Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 10:23 AM EST

PDB ID	:	2PVA
Title	:	OXIDIZED PENICILLIN V ACYLASE FROM B. SPHAERICUS
Authors	:	Suresh, C.G.; Pundle, A.V.; Rao, K.N.; SivaRaman, H.; Brannigan, J.A.; McVey, C.E.; Verma, C.S.; Dauter, Z.; Dodson, E.J.; Dodson, G.G.
Deposited on	:	1998-11-13
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 (i) 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 (i)) were used in the production of this report:

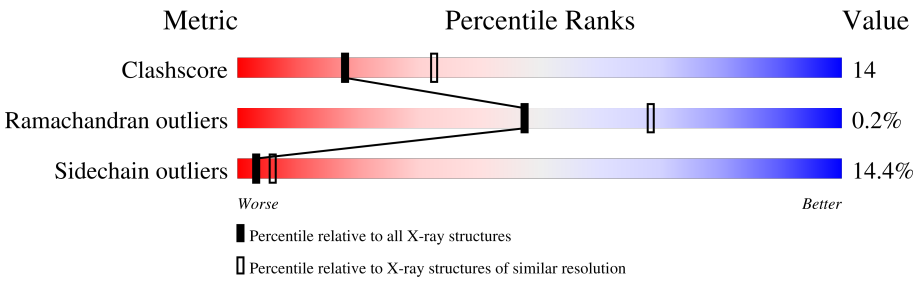
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	61% 28% 6% • •
1	B	345	65% 23% 7% • •
1	C	345	68% 21% 6% • •
1	D	345	59% 30% 6% • •

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
2	DTD	A	1001	X	-	-	-
2	DTD	B	1002	X	-	-	-
2	DTD	C	1003	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11209 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 PENICILLIN V ACYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2593	1648	423	509	13	0	0	0
1	B	332	2593	1648	423	509	13	0	0	0
1	C	332	2593	1648	423	509	13	0	0	0
1	D	332	2593	1648	423	509	13	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	OCS	CYS	modified residue	UNP P12256
A	74A	THR	-	insertion	UNP P12256
A	74B	TYR	-	insertion	UNP P12256
A	74C	ALA	-	insertion	UNP P12256
A	74D	ASP	-	insertion	UNP P12256
A	74E	GLU	-	insertion	UNP P12256
A	74F	PRO	-	insertion	UNP P12256
A	74G	LYS	-	insertion	UNP P12256
A	74H	LYS	-	insertion	UNP P12256
A	74I	GLY	-	insertion	UNP P12256
A	74J	THR	-	insertion	UNP P12256
B	1	OCS	CYS	modified residue	UNP P12256
B	74A	THR	-	insertion	UNP P12256
B	74B	TYR	-	insertion	UNP P12256
B	74C	ALA	-	insertion	UNP P12256
B	74D	ASP	-	insertion	UNP P12256
B	74E	GLU	-	insertion	UNP P12256
B	74F	PRO	-	insertion	UNP P12256
B	74G	LYS	-	insertion	UNP P12256
B	74H	LYS	-	insertion	UNP P12256
B	74I	GLY	-	insertion	UNP P12256

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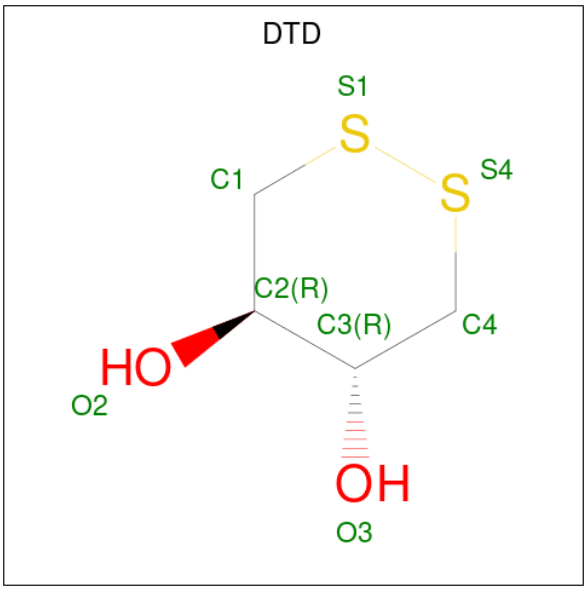
Chain	Residue	Modelled	Actual	Comment	Reference
B	74J	THR	-	insertion	UNP P12256
C	1	OCS	CYS	modified residue	UNP P12256
C	74A	THR	-	insertion	UNP P12256
C	74B	TYR	-	insertion	UNP P12256
C	74C	ALA	-	insertion	UNP P12256
C	74D	ASP	-	insertion	UNP P12256
C	74E	GLU	-	insertion	UNP P12256
C	74F	PRO	-	insertion	UNP P12256
C	74G	LYS	-	insertion	UNP P12256
C	74H	LYS	-	insertion	UNP P12256
C	74I	GLY	-	insertion	UNP P12256
C	74J	THR	-	insertion	UNP P12256
D	1	OCS	CYS	modified residue	UNP P12256
D	74A	THR	-	insertion	UNP P12256
D	74B	TYR	-	insertion	UNP P12256
D	74C	ALA	-	insertion	UNP P12256
D	74D	ASP	-	insertion	UNP P12256
D	74E	GLU	-	insertion	UNP P12256
D	74F	PRO	-	insertion	UNP P12256
D	74G	LYS	-	insertion	UNP P12256
D	74H	LYS	-	insertion	UNP P12256
D	74I	GLY	-	insertion	UNP P12256
D	74J	THR	-	insertion	UNP P12256

- Molecule 2 is DITHIANE DIOL (three-letter code: DTD) (formula: $C_4H_8O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	8	4	2	2	0	0
2	B	1	8	4	2	2	0	0
2	C	1	8	4	2	2	0	0
2	D	1	8	4	2	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	203	203	203	0	0
3	B	212	212	212	0	0
3	C	217	217	217	0	0
3	D	173	173	173	0	0

