W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2014 – 02:35 PM EST

PDB ID	:	4CD9
Title	:	Structure of SasG A-domain (residues 163-419) from Staphylococcus aureus
Authors	:	Atkin, K.E.; Brentnall, A.S.; Dodson, E.J.; Turkenburg, J.P.; Potts, J.R.
Deposited on	:	2013-10-30
Resolution	:	1.65 Å(reported)

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 1.65 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.
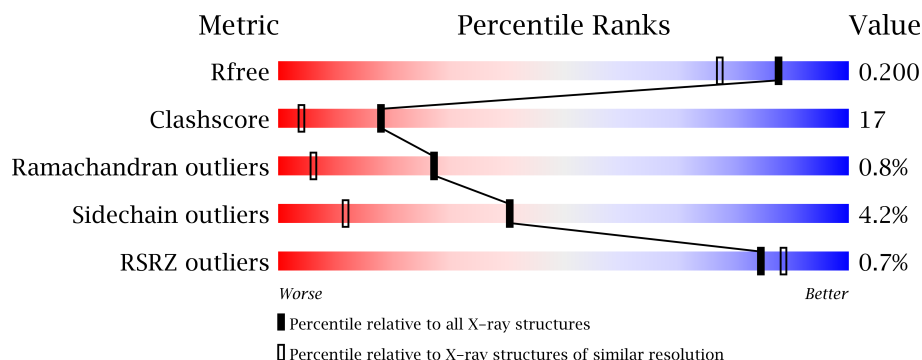
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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 >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	259	
1	B	259	
1	C	259	
1	D	259	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	1420	-	X

Full wwPDB X-ray Structure Validation Report

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8263 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SURFACE PROTEIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1981	1234	343	400	4			
1	B	255	Total	C	N	O	S	0	0	0
			1966	1225	340	397	4			
1	C	256	Total	C	N	O	S	0	0	0
			1975	1231	342	398	4			
1	D	254	Total	C	N	O	S	0	0	0
			1960	1222	339	395	4			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2
OH

C1

C2

HO

O1
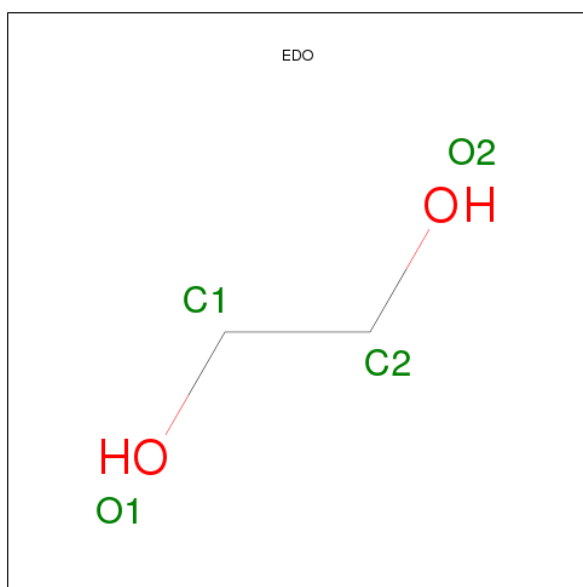
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total 98	O 98	0	3
4	B	80	Total 81	O 81	0	1
4	C	101	Total 102	O 102	0	1
4	D	84	Total 84	O 84	0	0

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: SURFACE PROTEIN G
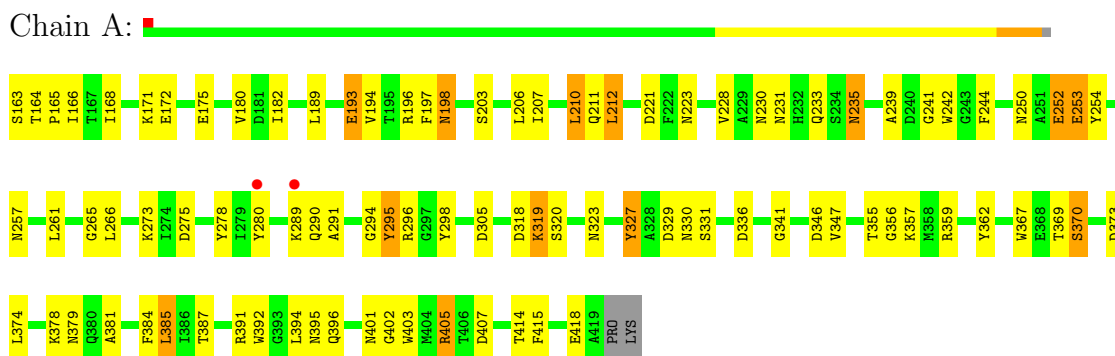
Chain A:

• Molecule 1: SURFACE PROTEIN G
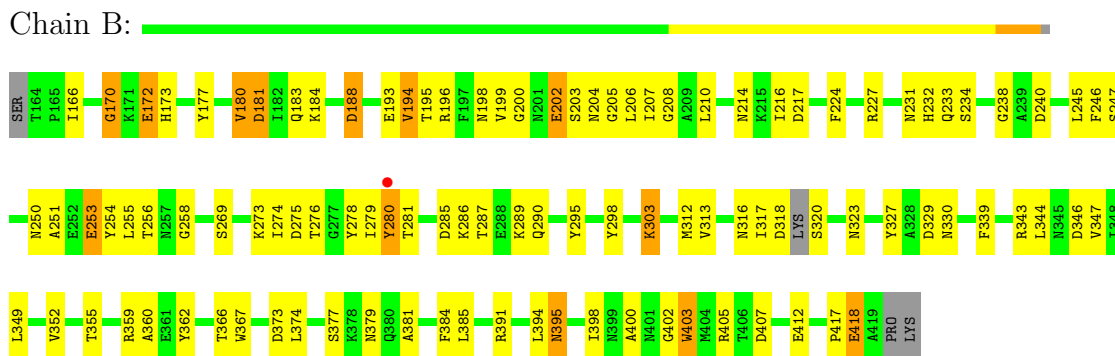
Chain B:

• Molecule 1: SURFACE PROTEIN G

Chain C:

• Molecule 1: SURFACE PROTEIN G

Chain D:

4 Data and refinement statistics (i)

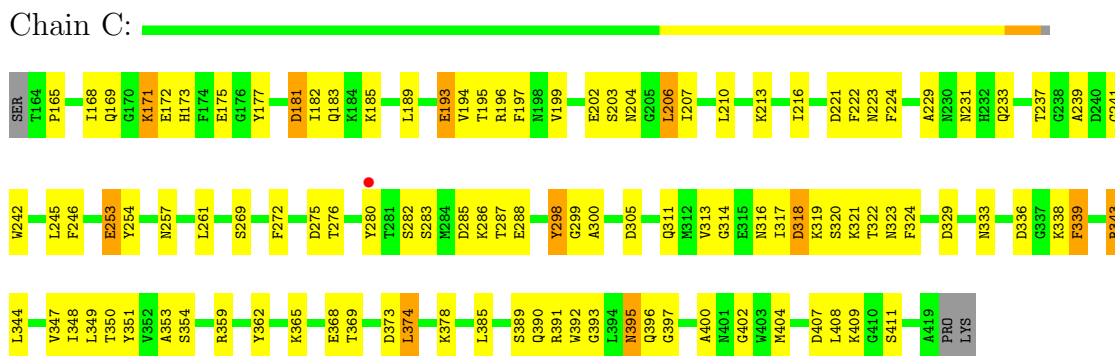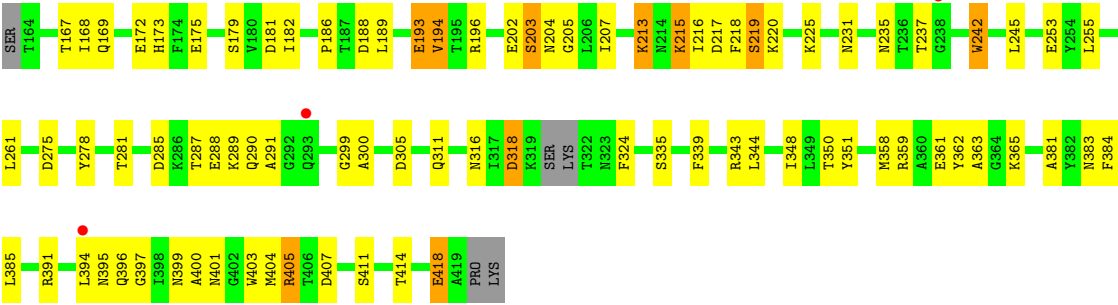| Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	63.21Å 63.21Å 273.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.37 – 1.65 57.37 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (57.37-1.65) 99.1 (57.37-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.185 , 0.243 0.206 , 0.200	Depositor DCC
R_{free} test set	6365 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 15.7	EDS
Estimated twinning fraction	0.506 for H, K, L 0.494 for K, H, -L 0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.506 for H, K, L 0.494 for K, H, -L	Depositor
L-test for twinning	$< |L| > = 0.40, < L^2 > = 0.22$	Xtriage
Outliers	0 of 126731 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8263	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 67.22 % 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 5.3298e-06.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.40	7/2018 (0.3%)	1.40	14/2718 (0.5%)
1	B	1.34	5/2002 (0.2%)	1.43	19/2696 (0.7%)
1	C	1.44	6/2012 (0.3%)	1.49	23/2710 (0.8%)
1	D	1.36	7/1996 (0.4%)	1.41	17/2688 (0.6%)
All	All	1.38	25/8028 (0.3%)	1.43	73/10812 (0.7%)

