



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 AM UTC

PDB ID : 2PVA / pdb_00002pva
Title : OXIDIZED PENICILLIN V ACYLASE FROM B. SPHAERICUS
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Deposited on : 1998-11-13
Resolution : 2.50 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

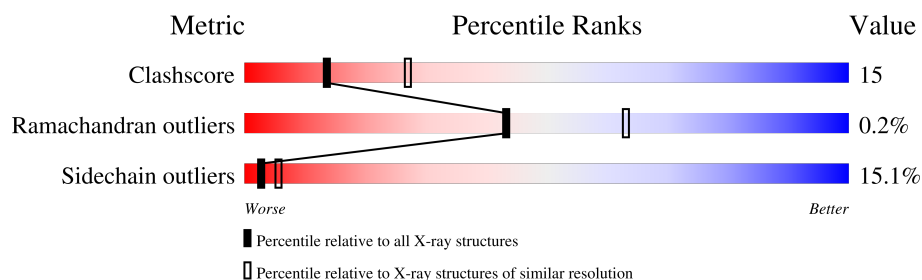
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	
1	C	345	
1	D	345	

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

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
1	A	332	Total	C	N	O	S	0	0	0
			2593	1648	423	509	13			
1	B	332	Total	C	N	O	S	0	0	0
			2593	1648	423	509	13			
1	C	332	Total	C	N	O	S	0	0	0
			2593	1648	423	509	13			
1	D	332	Total	C	N	O	S	0	0	0
			2593	1648	423	509	13			

There are 44 discrepancies between the modelled and reference sequences:

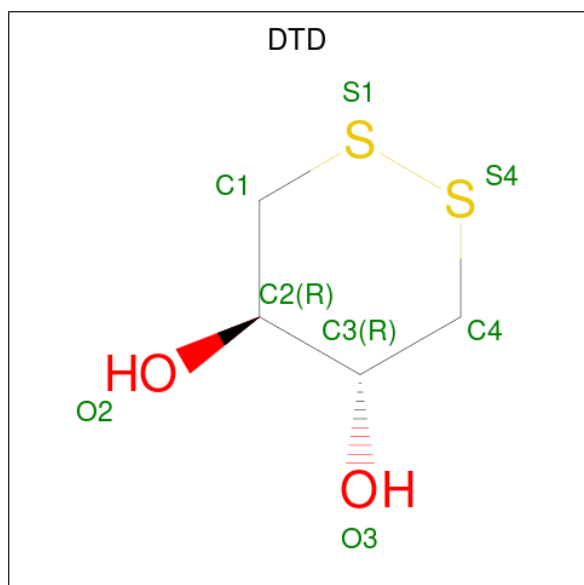
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	OCS	CYS	modified residue	UNP P12256
A	74A	THR	-	insertion	UNP P12256
A	74B	TYR	-	insertion	UNP P12256
A	74C	ALA	-	insertion	UNP P12256
A	74D	ASP	-	insertion	UNP P12256
A	74E	GLU	-	insertion	UNP P12256
A	74F	PRO	-	insertion	UNP P12256
A	74G	LYS	-	insertion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

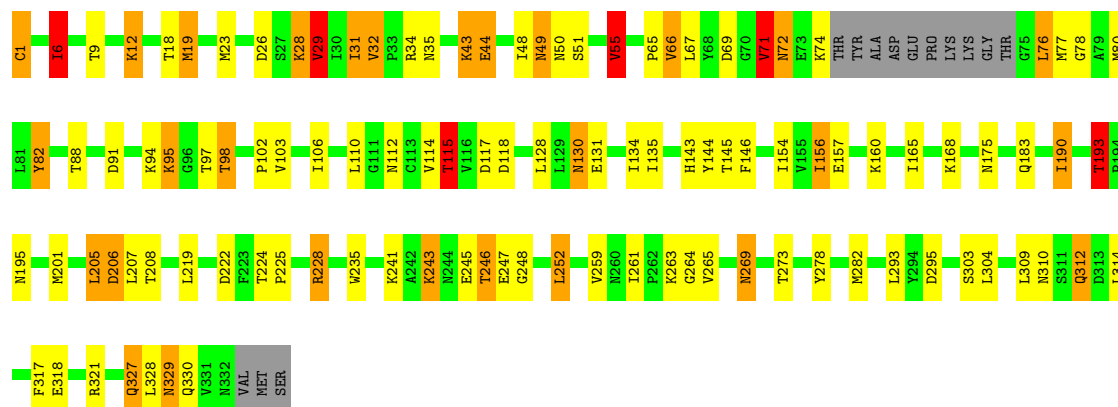
- Molecule 2 is DITHIANE DIOL (CCD ID: DTD) (formula: $C_4H_8O_2S_2$).