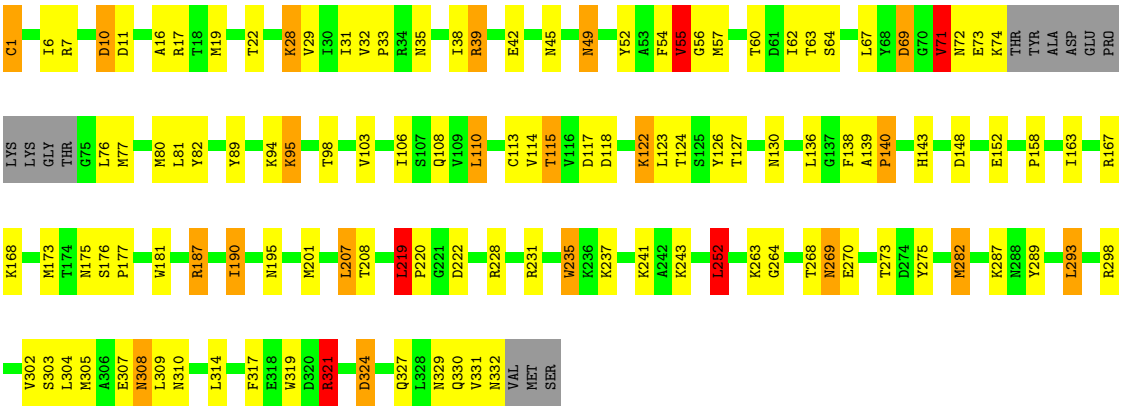
3 Residue-property plots (i)

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. 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: PENICILLIN V ACYLASE

Chain A:

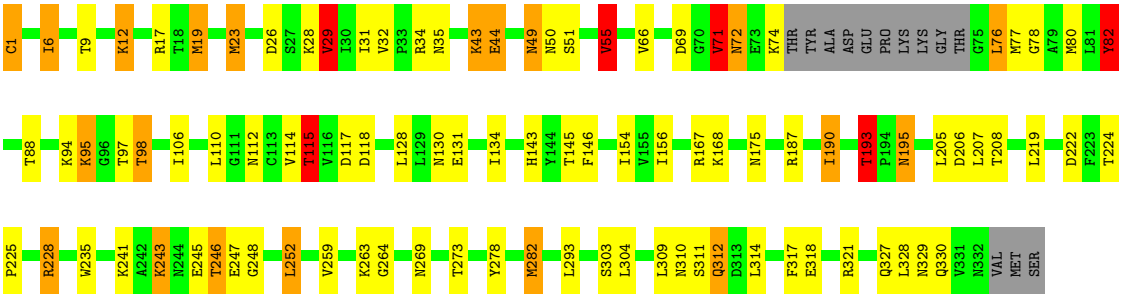


• Molecule 1: PENICILLIN V ACYLASE

Chain B:

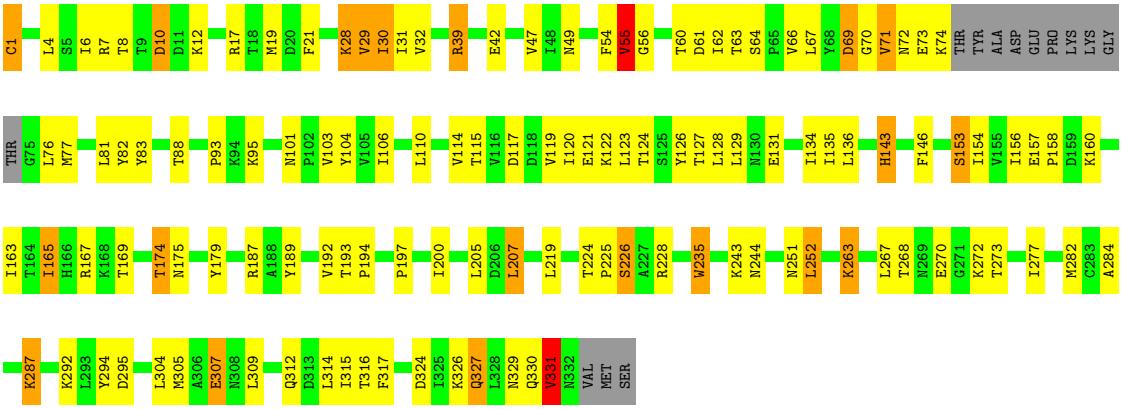
• Molecule 1: PENICILLIN V ACYLASE

Chain C:



- Molecule 1: PENICILLIN V ACYLASE

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	208.40Å 208.40Å 96.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.0 (20.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11209	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	0/2639	1.23	16/3589 (0.4%)
1	B	0.46	0/2639	1.23	13/3589 (0.4%)
1	C	0.49	0/2639	1.28	13/3589 (0.4%)
1	D	0.40	0/2639	1.09	14/3589 (0.4%)
All	All	0.46	0/10556	1.21	56/14356 (0.4%)

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	2
1	B	0	1
1	C	0	2
1	D	0	2
All	All	0	7