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	4
1	D	0	1
All	All	0	6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	253	GLU	CD-OE1	7.94	1.34	1.25
1	D	242	TRP	CE3-CZ3	-7.50	1.25	1.38
1	B	303	LYS	C-O	-7.21	1.09	1.23
1	B	269	SER	CB-OG	7.17	1.51	1.42
1	D	362	TYR	CB-CG	-6.76	1.41	1.51
1	D	219	SER	CB-OG	6.75	1.51	1.42
1	C	373	ASP	CB-CG	6.56	1.65	1.51
1	A	362	TYR	CE1-CZ	6.17	1.46	1.38
1	A	252	GLU	CD-OE1	6.05	1.32	1.25
1	D	172	GLU	CD-OE1	5.93	1.32	1.25
1	A	392	TRP	CB-CG	5.91	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ASP	CB-CG	5.88	1.64	1.51
1	A	379	ASN	CG-OD1	5.83	1.36	1.24
1	C	242	TRP	CZ3-CH2	5.70	1.49	1.40
1	A	327	TYR	CE1-CZ	-5.62	1.31	1.38
1	D	288	GLU	CD-OE2	-5.60	1.19	1.25
1	D	242	TRP	CE2-CZ2	-5.57	1.30	1.39
1	D	203	SER	CB-OG	-5.53	1.35	1.42
1	B	403	TRP	CB-CG	-5.52	1.40	1.50
1	B	170	GLY	C-N	-5.45	1.21	1.34
1	C	177	TYR	CB-CG	-5.36	1.43	1.51
1	B	412	GLU	CD-OE2	-5.35	1.19	1.25
1	A	370	SER	CB-OG	-5.33	1.35	1.42
1	C	272	PHE	CG-CD1	5.26	1.46	1.38
1	C	354	SER	CA-CB	-5.07	1.45	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	343	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	343	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	D	285	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	D	181	ASP	CB-CG-OD1	8.65	126.08	118.30
1	C	221	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	344	LEU	CB-CG-CD1	-8.21	97.05	111.00
1	D	217	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	C	318	ASP	CB-CG-OD1	-8.03	111.08	118.30
1	B	217	ASP	CB-CG-OD2	-7.98	111.11	118.30
1	D	245	LEU	CB-CG-CD1	-7.98	97.43	111.00
1	C	285	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	C	221	ASP	CB-CG-OD2	-7.66	111.40	118.30
1	B	407	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	336	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	C	253	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	C	206	LEU	CB-CG-CD2	-7.34	98.53	111.00
1	A	329	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	305	ASP	CB-CG-OD1	7.25	124.83	118.30
1	D	213	LYS	CD-CE-NZ	7.03	127.88	111.70
1	B	180	VAL	CB-CA-C	-6.99	98.11	111.40
1	A	210	LEU	CB-CG-CD2	-6.91	99.25	111.00
1	D	344	LEU	CA-CB-CG	6.91	131.19	115.30
1	A	212	LEU	CB-CG-CD2	6.82	122.59	111.00
1	C	343	ARG	NE-CZ-NH2	-6.77	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	285	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	253	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	C	285	ASP	CB-CG-OD1	6.64	124.28	118.30
1	D	305	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	385	LEU	CA-CB-CG	6.54	130.35	115.30
1	D	405	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	C	305	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	171	LYS	CB-CA-C	-6.47	97.47	110.40
1	B	395	ASN	N-CA-CB	6.34	122.02	110.60
1	A	221	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	181	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	373	ASP	CB-CG-OD1	-6.11	112.81	118.30
1	D	391	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	407	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	418	GLU	CB-CA-C	-5.90	98.60	110.40
1	C	329	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	329	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	407	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	280	TYR	CA-CB-CG	5.82	124.45	113.40
1	B	217	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	216	ILE	CG1-CB-CG2	-5.78	98.68	111.40
1	C	300	ALA	CB-CA-C	-5.74	101.50	110.10
1	C	374	LEU	CB-CG-CD2	5.72	120.73	111.00
1	A	346	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	253	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	B	246	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	B	394	LEU	N-CA-C	-5.55	96.02	111.00
1	C	385	LEU	CB-CG-CD2	-5.52	101.61	111.00
1	B	224	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	C	407	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	245	LEU	CB-CG-CD1	5.46	120.29	111.00
1	B	188	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	240	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	D	275	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	206	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	B	276	THR	CA-CB-CG2	-5.36	104.89	112.40