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

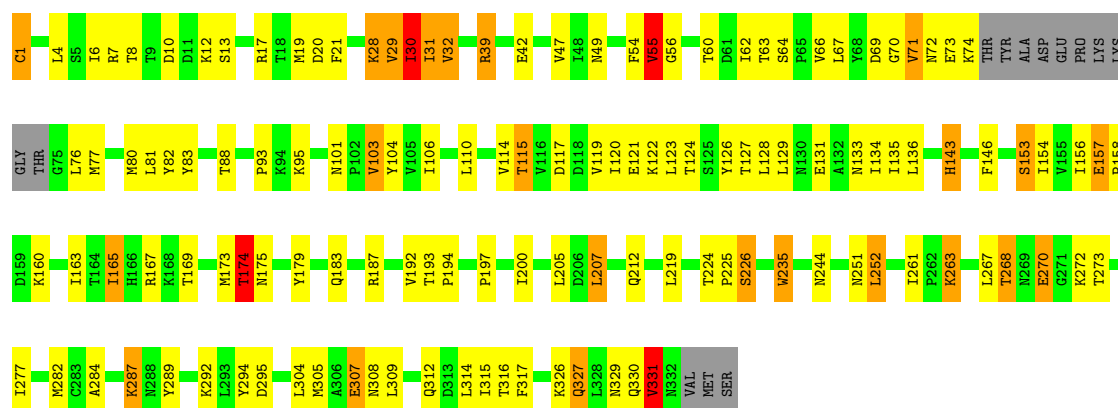
- Molecule 3 is water.

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



• Molecule 1: PENICILLIN V ACYLASE

Chain D: 58% 30% 7% . .



4 Data and refinement statistics

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	208.40 Å 208.40 Å 96.20 Å 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	0.58	0/2639	1.59	31/3589 (0.9%)
1	B	0.59	0/2639	1.56	31/3589 (0.9%)
1	C	0.63	0/2639	1.63	38/3589 (1.1%)
1	D	0.50	0/2639	1.42	16/3589 (0.4%)
All	All	0.58	0/10556	1.55	116/14356 (0.8%)