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	228	ARG	CD-NE-CZ	10.66	138.53	123.60
1	D	7	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	D	7	ARG	CD-NE-CZ	9.95	137.53	123.60
1	C	55	VAL	CB-CA-C	-8.60	95.06	111.40
1	C	34	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	B	321	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	199	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	321	ARG	CD-NE-CZ	7.72	134.40	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	VAL	CB-CA-C	-7.18	97.75	111.40
1	D	39	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	39	ARG	CD-NE-CZ	7.01	133.41	123.60
1	A	69	ASP	CB-CG-OD2	6.97	124.58	118.30
1	A	219	LEU	CA-CB-CG	6.86	131.08	115.30
1	D	189	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C	9	THR	C-N-CA	6.78	138.64	121.70
1	A	71	VAL	CB-CA-C	-6.72	98.62	111.40
1	A	187	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	A	321	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	148	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	282	MET	CA-CB-CG	6.48	124.32	113.30
1	C	71	VAL	CB-CA-C	-6.09	99.83	111.40
1	C	115	THR	N-CA-CB	-6.07	98.76	110.30
1	C	187	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	82	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	B	71	VAL	CB-CA-C	-6.01	99.97	111.40
1	B	61	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	324	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	328	LEU	C-N-CA	5.82	136.25	121.70
1	A	287	LYS	CA-CB-CG	5.79	126.13	113.40
1	D	228	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	321	ARG	CA-CB-CG	5.71	125.97	113.40
1	D	55	VAL	CB-CA-C	-5.65	100.66	111.40
1	D	69	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	222	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	62	ILE	N-CA-CB	5.63	123.75	110.80
1	C	193	THR	N-CA-CB	-5.60	99.66	110.30
1	A	324	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	287	LYS	CA-CB-CG	5.43	125.35	113.40
1	B	77	MET	CA-CB-CG	5.42	122.52	113.30
1	A	228	ARG	CD-NE-CZ	5.35	131.09	123.60
1	B	20	ASP	CB-CG-OD1	5.33	123.09	118.30
1	D	7	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	86	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	B	206	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	C	282	MET	CB-CA-C	-5.25	99.90	110.40
1	A	252	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	293	LEU	CA-CB-CG	5.21	127.27	115.30
1	D	189	TYR	CB-CG-CD1	5.19	124.12	121.00
1	B	115	THR	N-CA-CB	-5.19	100.44	110.30
1	B	208	THR	N-CA-CB	-5.18	100.46	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	26	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	10	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	10	ASP	CB-CA-C	-5.08	100.24	110.40
1	C	23	MET	CA-CB-CG	5.07	121.92	113.30
1	D	143	HIS	N-CA-CB	5.04	119.68	110.60
1	A	148	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	PRO	Mainchain
1	A	55	VAL	Mainchain
1	B	72	ASN	Mainchain
1	C	29	VAL	Mainchain
1	C	329	ASN	Mainchain
1	D	192	VAL	Mainchain
1	D	205	LEU	Mainchain

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	2593	0	2563	90	0
1	B	2593	0	2563	66	0
1	C	2593	0	2563	58	0
1	D	2593	0	2563	80	0
2	A	8	0	8	0	0
2	B	8	0	8	1	0
2	C	8	0	8	0	0
2	D	8	0	8	0	0
3	A	203	0	0	16	0
3	B	212	0	0	14	0
3	C	217	0	0	15	0
3	D	173	0	0	9	0
All	All	11209	0	10284	282	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 14.