1	B	275	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	206	LEU	CB-CG-CD1	5.34	120.08	111.00
1	C	409	LYS	C-N-CA	5.29	133.40	122.30
1	A	336	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	405	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	189	LEU	CB-CG-CD2	5.23	119.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	GLU	OE1-CD-OE2	5.16	129.50	123.30
1	A	193	GLU	CA-CB-CG	5.15	124.73	113.40
1	B	329	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	185	LYS	CD-CE-NZ	-5.10	99.97	111.70
1	C	194	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	D	384	PHE	CG-CD2-CE2	5.04	126.35	120.80
1	C	275	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	ARG	Mainchain
1	B	194	VAL	Peptide
1	B	238	GLY	Peptide
1	B	247	SER	Peptide
1	B	320	SER	Peptide
1	D	318	ASP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1981	0	1894	67	0
1	B	1966	0	1875	76	0
1	C	1975	0	1889	73	0
1	D	1960	0	1870	47	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	4	0	6	2	0
3	C	8	0	12	7	0
4	A	98	0	0	5	0
4	B	81	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	102	0	0	6	1
4	D	84	0	0	1	1
All	All	8263	0	7546	264	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (264) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:231:ASN:HD21	1:C:239:ALA:H	1.07	0.96
1:B:233:GLN:HG3	1:B:234:SER:H	1.27	0.95
1:C:175:GLU:HG2	1:C:213:LYS:HE3	1.48	0.93
1:B:233:GLN:HG3	1:B:234:SER:N	1.84	0.92
1:D:203:SER:O	1:D:395:ASN:C	2.11	0.89
1:A:231:ASN:HD22	1:A:402:GLY:HA2	1.38	0.86
1:C:378:LYS:NZ	3:C:1421:EDO:H21	1.90	0.86
1:D:350:THR:OG1	1:D:359:ARG:HB3	1.78	0.83
1:C:320:SER:HB2	1:C:322:THR:HG22	1.60	0.83
1:C:204:ASN:HD21	1:C:393:GLY:HA2	1.43	0.83
1:A:394:LEU:O	1:A:396:GLN:HG3	1.79	0.83
1:B:204:ASN:HA	1:B:395:ASN:HB3	1.61	0.81
1:B:286:LYS:O	1:B:289:LYS:N	2.16	0.77
1:A:323:ASN:HD22	1:A:367:TRP:HE1	1.31	0.76
1:A:280:TYR:HE1	1:A:396:GLN:HE22	1.34	0.75
1:A:391:ARG:HB3	1:A:394:LEU:HD12	1.68	0.75
1:A:197:PHE:O	1:A:198:ASN:HB2	1.87	0.74
1:C:378:LYS:HZ1	3:C:1421:EDO:H21	1.52	0.74
1:B:330:ASN:HB2	4:B:2059:HOH:O	1.87	0.74
1:C:395:ASN:C	1:C:396:GLN:HG3	2.09	0.72
1:D:361:GLU:HG3	4:D:2071:HOH:O	1.89	0.72
1:C:169:GLN:HB2	1:C:411:SER:O	1.90	0.72
1:A:194:VAL:HG21	1:A:405:ARG:HD2	1.73	0.71
1:B:278:TYR:HB2	1:B:290:GLN:HG2	1.73	0.70
1:B:352:VAL:HG13	1:B:355:THR:OG1	1.91	0.70
1:C:350:THR:OG1	1:C:359:ARG:HB3	1.92	0.69
1:D:204:ASN:HA	1:D:395:ASN:HA	1.75	0.68
1:C:195:THR:HG21	1:C:210:LEU:HD11	1.74	0.68
1:B:273:LYS:O	1:B:273:LYS:HG3	1.92	0.68
1:B:199:VAL:HG12	1:B:200:GLY:N	2.09	0.68
1:C:204:ASN:ND2	1:C:393:GLY:HA2	2.08	0.67
1:C:299:GLY:O	1:C:323:ASN:HB3	1.94	0.67
1:B:232:HIS:HE1	1:B:330:ASN:HD22	1.42	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:1420:EDO:H21	4:C:2101:HOH:O	1.94	0.66
1:B:195:THR:HG21	1:B:210:LEU:HD11	1.77	0.66
1:B:359:ARG:HD3	1:B:366:THR:CG2	2.26	0.66
1:C:182:ILE:CG2	1:C:193:GLU:HG3	2.26	0.65
1:C:165:PRO:HD3	4:C:2001:HOH:O	1.96	0.65
1:B:205:GLY:HA3	1:B:391:ARG:O	1.97	0.65
1:A:378:LYS:HD3	3:A:1420:EDO:H12	1.80	0.64
1:B:316:ASN:ND2	1:B:318:ASP:H	1.96	0.64
1:A:231:ASN:HD22	1:A:402:GLY:CA	2.07	0.64
1:D:182:ILE:HD12	1:D:193:GLU:OE2	1.98	0.64
1:D:196:ARG:HD2	1:D:403:TRP:CD2	2.33	0.63
1:C:233:GLN:NE2	1:C:400:ALA:HB1	2.13	0.63
1:A:235:ASN:HD22	1:A:235:ASN:C	2.01	0.62
1:B:278:TYR:CD1	1:B:290:GLN:HB3	2.34	0.62
1:D:339:PHE:CZ	1:D:363:ALA:HB2	2.34	0.62
1:C:199:VAL:O	1:C:206:LEU:HD13	1.99	0.62
1:B:317:ILE:HD11	1:B:359:ARG:NH1	2.14	0.61
1:C:395:ASN:O	1:C:396:GLN:HG3	1.99	0.61
1:B:278:TYR:HD1	1:B:290:GLN:HB3	1.64	0.61
1:A:289:LYS:O	1:A:291:ALA:N	2.33	0.61
1:B:273:LYS:HE3	1:B:298:TYR:CE1	2.36	0.60
1:B:274:ILE:HD13	1:B:362:TYR:CE2	2.36	0.60
1:D:316:ASN:HD21	1:D:318:ASP:HB2	1.67	0.60
1:B:172:GLU:HG2	1:B:173:HIS:CD2	2.37	0.59
1:D:202:GLU:O	1:D:397:GLY:HA2	2.01	0.59
1:B:208:GLY:O	1:B:254:TYR:HE2	1.85	0.59
1:D:215:LYS:HE2	1:D:383:ASN:HD21	1.67	0.58
1:C:183:GLN:HB2	1:C:196:ARG:CZ	2.32	0.58
1:B:202:GLU:HA	1:B:202:GLU:OE1	2.03	0.58
1:B:251:ALA:O	1:B:255:LEU:HG	2.03	0.58
1:C:350:THR:HG23	4:C:2088:HOH:O	2.01	0.58
1:A:369:THR:HG21	1:A:374:LEU:HD21	1.86	0.58
1:B:359:ARG:HH11	1:B:366:THR:HG21	1.66	0.58
1:C:181:ASP:OD1	1:C:196:ARG:HB3	2.03	0.58
1:C:320:SER:CB	1:C:322:THR:HG22	2.32	0.58
1:C:182:ILE:HG23	1:C:193:GLU:HG3	1.85	0.58
1:C:314:GLY:HA3	1:C:369:THR:HB	1.86	0.58