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 (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	VAL	CB-CA-C	-10.24	95.06	110.82
1	C	228	ARG	CD-NE-CZ	10.09	138.53	124.40
1	B	62	ILE	N-CA-CB	10.09	123.75	112.45
1	A	55	VAL	CB-CA-C	-9.40	97.75	111.19
1	D	7	ARG	CD-NE-CZ	9.38	137.53	124.40
1	C	9	THR	CA-C-N	8.82	138.64	121.18
1	C	9	THR	C-N-CA	8.82	138.64	121.18
1	C	295	ASP	CA-CB-CG	-7.85	104.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ILE	N-CA-C	7.75	115.22	107.55
1	A	71	VAL	CB-CA-C	-7.71	98.62	110.50
1	B	261	ILE	N-CA-C	7.62	115.09	107.55
1	D	32	VAL	N-CA-CB	7.40	120.21	112.37
1	B	32	VAL	CA-C-O	7.37	124.58	119.20
1	D	55	VAL	CB-CA-C	-7.36	100.66	111.19
1	B	208	THR	O-C-N	-7.35	115.82	121.55
1	C	115	THR	N-CA-CB	-7.35	98.76	111.55
1	A	143	HIS	CA-CB-CG	7.24	121.04	113.80
1	C	261	ILE	N-CA-C	7.23	115.86	107.77
1	A	321	ARG	CD-NE-CZ	7.14	134.40	124.40
1	B	71	VAL	CB-CA-C	-7.04	99.97	110.82
1	D	30	ILE	CB-CA-C	-7.00	102.89	111.08
1	B	66	VAL	N-CA-CB	6.94	119.32	110.99
1	C	71	VAL	CB-CA-C	-6.93	99.83	110.50
1	C	31	ILE	CA-C-N	-6.89	116.70	123.04
1	C	31	ILE	C-N-CA	-6.89	116.70	123.04
1	D	143	HIS	CA-CB-CG	6.81	120.61	113.80
1	C	29	VAL	N-CA-CB	6.80	118.75	111.00
1	C	328	LEU	CA-C-N	6.78	136.25	123.09
1	C	328	LEU	C-N-CA	6.78	136.25	123.09
1	B	10	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	219	LEU	CB-CA-C	6.74	117.60	109.31
1	C	32	VAL	CA-C-O	6.66	123.52	119.19
1	A	9	THR	CA-C-N	6.60	133.27	120.99
1	A	9	THR	C-N-CA	6.60	133.27	120.99
1	C	269	ASN	OD1-CG-ND2	6.60	129.20	122.60
1	A	308	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	B	31	ILE	CA-C-N	-6.53	116.23	123.02
1	B	31	ILE	C-N-CA	-6.53	116.23	123.02
1	D	39	ARG	CD-NE-CZ	6.43	133.41	124.40
1	C	193	THR	N-CA-CB	-6.40	99.66	111.18
1	C	157	GLU	CB-CG-CD	6.40	123.47	112.60
1	A	49	ASN	CA-CB-CG	-6.39	106.21	112.60
1	A	72	ASN	CA-CB-CG	6.39	118.99	112.60
1	B	115	THR	N-CA-CB	-6.38	100.44	111.55
1	C	32	VAL	CB-CA-C	6.37	117.28	110.53
1	A	29	VAL	N-CA-CB	6.37	117.47	110.53
1	C	66	VAL	N-CA-CB	6.37	119.48	111.46
1	D	20	ASP	CA-C-O	-6.35	113.46	120.38
1	A	114	VAL	CA-C-O	6.34	126.44	120.80
1	A	61	ASP	CA-C-O	-6.33	113.84	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	115	THR	N-CA-CB	-6.28	101.18	110.85
1	C	130	ASN	OD1-CG-ND2	6.15	128.75	122.60
1	B	32	VAL	N-CA-CB	6.11	118.75	111.23
1	B	143	HIS	CA-CB-CG	6.11	119.91	113.80
1	C	6	ILE	N-CA-CB	-6.04	102.29	112.44
1	B	31	ILE	CA-C-O	-6.03	113.61	120.66
1	A	287	LYS	CA-CB-CG	6.02	126.13	114.10
1	C	34	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	A	210	PHE	CA-CB-CG	5.96	119.76	113.80
1	A	268	THR	CA-C-O	-5.96	115.15	121.88
1	A	321	ARG	CA-CB-CG	5.93	125.97	114.10
1	B	62	ILE	N-CA-C	-5.91	101.61	108.82
1	B	30	ILE	CB-CA-C	-5.91	102.03	110.83
1	B	40	LEU	N-CA-C	-5.91	105.74	113.12
1	A	105	VAL	CA-C-O	-5.84	114.87	120.95
1	A	66	VAL	N-CA-CB	5.83	117.99	110.99
1	C	91	ASP	CA-CB-CG	-5.83	106.77	112.60
1	D	261	ILE	N-CA-C	5.78	113.78	107.60
1	D	157	GLU	CA-C-O	5.71	124.04	119.59
1	B	208	THR	CB-CA-C	5.63	117.78	109.22
1	D	287	LYS	CA-CB-CG	5.63	125.35	114.10
1	A	189	TYR	CA-C-N	5.58	132.02	121.97
1	A	189	TYR	C-N-CA	5.58	132.02	121.97
1	C	65	PRO	CA-C-N	-5.56	115.89	123.12
1	C	65	PRO	C-N-CA	-5.56	115.89	123.12
1	C	156	ILE	CB-CA-C	-5.54	102.91	110.77
1	B	65	PRO	CA-C-N	-5.53	115.96	122.93
1	B	65	PRO	C-N-CA	-5.53	115.96	122.93
1	B	162	GLY	N-CA-C	5.53	118.78	111.70
1	C	329	ASN	CB-CA-C	-5.53	101.00	112.44
1	B	208	THR	N-CA-CB	-5.50	100.46	110.63
1	B	157	GLU	CB-CG-CD	5.49	121.94	112.60
1	D	133	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	101	ASN	CA-C-N	5.47	125.81	119.47
1	A	101	ASN	C-N-CA	5.47	125.81	119.47
1	A	10	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	204	ASP	CA-CB-CG	-5.45	107.15	112.60
1	A	266	VAL	CA-C-O	-5.44	114.77	120.27
1	C	28	LYS	CA-C-N	-5.43	115.58	122.37
1	C	28	LYS	C-N-CA	-5.43	115.58	122.37
1	D	31	ILE	N-CA-CB	5.43	116.64	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	SER	CA-C-O	5.39	125.90	119.60
1	B	324	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	135	ILE	CA-C-O	-5.37	115.47	121.17
1	B	223	PHE	CA-CB-CG	-5.36	108.44	113.80
1	B	72	ASN	CB-CA-C	-5.34	100.41	110.51
1	A	189	TYR	CA-C-O	5.29	126.35	119.95
1	C	18	THR	N-CA-CB	5.24	119.16	110.52
1	B	84	ALA	CA-C-N	5.16	132.48	123.91
1	B	84	ALA	C-N-CA	5.16	132.48	123.91
1	B	72	ASN	CA-C-O	-5.16	115.86	121.89
1	D	212	GLN	CA-C-O	-5.14	115.88	121.89
1	D	268	THR	CA-C-O	-5.11	116.10	121.88
1	A	282	MET	CA-CB-CG	5.11	124.32	114.10
1	C	327	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	B	287	LYS	N-CA-CB	5.08	119.41	111.84
1	C	135	ILE	N-CA-C	5.08	115.29	110.42
1	C	102	PRO	CA-C-N	5.07	128.96	120.64
1	C	102	PRO	C-N-CA	5.07	128.96	120.64
1	D	174	THR	CB-CA-C	5.06	120.49	110.42
1	D	32	VAL	CA-C-O	5.05	122.64	119.51
1	C	183	GLN	OE1-CD-NE2	5.02	127.62	122.60
1	C	143	HIS	CA-CB-CG	5.02	118.82	113.80
1	B	167	ARG	N-CA-CB	-5.02	102.82	110.85
1	A	182	HIS	O-C-N	-5.01	116.91	122.07

