Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:11 am BST

PDB ID	:	1LVO
Title	:	Structure of coronavirus main proteinase reveals combination of a chymotrypsin fold with an extra alpha-helical domain
Authors	:	Anand, K.; Palm, G.J.; Mesters, J.R.; Siddell, S.G.; Ziebuhr, J.; Hilgenfeld, R.
Deposited on	:	2002-05-29
Resolution	:	1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

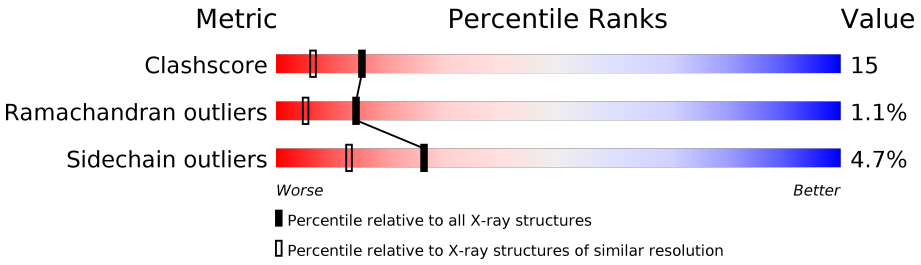
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.96 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	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	302	76% 19%
1	B	302	81% 16%
1	C	302	73% 25%
1	D	302	78% 19%
1	E	302	84% 12%
1	F	302	64% 29% 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	SO4	F	3010	-	-	X	-
3	DIO	C	2008	-	-	X	-
3	DIO	C	2009	-	-	X	-
3	DIO	E	2001	-	-	X	-
3	DIO	F	2003	-	-	X	-

2 Entry composition

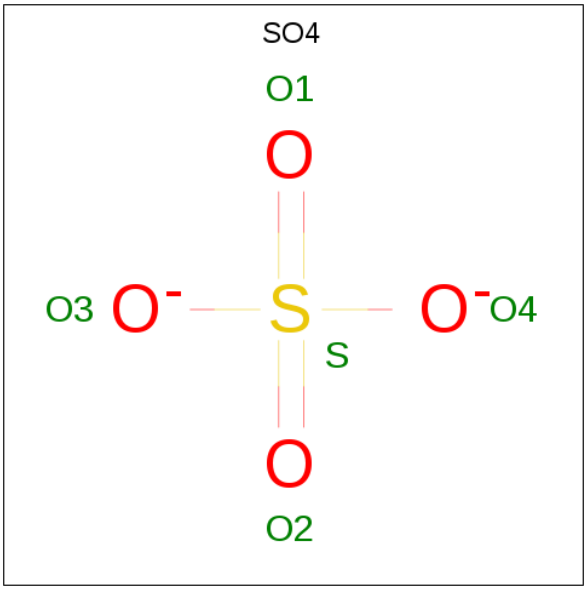
There are 5 unique types of molecules in this entry. The entry contains 15045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Replicase, hydrolase domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2297	1448	390	443	16			
1	B	300	Total	C	N	O	S	0	0	0
			2305	1452	392	445	16			
1	C	300	Total	C	N	O	S	0	0	0
			2305	1452	392	445	16			
1	D	301	Total	C	N	O	S	0	0	0
			2313	1458	393	446	16			
1	E	299	Total	C	N	O	S	0	0	0
			2297	1448	390	443	16			
1	F	299	Total	C	N	O	S	0	0	0
			2288	1441	388	443	16			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