All (282) 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:138:PHE:HB2	3:A:1177:HOH:O	1.46	1.12
1:C:312:GLN:HG3	3:C:1140:HOH:O	1.52	1.07
1:B:115:THR:HG22	1:B:118:ASP:H	1.26	0.96
1:B:116:VAL:HG21	1:B:152:GLU:HG2	1.50	0.94
1:B:241:LYS:HD2	3:B:1119:HOH:O	1.67	0.94
1:A:71:VAL:HG13	1:A:77:MET:HG2	1.49	0.94
1:A:71:VAL:HG22	1:A:282:MET:HG2	1.48	0.93
1:D:295:ASP:HB2	3:D:1005:HOH:O	1.70	0.91
1:B:292:LYS:HE3	3:C:1026:HOH:O	1.70	0.90
1:C:115:THR:HG22	1:C:118:ASP:H	1.40	0.86
1:C:98:THR:HG22	3:C:1194:HOH:O	1.77	0.84
1:C:71:VAL:HG13	1:C:77:MET:HG2	1.60	0.83
1:A:115:THR:HG22	1:A:118:ASP:H	1.44	0.83
1:B:95:LYS:HE2	1:B:95:LYS:H	1.43	0.82
1:C:72:ASN:HD21	1:C:76:LEU:H	1.27	0.82
1:A:98:THR:HG22	3:A:1131:HOH:O	1.78	0.82
1:B:196:PRO:HG2	1:C:269:ASN:HB3	1.62	0.82
1:D:39:ARG:HH11	1:D:63:THR:HG21	1.42	0.81
1:C:31:ILE:HG12	1:C:55:VAL:HG13	1.62	0.79
1:C:71:VAL:HG22	1:C:282:MET:HG2	1.64	0.79
3:A:1116:HOH:O	1:D:326:LYS:HE3	1.82	0.79
2:B:1002:DTD:S1	3:B:1183:HOH:O	2.40	0.79
1:D:55:VAL:HG22	1:D:304:LEU:HD13	1.65	0.78
1:A:263:LYS:HE2	3:A:1142:HOH:O	1.84	0.78
1:D:327:GLN:HB3	3:D:1176:HOH:O	1.85	0.77
1:C:72:ASN:ND2	1:C:76:LEU:H	1.82	0.77
1:D:31:ILE:HG12	1:D:55:VAL:HG13	1.68	0.75
1:D:29:VAL:HG13	1:D:317:PHE:HB2	1.69	0.74
1:A:330:GLN:HA	3:A:1109:HOH:O	1.88	0.73
1:C:190:ILE:HD11	1:D:207:LEU:O	1.89	0.72
1:D:307:GLU:HG3	1:D:315:ILE:HD13	1.71	0.72
1:D:62:ILE:CG1	3:D:1077:HOH:O	2.37	0.72
1:B:12:LYS:HE2	3:B:1123:HOH:O	1.90	0.71
1:A:55:VAL:HG22	1:A:304:LEU:HD13	1.74	0.70
1:A:324:ASP:CB	3:A:1140:HOH:O	2.39	0.70
1:C:55:VAL:HG22	1:C:304:LEU:HB2	1.72	0.69
1:A:94:LYS:HE2	1:A:95:LYS:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LYS:HG2	1:C:95:LYS:HD2	1.75	0.69
1:A:324:ASP:HB2	3:A:1140:HOH:O	1.91	0.68
1:A:308:ASN:ND2	1:A:310:ASN:H	1.92	0.67
1:A:122:LYS:HD3	1:A:126:TYR:HE2	1.60	0.66
1:B:72:ASN:HB3	1:B:74:LYS:H	1.60	0.66
1:B:205:LEU:HD13	1:B:207:LEU:HD11	1.77	0.66
1:A:39:ARG:HH11	1:A:63:THR:HG21	1.60	0.66
1:C:6:ILE:HD13	3:C:1166:HOH:O	1.95	0.66
1:D:71:VAL:HG22	1:D:282:MET:HG2	1.79	0.65
1:A:31:ILE:HG13	1:A:55:VAL:HG13	1.78	0.65
1:A:303:SER:HB2	1:D:331:VAL:HG21	1.79	0.64
1:D:62:ILE:HG12	3:D:1077:HOH:O	1.98	0.64
1:A:308:ASN:HD21	1:A:310:ASN:HB2	1.63	0.64
1:D:235:TRP:HA	1:D:235:TRP:CE3	2.33	0.63
1:D:235:TRP:HA	1:D:235:TRP:HE3	1.63	0.63
1:A:219:LEU:HD22	1:A:220:PRO:HD2	1.81	0.62
1:B:312:GLN:HG3	3:B:1176:HOH:O	1.99	0.62
1:B:330:GLN:HG2	3:B:1129:HOH:O	1.98	0.62
1:C:55:VAL:CG2	1:C:304:LEU:HB2	2.30	0.62
1:A:35:ASN:HA	1:A:49:ASN:HD22	1.66	0.61
1:C:6:ILE:CD1	3:C:1166:HOH:O	2.47	0.61
1:A:115:THR:HG22	1:A:118:ASP:N	2.15	0.61
1:C:318:GLU:HG3	3:C:1103:HOH:O	1.99	0.61
1:A:29:VAL:HG21	1:A:302:VAL:HG21	1.82	0.61
1:D:30:ILE:HG23	1:D:316:THR:HG22	1.83	0.60
1:C:190:ILE:HG12	1:D:200:ILE:HG12	1.83	0.60
1:C:193:THR:HG23	1:C:195:ASN:H	1.66	0.60
1:D:62:ILE:HG13	3:D:1077:HOH:O	1.97	0.60
1:C:50:ASN:HA	1:C:112:ASN:HD21	1.66	0.60
1:C:12:LYS:HE2	3:C:1219:HOH:O	2.02	0.59
1:C:115:THR:HG23	1:C:117:ASP:H	1.67	0.59
1:C:43:LYS:HD2	1:C:131:GLU:OE2	2.03	0.59
1:A:195:ASN:HD21	1:D:267:LEU:HD12	1.67	0.59
1:B:329:ASN:O	1:B:330:GLN:HB2	2.03	0.59
1:D:93:PRO:HA	1:D:127:THR:HG21	1.84	0.58
1:A:42:GLU:OE1	1:A:62:ILE:HB	2.03	0.58
1:B:94:LYS:HG2	1:B:95:LYS:HE2	1.86	0.58
1:C:310:ASN:HA	3:C:1186:HOH:O	2.02	0.58
1:D:71:VAL:HG13	1:D:77:MET:HB3	1.86	0.57
1:D:329:ASN:O	1:D:330:GLN:HB2	2.04	0.57
1:B:95:LYS:H	1:B:95:LYS:CE	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:THR:HG21	1:D:160:LYS:HG3	1.87	0.57
1:D:174:THR:CG2	1:D:175:ASN:H	2.17	0.57
1:A:115:THR:HG23	1:A:117:ASP:H	1.70	0.56
1:A:264:GLY:H	1:A:273:THR:HG23	1.71	0.56
1:A:158:PRO:HA	1:A:163:ILE:HD13	1.86	0.56
1:B:40:LEU:HB2	3:B:1127:HOH:O	2.05	0.56
1:A:39:ARG:HG2	1:A:64:SER:OG	2.06	0.56
1:C:264:GLY:H	1:C:273:THR:CG2	2.19	0.56
1:C:94:LYS:HD3	1:C:97:THR:HG23	1.87	0.56
1:D:174:THR:HG21	1:D:225:PRO:O	2.06	0.56
1:D:268:THR:OG1	1:D:270:GLU:HG2	2.07	0.55
1:B:9:THR:HB	1:B:243:LYS:HA	1.88	0.55
1:A:113:CYS:SG	1:A:122:LYS:HG3	2.47	0.55
1:A:305:MET:HG2	3:A:1080:HOH:O	2.05	0.55
1:C:35:ASN:HA	1:C:49:ASN:ND2	2.22	0.55
1:D:64:SER:HB2	1:D:104:TYR:CE1	2.42	0.54
1:D:72:ASN:O	1:D:287:LYS:HD2	2.08	0.54