1:B:194:VAL:HG21	1:B:405:ARG:HB3	1.85	0.58
1:A:233:GLN:HG2	1:A:401:ASN:O	2.04	0.57
1:B:280:TYR:CE2	1:B:281:THR:HG23	2.39	0.57
1:C:283:SER:O	1:C:287:THR:N	2.32	0.57
1:B:273:LYS:HE3	1:B:298:TYR:HE1	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:320:SER:O	1:C:321:LYS:HB2	2.04	0.57
1:A:231:ASN:HB3	1:A:403:TRP:O	2.04	0.57
1:D:348:ILE:HB	1:D:361:GLU:HB2	1.87	0.57
1:C:288:GLU:HG3	1:C:298:TYR:CE2	2.39	0.56
1:D:168:ILE:HD12	1:D:173:HIS:CG	2.40	0.56
1:D:350:THR:HG1	1:D:359:ARG:HB3	1.70	0.56
1:D:204:ASN:OD1	1:D:395:ASN:HB3	2.06	0.56
1:B:280:TYR:N	1:B:280:TYR:CD1	2.73	0.56
1:A:278:TYR:CE1	1:A:291:ALA:HB2	2.41	0.56
1:C:229:ALA:HB2	1:C:344:LEU:HD23	1.88	0.56
1:C:390:GLN:HG2	1:C:391:ARG:HG2	1.88	0.56
1:A:254:TYR:CZ	1:A:387:THR:HB	2.41	0.56
1:C:231:ASN:HD22	1:C:402:GLY:HA2	1.71	0.56
1:C:231:ASN:ND2	1:C:239:ALA:H	1.91	0.56
1:C:202:GLU:O	1:C:397:GLY:HA2	2.06	0.55
1:C:351:TYR:CZ	1:C:353:ALA:HA	2.42	0.55
1:B:231:ASN:HD22	1:B:402:GLY:HA2	1.72	0.55
1:D:188:ASP:O	1:D:343:ARG:NH1	2.38	0.55
1:B:347:VAL:HG22	1:B:362:TYR:CD1	2.42	0.55
1:C:347:VAL:HG22	1:C:362:TYR:CD1	2.41	0.55
1:B:359:ARG:HD3	1:B:366:THR:HG21	1.87	0.55
1:C:324:PHE:O	1:C:365:LYS:HE2	2.05	0.55
1:C:253:GLU:O	1:C:257:ASN:HB2	2.06	0.55
1:D:207:ILE:HG23	1:D:255:LEU:HD22	1.89	0.55
1:A:180:VAL:CG2	1:A:197:PHE:CD2	2.89	0.54
1:C:237:THR:HB	1:C:400:ALA:HB3	1.88	0.54
1:C:311:GLN:NE2	4:C:2066:HOH:O	2.40	0.54
1:B:199:VAL:HG12	1:B:200:GLY:H	1.70	0.54
1:B:359:ARG:HG3	1:B:367:TRP:O	2.07	0.54
1:A:171:LYS:HD2	1:A:182:ILE:HD11	1.88	0.54
1:A:355:THR:HG21	4:A:2085:HOH:O	2.08	0.54
1:B:280:TYR:HD1	1:B:280:TYR:H	1.56	0.54
1:B:227:ARG:HD2	1:B:346:ASP:OD1	2.07	0.53
1:B:203:SER:O	1:B:395:ASN:HB2	2.08	0.53
1:D:167:THR:HG23	1:D:414:THR:OG1	2.08	0.53
1:A:231:ASN:HD21	1:A:239:ALA:H	1.55	0.53
1:B:232:HIS:CE1	1:B:330:ASN:HD22	2.26	0.53
1:D:278:TYR:CE1	1:D:291:ALA:HB2	2.44	0.53
1:A:197:PHE:O	1:A:198:ASN:CB	2.55	0.53
1:A:381:ALA:CB	1:A:418:GLU:HB2	2.39	0.53
1:B:170:GLY:HA3	1:B:172:GLU:OE2	2.08	0.52
1:A:231:ASN:ND2	1:A:239:ALA:H	2.07	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:180:VAL:HG12	1:B:181:ASP:N	2.23	0.52
1:B:303:LYS:HD3	1:B:373:ASP:O	2.10	0.52
1:A:211:GLN:HG3	1:A:385:LEU:HD13	1.91	0.52
1:C:378:LYS:NZ	3:C:1421:EDO:C2	2.66	0.52
1:D:242:TRP:CZ2	1:D:404:MET:HB3	2.45	0.52
1:A:323:ASN:ND2	1:A:367:TRP:HE1	2.05	0.51
1:B:385:LEU:HD12	1:B:385:LEU:N	2.25	0.51
1:C:344:LEU:HD13	4:C:2031:HOH:O	2.11	0.51
1:C:317:ILE:HD13	1:C:368:GLU:HB2	1.93	0.51
1:A:384:PHE:C	1:A:385:LEU:HD22	2.31	0.51
1:B:199:VAL:CG1	1:B:200:GLY:N	2.74	0.50
1:A:381:ALA:HB2	1:A:418:GLU:HB2	1.93	0.50
1:A:180:VAL:HG22	1:A:197:PHE:CD2	2.46	0.50
1:D:169:GLN:HB3	1:D:411:SER:O	2.11	0.50
1:C:171:LYS:HD3	1:C:193:GLU:OE2	2.12	0.50
1:B:166:ILE:HG12	1:B:417:PRO:HD3	1.94	0.50
1:B:181:ASP:OD1	1:B:196:ARG:HB3	2.11	0.50
1:C:378:LYS:HZ3	3:C:1421:EDO:H21	1.76	0.50
1:C:333:ASN:O	1:C:336:ASP:HB3	2.12	0.50
1:A:378:LYS:HG2	4:A:2092:HOH:O	2.11	0.50
1:B:233:GLN:CG	1:B:234:SER:H	2.13	0.49
1:D:350:THR:O	1:D:358:MET:HA	2.13	0.49
1:B:206:LEU:HG	1:B:398:ILE:HG13	1.95	0.49
1:A:294:GLY:O	1:A:295:TYR:C	2.51	0.49
1:B:184:LYS:HG2	1:B:193:GLU:HB3	1.95	0.49
1:D:204:ASN:CG	1:D:395:ASN:HB3	2.32	0.49
1:A:385:LEU:HD22	1:A:385:LEU:N	2.27	0.49
1:B:286:LYS:O	1:B:287:THR:C	2.49	0.49
1:D:204:ASN:CB	1:D:395:ASN:HB3	2.43	0.48
1:A:257:ASN:O	1:A:265:GLY:HA2	2.13	0.48
1:C:241:GLY:HA2	1:C:276:THR:OG1	2.13	0.48
1:B:280:TYR:HD1	1:B:280:TYR:N	2.10	0.48
1:C:349:LEU:HD22	1:C:349:LEU:N	2.28	0.48
1:B:231:ASN:HB3	1:B:403:TRP:O	2.14	0.48
1:D:324:PHE:O	1:D:365:LYS:HE2	2.13	0.48
1:A:235:ASN:ND2	1:A:235:ASN:C	2.67	0.48
1:A:359:ARG:HA	1:A:367:TRP:O	2.13	0.48
1:A:356:GLY:O	1:A:370:SER:HA	2.13	0.48
3:A:1420:EDO:H11	4:A:2056:HOH:O	2.13	0.48
1:B:177:TYR:HB3	1:B:255:LEU:HD11	1.94	0.48
1:B:313:VAL:HG21	1:B:374:LEU:HD23	1.95	0.48
1:A:289:LYS:O	1:A:291:ALA:O	2.32	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:208:GLY:O	1:B:254:TYR:CE2	2.67	0.47
1:B:360:ALA:O	1:B:367:TRP:HE3	1.97	0.47
1:A:244:PHE:CZ	1:A:347:VAL:HG21	2.50	0.47
1:C:316:ASN:HD21	1:C:318:ASP:HB2	1.79	0.47
1:A:230:ASN:HD22	1:A:242:TRP:HE1	1.62	0.47
1:B:279:ILE:N	1:B:285:ASP:OD2	2.46	0.47
1:C:206:LEU:O	1:C:392:TRP:HB2	2.15	0.47
1:D:316:ASN:ND2	1:D:318:ASP:HB2	2.29	0.47