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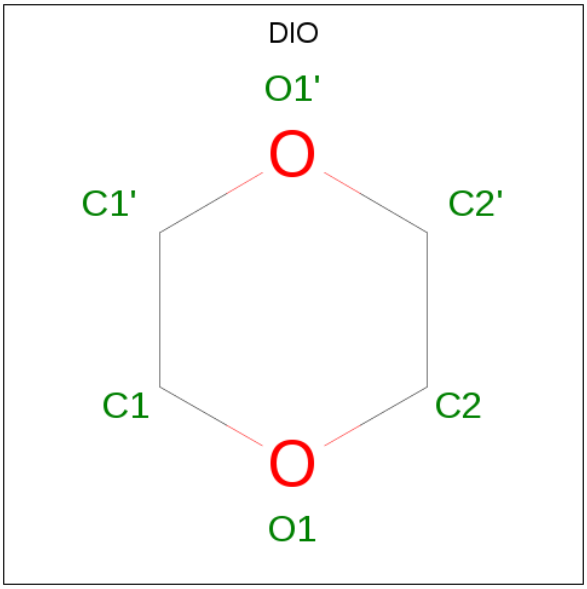
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 4 2	0	0
3	A	1	Total C O 6 4 2	0	0
3	A	1	Total C O 6 4 2	0	0
3	B	1	Total C O 6 4 2	0	0
3	C	1	Total C O 6 4 2	0	0
3	C	1	Total C O 6 4 2	0	0

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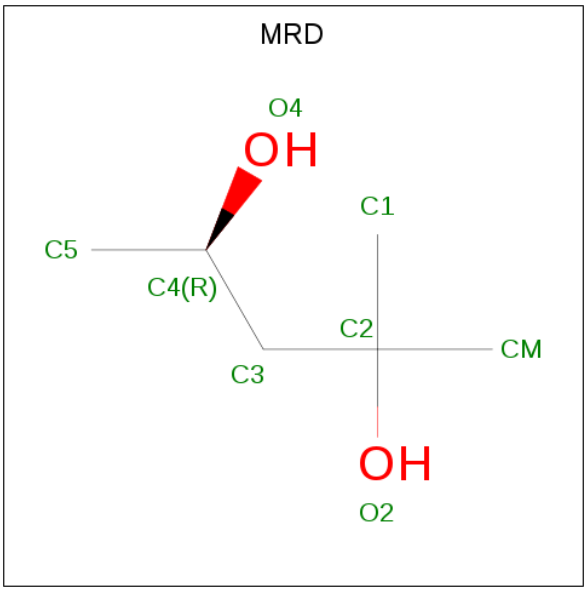
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 6 4 2	0	0
3	E	1	Total C O 6 4 2	0	0
3	F	1	Total C O 6 4 2	0	0

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	220	Total O 220 220	0	0
5	C	122	Total O 122 122	0	0
5	D	165	Total O 165 165	0	0
5	E	225	Total O 225 225	0	0
5	F	105	Total O 105 105	0	0

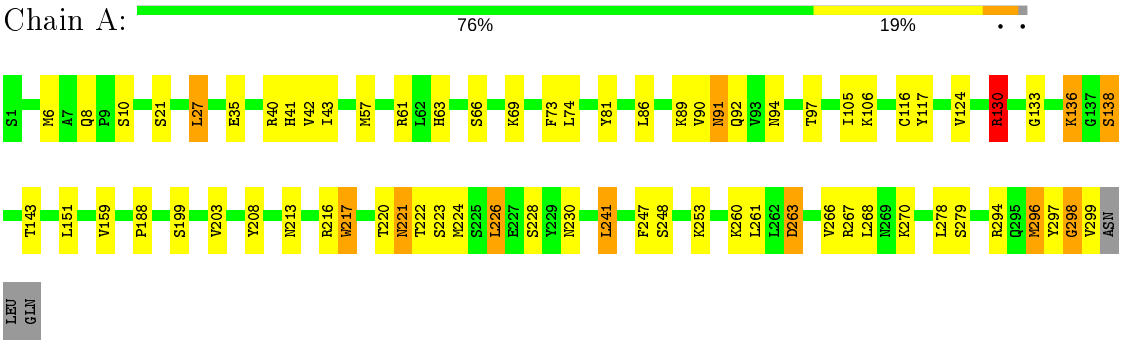
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