1:D:39:ARG:NH1	1:D:63:THR:HG21	2.19	0.54
1:A:324:ASP:CG	3:A:1140:HOH:O	2.47	0.54
1:A:321:ARG:HH11	1:A:321:ARG:HB3	1.73	0.54
1:A:329:ASN:OD1	1:A:331:VAL:HG12	2.07	0.54
1:D:154:ILE:HG22	1:D:167:ARG:HA	1.90	0.53
1:A:31:ILE:CG1	1:A:55:VAL:HG13	2.39	0.53
1:C:95:LYS:NZ	1:C:95:LYS:H	2.06	0.53
1:A:187:ARG:HB3	1:B:208:THR:O	2.08	0.53
1:A:263:LYS:HE3	1:A:275:TYR:CE2	2.43	0.53
1:B:28:LYS:HG2	1:B:30:ILE:HD13	1.89	0.53
1:B:72:ASN:HB2	1:B:76:LEU:H	1.74	0.53
1:A:264:GLY:H	1:A:273:THR:CG2	2.22	0.53
1:D:28:LYS:HB2	1:D:317:PHE:O	2.10	0.52
1:C:44:GLU:HG2	3:C:1173:HOH:O	2.08	0.52
1:D:165:ILE:O	1:D:165:ILE:HG13	2.09	0.52
1:B:74:LYS:HG3	1:B:114:VAL:HG22	1.92	0.52
1:D:62:ILE:HG22	1:D:134:ILE:HG22	1.91	0.52
1:D:292:LYS:NZ	3:D:1079:HOH:O	2.42	0.52
1:C:246:THR:HG23	3:C:1185:HOH:O	2.10	0.51
1:C:310:ASN:CA	3:C:1186:HOH:O	2.59	0.51
1:A:39:ARG:HH21	1:A:45:ASN:HA	1.76	0.51
1:A:303:SER:HB2	1:D:331:VAL:CG2	2.40	0.51
1:B:263:LYS:HE2	1:B:294:TYR:CE2	2.45	0.51
1:D:21:PHE:HB3	1:D:277:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LYS:HB3	1:D:114:VAL:HG13	1.92	0.51
1:D:135:ILE:HG13	1:D:136:LEU:HG	1.93	0.51
1:C:12:LYS:HE3	1:C:245:GLU:HB2	1.93	0.51
1:B:40:LEU:HD11	1:B:48:ILE:HD11	1.93	0.50
1:B:45:ASN:ND2	3:B:1079:HOH:O	2.43	0.50
1:B:115:THR:HG22	1:B:118:ASP:N	2.11	0.50
1:D:4:LEU:HD21	1:D:252:LEU:HD12	1.92	0.50
1:A:35:ASN:HA	1:A:49:ASN:ND2	2.25	0.50
1:D:31:ILE:CG1	1:D:55:VAL:HG13	2.40	0.50
1:D:56:GLY:HA3	1:D:69:ASP:O	2.12	0.50
1:B:168:LYS:HA	3:B:1075:HOH:O	2.11	0.50
1:D:54:PHE:HE1	1:D:67:LEU:HD13	1.76	0.50
1:B:177:PRO:HD2	1:B:182:HIS:CE1	2.45	0.50
1:B:119:VAL:HG12	1:B:123:LEU:HD12	1.94	0.49
1:A:269:ASN:C	1:A:269:ASN:HD22	2.16	0.49
1:B:152:GLU:OE1	1:B:167:ARG:NE	2.45	0.49
1:D:174:THR:CG2	1:D:175:ASN:N	2.75	0.49
1:A:22:THR:HG21	1:A:268:THR:HG21	1.94	0.49
1:D:193:THR:HB	1:D:194:PRO:CD	2.43	0.49
1:C:145:THR:HG23	3:C:1189:HOH:O	2.12	0.49
1:A:52:TYR:HB3	1:A:73:GLU:HG2	1.94	0.49
1:B:331:VAL:HA	1:C:303:SER:HB2	1.95	0.49
1:A:80:MET:HE3	1:A:106:ILE:HG12	1.95	0.49
1:B:51:SER:H	1:B:112:ASN:ND2	2.10	0.49
1:C:19:MET:HG3	1:C:278:TYR:CE2	2.48	0.49
1:C:243:LYS:HB2	1:C:247:GLU:OE1	2.13	0.48
1:B:64:SER:HB3	1:B:65:PRO:HD2	1.94	0.48
1:D:193:THR:HB	1:D:194:PRO:HD2	1.95	0.48
1:B:115:THR:HG23	1:B:117:ASP:H	1.79	0.48
1:C:146:PHE:N	3:C:1189:HOH:O	2.46	0.48
1:B:269:ASN:ND2	1:B:269:ASN:H	2.12	0.48
1:B:127:THR:HG22	1:B:129:LEU:HD23	1.96	0.47
1:C:228:ARG:HG2	1:C:259:VAL:HG12	1.96	0.47
1:B:176:SER:HB3	1:B:177:PRO:HA	1.95	0.47
1:D:30:ILE:HD12	1:D:60:THR:HG23	1.97	0.47
1:D:158:PRO:HA	1:D:163:ILE:HD13	1.96	0.47
1:B:51:SER:H	1:B:112:ASN:HD21	1.62	0.47
1:A:235:TRP:CE3	1:A:235:TRP:HA	2.50	0.47
1:B:36:TYR:CE2	1:B:314:LEU:HD13	2.49	0.47
1:A:139:ALA:N	3:A:1177:HOH:O	2.46	0.47
1:D:42:GLU:H	1:D:131:GLU:CD	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:THR:HG23	1:C:195:ASN:N	2.29	0.46
1:D:226:SER:HB2	3:D:1063:HOH:O	2.15	0.46
1:B:115:THR:O	1:B:119:VAL:HG23	2.15	0.46
1:B:166:HIS:HD2	3:B:1087:HOH:O	1.98	0.46
1:D:83:TYR:CZ	1:D:157:GLU:HG2	2.50	0.46
1:A:269:ASN:ND2	1:A:270:GLU:OE1	2.49	0.46
1:A:309:LEU:HB2	3:A:1135:HOH:O	2.14	0.46
1:B:98:THR:HG22	3:B:1153:HOH:O	2.15	0.46
1:C:72:ASN:ND2	1:C:76:LEU:N	2.59	0.46
1:D:307:GLU:CG	1:D:315:ILE:HD13	2.43	0.46
1:A:56:GLY:HA3	1:A:69:ASP:O	2.16	0.46
1:A:237:LYS:O	1:A:237:LYS:HG2	2.16	0.46
1:A:241:LYS:NZ	3:A:1100:HOH:O	2.47	0.46
1:C:35:ASN:OD1	1:C:49:ASN:ND2	2.48	0.46
1:D:10:ASP:OD2	1:D:244:ASN:HA	2.15	0.46
1:D:55:VAL:CG2	1:D:304:LEU:HB2	2.46	0.46
1:D:235:TRP:CE3	1:D:235:TRP:CA	2.98	0.46
1:A:106:ILE:HG22	1:A:110:LEU:HD22	1.98	0.46
1:D:122:LYS:HD2	1:D:126:TYR:HE2	1.81	0.46
1:C:69:ASP:HA	1:C:78:GLY:O	2.16	0.45
1:D:62:ILE:HD11	1:D:66:VAL:CG1	2.46	0.45
1:D:121:GLU:O	1:D:124:THR:HB	2.16	0.45
1:B:59:SER:OG	3:B:1093:HOH:O	2.20	0.45
1:C:115:THR:HG23	1:C:117:ASP:N	2.31	0.45
1:C:145:THR:C	3:C:1189:HOH:O	2.53	0.45
1:D:224:THR:HB	1:D:225:PRO:HD2	1.97	0.45
1:A:207:LEU:HB3	1:B:190:ILE:HG21	1.98	0.45
1:C:154:ILE:HD12	1:C:156:ILE:HD11	1.98	0.45
1:D:169:THR:HB	1:D:179:TYR:CZ	2.51	0.45
1:A:32:VAL:HA	1:A:33:PRO:HD3	1.84	0.45
1:B:71:VAL:HG22	1:B:282:MET:HB2	1.99	0.45
1:A:298:ARG:NH1	1:D:326:LYS:HD2	2.31	0.45
1:C:248:GLY:O	1:C:252:LEU:HD22	2.17	0.45