1:C:189:LEU:O	1:D:335:SER:HB2	2.15	0.47
1:A:203:SER:O	1:A:395:ASN:HA	2.14	0.47
1:D:175:GLU:HG2	1:D:213:LYS:HE3	1.95	0.47
1:C:171:LYS:HE3	1:C:171:LYS:HB2	1.79	0.47
1:C:181:ASP:CG	1:C:199:VAL:HG11	2.35	0.47
1:D:202:GLU:HB2	1:D:205:GLY:O	2.15	0.47
1:D:215:LYS:HD3	1:D:418:GLU:OE1	2.15	0.47
1:A:252:GLU:HA	1:A:252:GLU:OE1	2.15	0.46
1:A:318:ASP:O	1:A:320:SER:N	2.47	0.46
1:B:381:ALA:HB2	1:B:418:GLU:HB2	1.97	0.46
1:C:378:LYS:HZ3	3:C:1421:EDO:C2	2.27	0.46
1:A:250:ASN:OD1	1:A:250:ASN:C	2.54	0.46
1:B:352:VAL:O	1:B:352:VAL:HG13	2.16	0.46
1:A:168:ILE:HD11	1:A:415:PHE:HE1	1.81	0.46
1:C:169:GLN:CB	1:C:411:SER:O	2.63	0.46
1:D:218:PHE:O	1:D:351:TYR:OH	2.21	0.46
1:B:188:ASP:N	1:B:188:ASP:OD1	2.48	0.46
1:C:343:ARG:NH2	1:D:335:SER:OG	2.48	0.46
1:D:203:SER:O	1:D:395:ASN:CA	2.64	0.46
1:B:295:TYR:O	1:B:327:TYR:CD2	2.69	0.46
1:A:241:GLY:HA3	1:A:261:LEU:CD2	2.45	0.45
1:C:207:ILE:HG13	1:C:389:SER:HB3	1.97	0.45
1:C:261:LEU:HA	1:C:261:LEU:HD23	1.84	0.45
1:C:288:GLU:HG3	1:C:298:TYR:CD2	2.52	0.45
1:C:347:VAL:HG12	1:C:349:LEU:HD21	1.98	0.45
1:C:390:GLN:O	1:C:391:ARG:C	2.55	0.45
1:A:166:ILE:O	1:A:414:THR:HA	2.17	0.45
1:A:163:SER:HB3	4:A:2001:HOH:O	2.17	0.45
1:A:180:VAL:HG21	1:A:197:PHE:CD2	2.52	0.45
1:C:197:PHE:HB2	1:C:404:MET:HB2	1.98	0.45
1:A:250:ASN:OD1	1:A:253:GLU:HG3	2.16	0.44
1:B:199:VAL:CG1	1:B:200:GLY:H	2.28	0.44
1:B:312:MET:HE1	1:B:323:ASN:HD21	1.82	0.44
1:C:316:ASN:HD22	1:C:321:LYS:CA	2.30	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:246:PHE:O	1:C:269:SER:HB3	2.17	0.44
1:B:183:GLN:HB2	1:B:196:ARG:CZ	2.48	0.44
1:C:339:PHE:CD1	1:C:339:PHE:C	2.90	0.44
1:A:327:TYR:O	1:A:341:GLY:HA3	2.18	0.44
1:D:299:GLY:O	1:D:300:ALA:HB2	2.18	0.44
1:B:232:HIS:HE1	1:B:330:ASN:ND2	2.11	0.43
1:A:172:GLU:CD	1:A:172:GLU:H	2.22	0.43
1:D:219:SER:O	1:D:220:LYS:HD3	2.18	0.43
1:B:254:TYR:O	1:B:258:GLY:N	2.49	0.43
1:C:168:ILE:HD12	1:C:173:HIS:CG	2.53	0.43
1:C:182:ILE:HD13	1:C:195:THR:HA	2.00	0.43
1:C:347:VAL:HG12	1:C:349:LEU:CD2	2.49	0.43
1:D:189:LEU:HD11	1:D:405:ARG:CZ	2.48	0.43
1:D:220:LYS:HD3	1:D:220:LYS:HA	1.74	0.43
1:A:289:LYS:C	1:A:291:ALA:N	2.72	0.43
1:B:206:LEU:HG	1:B:398:ILE:CG1	2.49	0.43
1:A:180:VAL:HG13	1:A:196:ARG:O	2.17	0.43
1:A:207:ILE:HD11	1:A:254:TYR:CE2	2.54	0.43
1:D:216:ILE:O	1:D:381:ALA:HA	2.19	0.43
1:C:316:ASN:HD22	1:C:321:LYS:C	2.22	0.43
1:A:294:GLY:O	1:A:296:ARG:N	2.52	0.43
1:D:204:ASN:HA	1:D:395:ASN:CB	2.49	0.42
1:D:399:ASN:O	1:D:400:ALA:HB2	2.18	0.42
1:B:232:HIS:CE1	1:B:330:ASN:ND2	2.87	0.42
1:A:164:THR:HG22	1:A:165:PRO:O	2.18	0.42
1:C:210:LEU:HD13	1:C:408:LEU:HD11	2.01	0.42
1:A:355:THR:OG1	1:A:357:LYS:HG2	2.20	0.42
1:C:408:LEU:HD23	1:C:408:LEU:HA	1.80	0.42
1:B:233:GLN:CG	1:B:234:SER:N	2.65	0.42
1:C:313:VAL:HG21	1:C:374:LEU:HD23	2.01	0.42
1:D:186:PRO:HG3	1:D:194:VAL:HG22	2.00	0.42
1:D:225:LYS:HG3	1:D:348:ILE:HD13	2.02	0.42
1:A:298:TYR:HA	1:A:323:ASN:O	2.19	0.42
1:A:330:ASN:O	1:A:331:SER:C	2.57	0.42
3:C:1420:EDO:H22	4:C:2009:HOH:O	2.19	0.42
1:D:203:SER:HA	1:D:397:GLY:HA2	2.02	0.42
1:B:250:ASN:OD1	1:B:253:GLU:HG3	2.19	0.41
1:B:280:TYR:CD2	1:B:281:THR:HG23	2.55	0.41
1:A:175:GLU:O	1:A:210:LEU:HA	2.20	0.41
1:A:273:LYS:HE3	1:A:298:TYR:CE2	2.55	0.41
1:D:225:LYS:HB3	1:D:225:LYS:HE2	1.86	0.41
1:D:203:SER:O	1:D:396:GLN:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:242:TRP:O	1:D:261:LEU:HD21	2.20	0.41
1:A:228:VAL:HB	1:A:242:TRP:CZ2	2.55	0.41
1:B:273:LYS:CE	1:B:298:TYR:HE1	2.33	0.41
1:B:216:ILE:CD1	1:B:384:PHE:HB2	2.51	0.41
1:B:233:GLN:NE2	1:B:400:ALA:HB1	2.36	0.41
1:C:223:ASN:HA	1:C:349:LEU:O	2.21	0.41
1:C:224:PHE:O	1:C:348:ILE:HA	2.21	0.41
1:D:225:LYS:HG3	1:D:348:ILE:CD1	2.50	0.41
1:A:168:ILE:HD11	1:A:415:PHE:CE1	2.56	0.41
1:A:319:LYS:H	1:A:319:LYS:HG2	1.62	0.41
1:B:379:ASN:C	1:B:379:ASN:OD1	2.59	0.41
1:A:212:LEU:HD21	1:A:415:PHE:CZ	2.55	0.40
1:B:207:ILE:HG13	1:B:208:GLY:N	2.35	0.40
1:B:359:ARG:HD3	1:B:366:THR:HG23	2.01	0.40
1:C:245:LEU:HD12	1:C:246:PHE:N	2.36	0.40
1:A:356:GLY:HA2	4:A:2084:HOH:O	2.21	0.40
1:B:202:GLU:HB2	1:B:206:LEU:HD23	2.03	0.40
1:D:235:ASN:ND2	1:D:290:GLN:O	2.53	0.40
1:A:197:PHE:CZ	1:A:210:LEU:HG	2.55	0.40
1:A:168:ILE:CD1	1:A:415:PHE:HE1	2.34	0.40
1:C:283:SER:HA	1:C:286:LYS:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:2047[B]:HOH:O	4:D:2034:HOH:O[4_554]	2.12	0.08