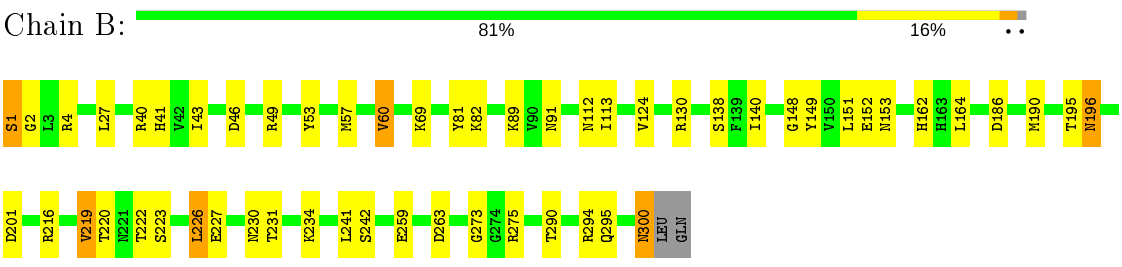
- Molecule 1: Replicase, hydrolase domain

Chain A:



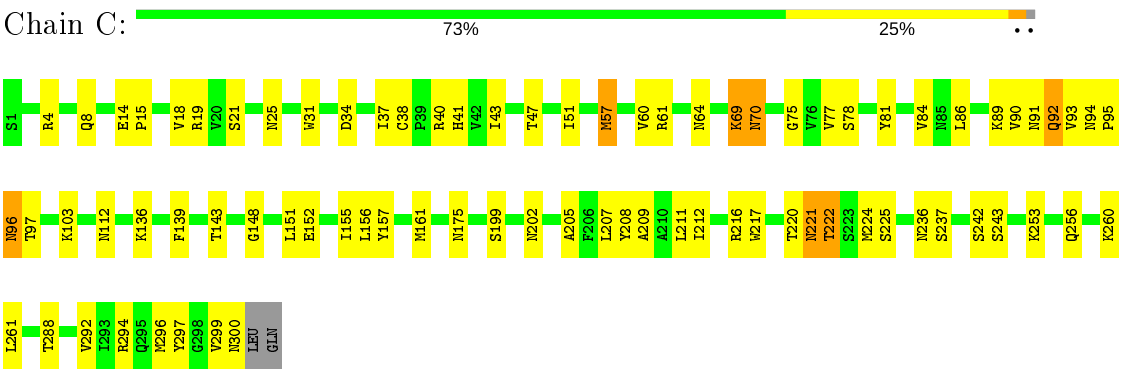
- Molecule 1: Replicase, hydrolase domain

Chain B:



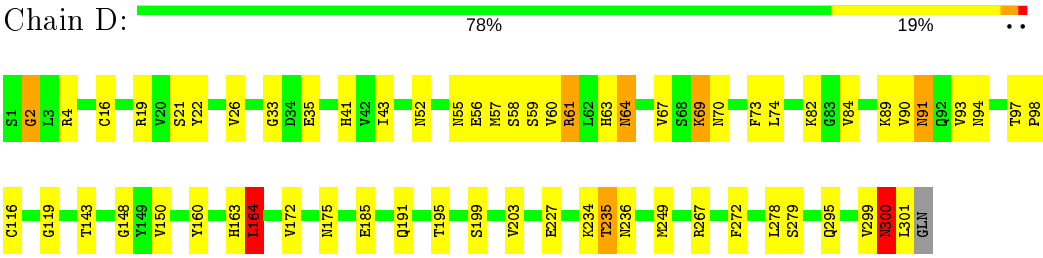
- Molecule 1: Replicase, hydrolase domain

Chain C:



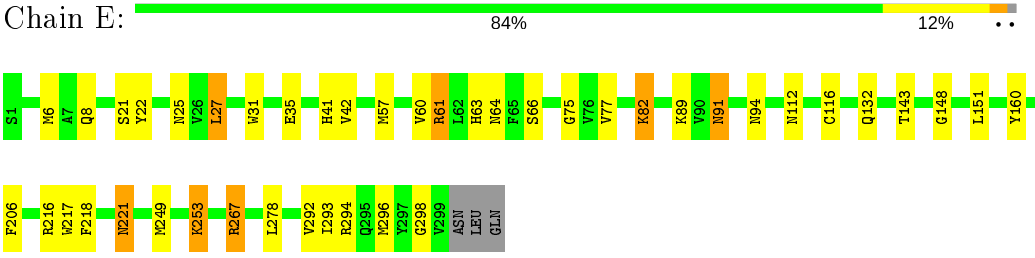
- Molecule 1: Replicase, hydrolase domain