1:A:54:PHE:HE1	1:A:67:LEU:HD13	1.82	0.45
1:C:190:ILE:CG2	1:D:197:PRO:HG2	2.47	0.45
1:C:222:ASP:OD1	1:C:224:THR:HG23	2.17	0.45
1:A:38:ILE:HB	1:A:108:GLN:NE2	2.32	0.45
1:A:106:ILE:HB	3:A:1007:HOH:O	2.17	0.45
1:B:106:ILE:O	1:B:110:LEU:HB2	2.17	0.45
1:D:167:ARG:HE	1:D:167:ARG:HB3	1.63	0.45
1:B:131:GLU:O	1:B:139:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:VAL:HG23	1:A:332:ASN:O	2.16	0.44
1:B:6:ILE:HG12	1:B:252:LEU:HD13	1.99	0.44
1:B:12:LYS:HG2	1:B:283:CYS:SG	2.57	0.44
1:C:224:THR:HB	1:C:225:PRO:HD2	1.99	0.44
1:D:174:THR:HG23	1:D:175:ASN:H	1.82	0.44
1:C:74:LYS:HG3	1:C:114:VAL:HG22	1.99	0.44
1:A:10:ASP:O	1:A:11:ASP:HB2	2.17	0.44
1:A:54:PHE:HB3	1:A:72:ASN:HA	2.00	0.44
1:B:28:LYS:HG3	1:B:316:THR:HB	2.00	0.44
1:A:195:ASN:ND2	1:D:267:LEU:HD12	2.31	0.44
1:A:219:LEU:HD11	1:A:231:ARG:HG2	1.99	0.44
1:B:46:VAL:HB	3:B:1127:HOH:O	2.18	0.44
1:D:115:THR:O	1:D:119:VAL:HG23	2.18	0.44
1:A:1:OCS:HB3	1:A:81:LEU:HD23	1.99	0.44
1:A:39:ARG:HD3	1:A:63:THR:HG21	2.00	0.43
1:D:21:PHE:HB3	1:D:277:ILE:CD1	2.48	0.43
1:A:175:ASN:HB3	3:A:1186:HOH:O	2.17	0.43
1:B:143:HIS:HB2	1:B:157:GLU:HG2	1.99	0.43
1:B:248:GLY:O	1:B:252:LEU:HB2	2.18	0.43
1:C:80:MET:HE3	1:C:106:ILE:HG12	1.99	0.43
1:D:263:LYS:HD3	1:D:294:TYR:CZ	2.53	0.43
1:A:31:ILE:HD13	1:A:307:GLU:HG3	2.01	0.43
1:B:219:LEU:HD22	1:B:220:PRO:HD2	2.00	0.43
1:D:115:THR:HG22	1:D:117:ASP:H	1.83	0.43
1:A:327:GLN:HE21	1:A:331:VAL:N	2.16	0.43
1:A:60:THR:HA	3:A:1168:HOH:O	2.18	0.43
1:B:121:GLU:O	1:B:124:THR:HB	2.19	0.43
1:B:263:LYS:HD3	1:B:275:TYR:CG	2.54	0.43
1:D:106:ILE:O	1:D:110:LEU:HB2	2.19	0.43
1:D:101:ASN:HB2	1:D:131:GLU:OE1	2.19	0.43
1:A:308:ASN:HD22	1:A:310:ASN:H	1.64	0.43
1:C:29:VAL:HG13	1:C:317:PHE:HB2	2.00	0.43
1:D:120:ILE:CD1	1:D:167:ARG:HH11	2.32	0.43
1:A:39:ARG:NH2	1:A:45:ASN:HA	2.33	0.42
1:B:1:OCS:HB3	1:B:81:LEU:HD23	2.01	0.42
1:C:246:THR:CG2	3:C:1185:HOH:O	2.66	0.42
1:A:304:LEU:O	1:A:309:LEU:HD11	2.19	0.42
1:A:293:LEU:HD21	1:A:319:TRP:HB3	2.00	0.42
1:B:20:ASP:HA	1:B:275:TYR:O	2.20	0.42
1:C:95:LYS:HD2	1:C:95:LYS:N	2.34	0.42
1:D:8:THR:OG1	1:D:12:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:CD2	1:B:220:PRO:HD2	2.50	0.42
1:A:235:TRP:HA	1:A:235:TRP:HE3	1.83	0.42
1:C:115:THR:CG2	1:C:118:ASP:H	2.23	0.42
1:D:128:LEU:N	3:D:1170:HOH:O	2.51	0.42
1:A:177:PRO:HG2	1:A:181:TRP:CD2	2.55	0.42
1:C:1:OCS:OD1	1:C:82:TYR:HB2	2.19	0.42
1:C:264:GLY:H	1:C:273:THR:HG21	1.84	0.42
1:D:77:MET:HE1	1:D:284:ALA:HB2	2.02	0.42
1:B:80:MET:HE3	1:B:106:ILE:HG12	2.01	0.42
1:B:12:LYS:HE3	1:B:245:GLU:HB2	2.02	0.41
1:C:208:THR:O	1:D:187:ARG:HB3	2.20	0.41
1:D:1:OCS:HB3	1:D:81:LEU:HD23	2.01	0.41
1:D:146:PHE:O	1:D:153:SER:HA	2.19	0.41
1:B:39:ARG:O	1:B:108:GLN:NE2	2.53	0.41
1:A:16:ALA:CB	1:A:252:LEU:HG	2.50	0.41
1:A:55:VAL:CG2	1:A:304:LEU:HB2	2.51	0.41
1:A:57:MET:HB2	1:A:289:TYR:OH	2.21	0.41
1:D:154:ILE:HD13	1:D:156:ILE:HD11	2.02	0.41
1:A:74:LYS:HB3	1:A:114:VAL:HG13	2.01	0.41
1:B:172:VAL:N	3:B:1080:HOH:O	2.34	0.41
1:B:329:ASN:O	1:B:330:GLN:CB	2.66	0.41
1:A:22:THR:HA	1:A:273:THR:O	2.21	0.41
1:A:55:VAL:HG22	1:A:304:LEU:HB2	2.03	0.41
1:B:32:VAL:HG13	1:B:54:PHE:CE1	2.56	0.41
1:B:246:THR:HG23	3:B:1144:HOH:O	2.19	0.41
1:A:136:LEU:HD12	1:A:140:PRO:HG3	2.02	0.41
1:A:176:SER:HB3	1:A:177:PRO:HA	2.02	0.41
1:B:263:LYS:HD3	1:B:275:TYR:CD2	2.56	0.41
1:A:89:TYR:HD2	1:A:130:ASN:HD22	1.69	0.41
1:D:70:GLY:O	1:D:77:MET:HA	2.21	0.41
1:A:152:GLU:OE1	1:A:167:ARG:NH2	2.50	0.40
1:A:177:PRO:HG2	1:A:181:TRP:CE3	2.56	0.40
1:A:127:THR:HA	3:A:1075:HOH:O	2.22	0.40
1:A:321:ARG:HH11	1:A:321:ARG:CG	2.35	0.40
1:A:28:LYS:HB2	1:A:317:PHE:O	2.20	0.40
1:A:81:LEU:HD13	1:A:173:MET:CE	2.51	0.40
1:C:175:ASN:HB2	1:C:225:PRO:HB3	2.03	0.40
1:D:251:ASN:ND2	3:D:1025:HOH:O	2.32	0.40
1:A:190:ILE:H	1:A:190:ILE:HG22	1.56	0.40
1:B:115:THR:CG2	1:B:117:ASP:HB2	2.52	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	330/345 (96%)	315 (96%)	15 (4%)	0	100	100
1	B	330/345 (96%)	316 (96%)	13 (4%)	1 (0%)	41	61
1	C	330/345 (96%)	317 (96%)	13 (4%)	0	100	100
1	D	330/345 (96%)	305 (92%)	24 (7%)	1 (0%)	41	61
All	All	1320/1380 (96%)	1253 (95%)	65 (5%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	330	GLN
1	D	331	VAL