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	255/259 (98%)	228 (89%)	22 (9%)	5 (2%)	11	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	251/259 (97%)	233 (93%)	17 (7%)	1 (0%)	43	19
1	C	254/259 (98%)	231 (91%)	21 (8%)	2 (1%)	27	6
1	D	250/259 (96%)	226 (90%)	24 (10%)	0	100	100
All	All	1010/1036 (98%)	918 (91%)	84 (8%)	8 (1%)	27	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	TYR
1	A	198	ASN
1	A	319	LYS
1	B	198	ASN
1	A	290	GLN
1	A	266	LEU
1	C	172	GLU
1	C	395	ASN

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	211/213 (99%)	207 (98%)	4 (2%)	69	43
1	B	209/213 (98%)	200 (96%)	9 (4%)	40	11
1	C	210/213 (99%)	200 (95%)	10 (5%)	35	9
1	D	208/213 (98%)	196 (94%)	12 (6%)	28	5
All	All	838/852 (98%)	803 (96%)	35 (4%)	40	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	A	223	ASN
1	A	235	ASN
1	A	385	LEU

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Mol	Chain	Res	Type
1	B	172	GLU
1	B	202	GLU
1	B	214	ASN
1	B	256	THR
1	B	280	TYR
1	B	339	PHE
1	B	349	LEU
1	B	377	SER
1	B	418	GLU
1	C	181	ASP
1	C	193	GLU
1	C	203	SER
1	C	222	PHE
1	C	254	TYR
1	C	282	SER
1	C	298	TYR
1	C	319	LYS
1	C	338	LYS
1	C	339	PHE
1	D	179	SER
1	D	193	GLU
1	D	194	VAL
1	D	215	LYS
1	D	231	ASN
1	D	237	THR
1	D	281	THR
1	D	287	THR
1	D	289	LYS
1	D	311	GLN
1	D	394	LEU
1	D	401	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	230	ASN
1	A	231	ASN
1	A	235	ASN
1	A	309	ASN
1	A	316	ASN
1	A	323	ASN

