (0%)	52	43
All	All	1749/1832 (96%)	1689 (97%)	59 (3%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	184	GLY

### 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	364/377 (97%)	357 (98%)	7 (2%)	65	58
1	B	365/377 (97%)	358 (98%)	7 (2%)	65	58
1	C	364/377 (97%)	356 (98%)	8 (2%)	60	51
1	D	364/377 (97%)	358 (98%)	6 (2%)	70	66
All	All	1457/1508 (97%)	1429 (98%)	28 (2%)	65	58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	25	ASN
1	A	208	ARG
1	A	314	ASP
1	A	367	ARG
1	A	425	ASP
1	A	429	GLN

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Mol	Chain	Res	Type
1	B	9	ASP
1	B	37	ASN
1	B	228	ASN
1	B	272	GLN
1	B	321	LEU
1	B	323	GLN
1	B	367	ARG
1	C	9	ASP
1	C	37	ASN
1	C	87	GLU
1	C	198	ARG
1	C	203	ASP
1	C	258	GLN
1	C	367	ARG
1	C	394	LEU
1	D	9	ASP
1	D	14	LEU
1	D	37	ASN
1	D	98	SER
1	D	313	ASP
1	D	367	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	34	GLN
1	A	44	GLN
1	A	178	ASN
1	A	226	GLN
1	A	236	GLN
1	A	249	ASN
1	A	276	ASN
1	A	415	GLN
1	A	432	ASN
1	B	31	HIS
1	B	37	ASN
1	B	44	GLN
1	B	178	ASN
1	B	226	GLN
1	B	228	ASN
1	B	230	GLN

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Mol	Chain	Res	Type
1	B	236	GLN
1	B	249	ASN
1	B	272	GLN
1	B	323	GLN
1	C	34	GLN
1	C	37	ASN
1	C	44	GLN
1	C	84	GLN
1	C	178	ASN
1	C	185	HIS
1	C	226	GLN
1	C	249	ASN
1	C	258	GLN
1	C	336	ASN
1	C	432	ASN
1	D	37	ASN
1	D	44	GLN
1	D	84	GLN
1	D	95	HIS
1	D	154	ASN
1	D	178	ASN
1	D	180	ASN
1	D	226	GLN
1	D	249	ASN
1	D	276	ASN
1	D	328	HIS
1	D	432	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	SUO	A	1001	-	9,15,15	0.43	0	8,18,18	0.33	0
3	SUO	B	1002	-	9,15,15	0.24	0	8,18,18	0.47	0
3	SUO	C	1003	-	9,15,15	0.33	0	8,18,18	0.34	0
3	SUO	D	1004	-	9,15,15	0.34	0	8,18,18	0.48	0

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
3	SUO	A	1001	-	-	0/11/17/17	0/0/0/0
3	SUO	B	1002	-	-	0/11/17/17	0/0/0/0
3	SUO	C	1003	-	-	0/11/17/17	0/0/0/0
3	SUO	D	1004	-	-	0/11/17/17	0/0/0/0

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	SUO	1	0
3	B	1002	SUO	1	0
3	C	1003	SUO	1	0
3	D	1004	SUO	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	439/458 (95%)	0.19	8 (1%) 71 80	11, 23, 38, 48	0
1	B	440/458 (96%)	0.17	8 (1%) 71 80	12, 22, 38, 49	0
1	C	439/458 (95%)	0.48	18 (4%) 41 52	15, 29, 41, 49	0
1	D	439/458 (95%)	0.25	9 (2%) 67 75	13, 25, 39, 49	0
All	All	1757/1832 (95%)	0.27	43 (2%) 62 72	11, 25, 40, 49	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	292	THR	6.2
1	B	378	ARG	4.2
1	A	91	ARG	4.1
1	A	4	TRP	4.1
1	C	4	TRP	4.1
1	D	378	ARG	4.0
1	C	378	ARG	3.9
1	C	342	ASP	3.9
1	C	329	ALA	3.8
1	B	2	ASN	3.7
1	C	95	HIS	3.6
1	B	313	ASP	3.6
1	C	269	ARG	3.6
1	C	230	GLN	3.2
1	D	412	ALA	3.1
1	A	282	ASN	3.1
1	A	314	ASP	3.0
1	B	4	TRP	2.9
1	C	201	GLY	2.9
1	A	313	ASP	2.8
1	C	96	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	203	ASP	2.8
1	B	418	ARG	2.7
1	C	405	ARG	2.7
1	C	91	ARG	2.6
1	D	4	TRP	2.6
1	D	91	ARG	2.6
1	B	272	GLN	2.6
1	C	338	LEU	2.5
1	D	441	ARG	2.5
1	D	228	ASN	2.4
1	B	32	ARG	2.4
1	C	157	GLU	2.3
1	C	156	GLU	2.3
1	B	95	HIS	2.3
1	C	341	ALA	2.3
1	D	276	ASN	2.2
1	A	230	GLN	2.2
1	A	203	ASP	2.2
1	D	32	ARG	2.1
1	C	313	ASP	2.1
1	D	435	SER	2.0
1	A	184	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SUO	A	1001	16/16	0.95	0.13	2.70	12,16,20,25	0
3	SUO	C	1003	16/16	0.94	0.11	1.27	19,21,25,26	0
2	K	C	2003	1/1	0.45	0.23	0.58	72,72,72,72	0
2	K	B	2002	1/1	0.98	0.14	0.39	43,43,43,43	0
3	SUO	D	1004	16/16	0.96	0.10	-0.05	15,18,21,26	0
3	SUO	B	1002	16/16	0.96	0.10	-0.10	14,16,20,22	0
2	K	D	2004	1/1	0.97	0.11	-1.00	63,63,63,63	0
2	K	A	2001	1/1	0.95	0.06	-2.43	41,41,41,41	0

## 6.5 Other polymers

There are no such residues in this entry.