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	288/299 (96%)	255 (88%)	33 (12%)	5	11
1	B	288/299 (96%)	244 (85%)	44 (15%)	2	5
1	C	288/299 (96%)	238 (83%)	50 (17%)	2	3
1	D	288/299 (96%)	249 (86%)	39 (14%)	4	7
All	All	1152/1196 (96%)	986 (86%)	166 (14%)	3	6

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	7	ARG
1	A	17	ARG
1	A	19	MET
1	A	28	LYS
1	A	39	ARG
1	A	49	ASN
1	A	55	VAL
1	A	71	VAL
1	A	76	LEU
1	A	82	TYR
1	A	95	LYS
1	A	103	VAL
1	A	110	LEU
1	A	115	THR
1	A	122	LYS
1	A	123	LEU
1	A	124	THR
1	A	143	HIS
1	A	168	LYS
1	A	190	ILE
1	A	201	MET
1	A	207	LEU
1	A	208	THR
1	A	219	LEU
1	A	235	TRP
1	A	243	LYS
1	A	252	LEU
1	A	269	ASN
1	A	293	LEU
1	A	308	ASN
1	A	314	LEU
1	A	321	ARG
1	B	9	THR
1	B	12	LYS
1	B	17	ARG
1	B	19	MET
1	B	28	LYS
1	B	29	VAL
1	B	32	VAL
1	B	44	GLU
1	B	47	VAL
1	B	66	VAL