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Mol	Chain	Res	Type
1	A	383	ASN
1	A	396	GLN
1	B	173	HIS
1	B	183	GLN
1	B	230	ASN
1	B	231	ASN
1	B	232	HIS
1	B	233	GLN
1	B	257	ASN
1	B	316	ASN
1	B	323	ASN
1	B	330	ASN
1	B	383	ASN
1	C	198	ASN
1	C	231	ASN
1	C	311	GLN
1	C	316	ASN
1	C	323	ASN
1	C	333	ASN
1	C	383	ASN
1	D	169	GLN
1	D	198	ASN
1	D	230	ASN
1	D	309	ASN
1	D	311	GLN
1	D	316	ASN
1	D	326	ASN
1	D	330	ASN
1	D	333	ASN
1	D	383	ASN
1	D	396	GLN

5.3.3   RNA ⓘ

There are no RNA chains 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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	EDO	A	1420	-	3,3,3	0.76	0	2,2,2	0.50	0
3	EDO	C	1420	-	3,3,3	0.44	0	2,2,2	0.78	0
3	EDO	C	1421	-	3,3,3	0.50	0	2,2,2	0.40	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	EDO	A	1420	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1420	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1421	-	-	0/1/1/1	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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	257/259 (99%)	-0.04	2 (0%)	83	87	6, 15, 28, 40	0
1	B	255/259 (98%)	0.03	1 (0%)	90	94	7, 16, 29, 34	0
1	C	256/259 (98%)	-0.11	1 (0%)	90	94	7, 15, 28, 37	0
1	D	254/259 (98%)	0.03	3 (1%)	75	79	6, 17, 29, 40	0
All	All	1022/1036 (98%)	-0.02	7 (0%)	84	88	6, 16, 29, 40	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	293	GLN	3.9
1	A	280	TYR	3.5
1	D	238	GLY	2.9
1	C	280	TYR	2.9
1	A	289	LYS	2.7
1	B	280	TYR	2.4
1	D	394	LEU	2.1

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 ⓘ

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, 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.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	EDO	A	1420	4/4	0.16	2.04	20,24,24,27	0
3	EDO	C	1421	4/4	0.08	-0.85	16,16,17,18	0
2	CA	B	500	1/1	0.07	-1.36	18,18,18,18	0
2	CA	C	500	1/1	0.06	-2.03	16,16,16,16	0
3	EDO	C	1420	4/4	0.06	-2.09	10,13,13,14	0
2	CA	D	500	1/1	0.06	-2.64	19,19,19,19	0
2	CA	A	500	1/1	0.04	-2.88	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.