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

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	96	0
1	B	2593	0	2563	68	0
1	C	2593	0	2563	62	0
1	D	2593	0	2563	88	0
2	A	8	0	8	1	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	18	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	301	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 15.

All (301) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:80:MET:HE1	1:D:103:VAL:HA	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:77:MET:HE2	1:A:284:ALA:HB2	1.83	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:D:282:MET:HE2	1:D:289:TYR:HE1	1.67	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:A:324:ASP:CG	3:A:1140:HOH:O	2.47	0.58
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
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:D:77:MET:HE2	1:D:284:ALA:HB2	1.86	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:13:SER:O	1:D:77:MET:HE1	2.06	0.55
1:A:269:ASN:C	1:A:269:ASN:HD22	2.16	0.54
1:D:64:SER:HB2	1:D:104:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:42:GLU:H	1:D:131:GLU:CD	2.19	0.51
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
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:C:145:THR:C	3:C:1189:HOH:O	2.53	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:D:143:HIS:NE2	1:D:173:MET:HE3	2.27	0.50
1:B:119:VAL:HG12	1:B:123:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLU:OE1	1:B:167:ARG:NE	2.45	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: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:D:143:HIS:CD2	1:D:173:MET:HE3	2.48	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:A:282:MET:HE2	1:A:289:TYR:CE1	2.48	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:D:174:THR:CG2	1:D:175:ASN:N	2.75	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:A:292:LYS:NZ	3:A:1030:HOH:O	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:80:MET:HE3	1:A:106:ILE:HG12	1.98	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:143:HIS:CE1	1:D:173:MET:HE3	2.52	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
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:B:80:MET:HE3	1:B:106:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ARG:C	1:D:17:ARG:HD3	2.43	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: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:72:ASN:HD22	1:C:72:ASN:C	2.27	0.42
1:C:80:MET:HE2	1:C:144:TYR:HE1	1.84	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
1:B:219:LEU:CD2	1:B:220:PRO:HD2	2.50	0.42
1:A:19:MET:HE1	2:A:1001:DTD:H31	2.02	0.42
1:A:235:TRP:HA	1:A:235:TRP:HE3	1.83	0.42
1:A:274:ASP:CG	3:A:1194:HOH:O	2.62	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:B:12:LYS:HE3	1:B:245:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:329:ASN:O	1:A:330:GLN:C	2.63	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:C:205:LEU:HD11	1:D:183:GLN:CD	2.45	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:C:201:MET:HE3	1:C:206:ASP:CG	2.46	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:B:19:MET:HE3	1:B:19:MET:HB3	1.91	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:C:80:MET:HE3	1:C:106:ILE:HG12	2.04	0.40
1:A:28:LYS:HB2	1:A:317:PHE:O	2.20	0.40
1:B:13:SER:O	1:B:77:MET:HE1	2.21	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