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Mol	Chain	Res	Type
1	B	71	VAL
1	B	72	ASN
1	B	76	LEU
1	B	82	TYR
1	B	88	THR
1	B	91	ASP
1	B	95	LYS
1	B	98	THR
1	B	110	LEU
1	B	115	THR
1	B	130	ASN
1	B	134	ILE
1	B	135	ILE
1	B	143	HIS
1	B	163	ILE
1	B	190	ILE
1	B	201	MET
1	B	205	LEU
1	B	207	LEU
1	B	208	THR
1	B	219	LEU
1	B	241	LYS
1	B	243	LYS
1	B	252	LEU
1	B	263	LYS
1	B	269	ASN
1	B	287	LYS
1	B	292	LYS
1	B	293	LEU
1	B	309	LEU
1	B	314	LEU
1	B	318	GLU
1	B	322	LYS
1	B	331	VAL
1	C	6	ILE
1	C	12	LYS
1	C	17	ARG
1	C	19	MET
1	C	23	MET
1	C	28	LYS
1	C	29	VAL
1	C	32	VAL

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Mol	Chain	Res	Type
1	C	43	LYS
1	C	44	GLU
1	C	49	ASN
1	C	51	SER
1	C	55	VAL
1	C	66	VAL
1	C	71	VAL
1	C	72	ASN
1	C	76	LEU
1	C	82	TYR
1	C	88	THR
1	C	95	LYS
1	C	98	THR
1	C	110	LEU
1	C	115	THR
1	C	128	LEU
1	C	130	ASN
1	C	134	ILE
1	C	143	HIS
1	C	167	ARG
1	C	168	LYS
1	C	190	ILE
1	C	193	THR
1	C	195	ASN
1	C	205	LEU
1	C	206	ASP
1	C	207	LEU
1	C	219	LEU
1	C	235	TRP
1	C	241	LYS
1	C	243	LYS
1	C	246	THR
1	C	252	LEU
1	C	263	LYS
1	C	293	LEU
1	C	309	LEU
1	C	311	SER
1	C	312	GLN
1	C	314	LEU
1	C	321	ARG
1	C	327	GLN
1	C	330	GLN

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Mol	Chain	Res	Type
1	D	6	ILE
1	D	17	ARG
1	D	19	MET
1	D	28	LYS
1	D	29	VAL
1	D	30	ILE
1	D	32	VAL
1	D	47	VAL
1	D	49	ASN
1	D	55	VAL
1	D	61	ASP
1	D	71	VAL
1	D	73	GLU
1	D	76	LEU
1	D	82	TYR
1	D	95	LYS
1	D	103	VAL
1	D	123	LEU
1	D	129	LEU
1	D	143	HIS
1	D	153	SER
1	D	165	ILE
1	D	174	THR
1	D	207	LEU
1	D	219	LEU
1	D	226	SER
1	D	235	TRP
1	D	243	LYS
1	D	252	LEU
1	D	263	LYS
1	D	272	LYS
1	D	273	THR
1	D	305	MET
1	D	307	GLU
1	D	309	LEU
1	D	312	GLN
1	D	314	LEU
1	D	327	GLN
1	D	331	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	ASN
1	A	130	ASN
1	A	185	ASN
1	A	195	ASN
1	A	198	GLN
1	A	251	ASN
1	A	260	ASN
1	A	269	ASN
1	A	308	ASN
1	A	327	GLN
1	B	72	ASN
1	B	112	ASN
1	B	130	ASN
1	B	185	ASN
1	B	195	ASN
1	B	251	ASN
1	B	260	ASN
1	B	269	ASN
1	B	308	ASN
1	C	35	ASN
1	C	49	ASN
1	C	72	ASN
1	C	112	ASN
1	C	185	ASN
1	C	198	GLN
1	C	260	ASN
1	C	308	ASN
1	D	35	ASN
1	D	49	ASN
1	D	185	ASN
1	D	251	ASN
1	D	308	ASN
1	D	327	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	OCS	B	1	1	7,8,9	0.98	0	6,11,13	2.62	3 (50%)
1	OCS	D	1	1	7,8,9	1.34	0	6,11,13	2.70	3 (50%)
1	OCS	A	1	1	7,8,9	1.17	0	6,11,13	1.83	2 (33%)
1	OCS	C	1	1	7,8,9	1.31	1 (14%)	6,11,13	1.81	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
1	OCS	B	1	1	-	2/4/7/9	-
1	OCS	D	1	1	-	0/4/7/9	-
1	OCS	A	1	1	-	3/4/7/9	-
1	OCS	C	1	1	-	3/4/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	OCS	CB-CA	-2.49	1.51	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	OCS	OD1-SG-CB	5.86	113.91	106.94
1	B	1	OCS	OD1-SG-CB	4.87	112.73	106.94
1	A	1	OCS	OD3-SG-CB	3.25	110.81	106.94
1	C	1	OCS	OD2-SG-CB	2.86	110.30	105.74
1	C	1	OCS	OD1-SG-CB	2.82	110.29	106.94
1	B	1	OCS	OD2-SG-CB	2.71	110.06	105.74
1	A	1	OCS	OD2-SG-OD3	-2.54	105.06	111.27
1	D	1	OCS	OD3-SG-OD1	-2.28	106.06	113.95
1	B	1	OCS	OD2-SG-OD1	-2.07	106.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	OCS	OD3-SG-CB	2.01	109.33	106.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	OCS	CA-CB-SG-OD1
1	A	1	OCS	CA-CB-SG-OD2
1	A	1	OCS	CA-CB-SG-OD3
1	B	1	OCS	N-CA-CB-SG
1	C	1	OCS	CA-CB-SG-OD1
1	C	1	OCS	CA-CB-SG-OD2
1	C	1	OCS	CA-CB-SG-OD3
1	B	1	OCS	CA-CB-SG-OD3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	OCS	1	0
1	D	1	OCS	1	0
1	A	1	OCS	1	0
1	C	1	OCS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	DTD	A	1001	-	6,8,8	0.58	0	6,10,10	0.89	0
2	DTD	B	1002	-	6,8,8	0.49	0	6,10,10	1.28	1 (16%)
2	DTD	D	1004	-	6,8,8	0.55	0	6,10,10	1.15	1 (16%)
2	DTD	C	1003	-	6,8,8	0.67	0	6,10,10	1.17	1 (16%)

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
2	DTD	A	1001	-	1/1/2/2	-	0/0/1/1
2	DTD	B	1002	-	1/1/2/2	-	0/0/1/1
2	DTD	D	1004	-	-	-	0/0/1/1
2	DTD	C	1003	-	1/1/2/2	-	0/0/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1004	DTD	O3-C3-C2	-2.49	104.70	110.22
2	C	1003	DTD	O3-C3-C2	-2.31	105.10	110.22
2	B	1002	DTD	O2-C2-C1	-2.09	106.30	109.91

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	DTD	C2
2	B	1002	DTD	C2
2	C	1003	DTD	C2

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	DTD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.