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	330/345 (96%)	315 (96%)	15 (4%)	0	100	100
1	B	330/345 (96%)	316 (96%)	13 (4%)	1 (0%)	36	55
1	C	330/345 (96%)	317 (96%)	13 (4%)	0	100	100
1	D	330/345 (96%)	305 (92%)	24 (7%)	1 (0%)	36	55
All	All	1320/1380 (96%)	1253 (95%)	65 (5%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

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

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	288/299 (96%)	250 (87%)	38 (13%)	4	8
1	B	288/299 (96%)	241 (84%)	47 (16%)	2	4
1	C	288/299 (96%)	237 (82%)	51 (18%)	2	3
1	D	288/299 (96%)	250 (87%)	38 (13%)	4	8
All	All	1152/1196 (96%)	978 (85%)	174 (15%)	3	5

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	7	ARG
1	A	9	THR
1	A	28	LYS
1	A	29	VAL
1	A	32	VAL
1	A	39	ARG
1	A	49	ASN
1	A	55	VAL
1	A	66	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	130	ASN
1	A	152	GLU
1	A	168	LYS
1	A	180	GLU
1	A	190	ILE
1	A	201	MET
1	A	207	LEU
1	A	208	THR
1	A	219	LEU
1	A	241	LYS
1	A	243	LYS
1	A	252	LEU
1	A	269	ASN
1	A	293	LEU
1	A	314	LEU
1	A	321	ARG
1	A	322	LYS
1	A	331	VAL
1	B	9	THR
1	B	12	LYS
1	B	19	MET
1	B	29	VAL
1	B	32	VAL

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Mol	Chain	Res	Type
1	B	43	LYS
1	B	44	GLU
1	B	45	ASN
1	B	47	VAL
1	B	66	VAL
1	B	71	VAL
1	B	72	ASN
1	B	76	LEU
1	B	82	TYR
1	B	88	THR
1	B	95	LYS
1	B	98	THR
1	B	103	VAL
1	B	110	LEU
1	B	115	THR
1	B	121	GLU
1	B	134	ILE
1	B	135	ILE
1	B	163	ILE
1	B	190	ILE
1	B	198	GLN
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	265	VAL
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	321	ARG
1	B	322	LYS
1	B	331	VAL
1	B	332	ASN

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Mol	Chain	Res	Type
1	C	6	ILE
1	C	12	LYS
1	C	19	MET
1	C	23	MET
1	C	28	LYS
1	C	29	VAL
1	C	32	VAL
1	C	43	LYS
1	C	44	GLU
1	C	48	ILE
1	C	49	ASN
1	C	51	SER
1	C	55	VAL
1	C	66	VAL
1	C	67	LEU
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	103	VAL
1	C	110	LEU
1	C	115	THR
1	C	128	LEU
1	C	130	ASN
1	C	134	ILE
1	C	160	LYS
1	C	165	ILE
1	C	168	LYS
1	C	190	ILE
1	C	193	THR
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

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Mol	Chain	Res	Type
1	C	263	LYS
1	C	265	VAL
1	C	293	LEU
1	C	309	LEU
1	C	312	GLN
1	C	314	LEU
1	C	321	ARG
1	C	327	GLN
1	C	330	GLN
1	D	6	ILE
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	71	VAL
1	D	73	GLU
1	D	76	LEU
1	D	82	TYR
1	D	95	LYS
1	D	103	VAL
1	D	115	THR
1	D	123	LEU
1	D	129	LEU
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	252	LEU
1	D	263	LYS
1	D	270	GLU
1	D	272	LYS
1	D	273	THR
1	D	305	MET
1	D	307	GLU
1	D	308	ASN

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Mol	Chain	Res	Type
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 (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	ASN
1	A	130	ASN
1	A	182	HIS
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	310	ASN
1	A	327	GLN
1	B	45	ASN
1	B	72	ASN
1	B	112	ASN
1	B	166	HIS
1	B	185	ASN
1	B	195	ASN
1	B	251	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	195	ASN
1	C	198	GLN
1	C	308	ASN
1	D	35	ASN
1	D	45	ASN
1	D	49	ASN

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Mol	Chain	Res	Type
1	D	183	GLN
1	D	251	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	1	1	6,8,9	1.56	1 (16%)	7,11,13	2.22	2 (28%)
1	OCS	C	1	1	6,8,9	1.62	1 (16%)	7,11,13	1.48	2 (28%)
1	OCS	A	1	1	6,8,9	1.34	1 (16%)	7,11,13	1.56	2 (28%)
1	OCS	B	1	1	6,8,9	1.08	0	7,11,13	2.20	3 (42%)

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	D	1	1	-	0/4/7/9	-
1	OCS	C	1	1	-	3/4/7/9	-
1	OCS	A	1	1	-	3/4/7/9	-
1	OCS	B	1	1	-	3/4/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	OCS	CB-CA	-3.15	1.51	1.53
1	A	1	OCS	CB-CA	-2.36	1.51	1.53
1	D	1	OCS	CB-CA	-2.29	1.52	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	OCS	OD1-SG-CB	4.79	113.91	106.76
1	B	1	OCS	OD1-SG-CB	4.00	112.73	106.76
1	A	1	OCS	OD3-SG-CB	2.71	110.81	106.76
1	A	1	OCS	OD2-SG-OD3	-2.53	105.06	111.40
1	D	1	OCS	OD3-SG-OD1	-2.39	106.06	113.82
1	C	1	OCS	OD1-SG-CB	2.37	110.29	106.76
1	C	1	OCS	OD2-SG-CB	2.24	110.30	105.97
1	B	1	OCS	OD2-SG-CB	2.12	110.06	105.97
1	B	1	OCS	OD2-SG-OD1	-2.07	106.22	111.40

There are no chirality outliers.

All (9) 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
1	B	1	OCS	CA-CB-SG-OD1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DTD	B	1002	-	8,8,8	0.56	0	6,10,10	1.28	1 (16%)
2	DTD	C	1003	-	8,8,8	0.68	0	6,10,10	1.17	1 (16%)
2	DTD	D	1004	-	8,8,8	0.55	0	6,10,10	1.16	1 (16%)
2	DTD	A	1001	-	8,8,8	0.66	0	6,10,10	0.90	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
2	DTD	B	1002	-	1/1/2/2	-	1/1/1/1
2	DTD	C	1003	-	1/1/2/2	-	1/1/1/1
2	DTD	D	1004	-	-	-	0/1/1/1
2	DTD	A	1001	-	1/1/2/2	-	1/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1004	DTD	O3-C3-C2	-2.51	104.70	110.20
2	C	1003	DTD	O3-C3-C2	-2.33	105.10	110.20
2	B	1002	DTD	O2-C2-C1	-2.09	106.30	109.81

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.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DTD	C1-C2-C3-C4-S1-S4
2	B	1002	DTD	C1-C2-C3-C4-S1-S4
2	C	1003	DTD	C1-C2-C3-C4-S1-S4

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	DTD	1	0
2	A	1001	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.