Chain D:



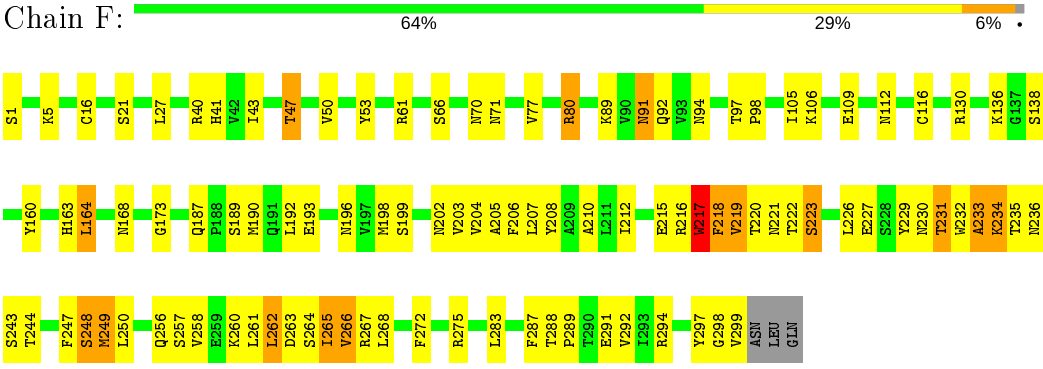
• Molecule 1: Replicase, hydrolase domain

Chain E:



• Molecule 1: Replicase, hydrolase domain

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.82Å 160.13Å 88.96Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	27.42 – 1.96	Depositor
% Data completeness (in resolution range)	92.3 (27.42-1.96)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15045	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.83	0/2343	0.92	5/3171 (0.2%)
1	B	0.92	2/2351 (0.1%)	0.91	2/3182 (0.1%)
1	C	0.76	0/2351	0.87	0/3182
1	D	0.83	0/2359	0.88	4/3193 (0.1%)
1	E	0.92	0/2343	0.91	4/3171 (0.1%)
1	F	0.68	0/2334	0.81	0/3161
All	All	0.83	2/14081 (0.0%)	0.88	15/19060 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	TYR	CD1-CE1	5.12	1.47	1.39
1	B	149	TYR	CD2-CE2	5.09	1.47	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	267	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	E	267	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	130	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	B	69	LYS	C-N-CA	-6.56	105.31	121.70
1	D	267	ARG	NE-CZ-NH2	-5.89	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	164	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	298	GLY	N-CA-C	5.69	127.32	113.10
1	E	82	LYS	N-CA-C	-5.60	95.89	111.00
1	A	138	SER	N-CA-C	-5.36	96.54	111.00
1	D	267	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	82	LYS	N-CA-C	-5.24	96.85	111.00
1	A	263	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	164	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	241	LEU	CA-CB-CG	5.04	126.88	115.30
1	D	82	LYS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	TYR	Sidechain

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	2297	0	2247	60	0
1	B	2305	0	2253	51	0
1	C	2305	0	2253	80	0
1	D	2313	0	2264	61	0
1	E	2297	0	2247	48	0
1	F	2288	0	2224	125	0
2	A	25	0	0	2	0
2	B	20	0	0	0	0
2	C	25	0	0	1	0
2	D	25	0	0	0	0
2	E	20	0	0	0	0
2	F	20	0	0	3	0
3	A	18	0	24	2	0
3	B	6	0	8	1	0
3	C	12	0	16	12	0
3	E	12	0	16	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	6	0	8	5	0
4	A	8	0	14	5	0
4	B	8	0	14	5	0
4	C	8	0	14	3	0
4	D	8	0	14	1	0
4	E	8	0	14	2	0
4	F	8	0	14	3	0
5	A	166	0	0	6	0
5	B	220	0	0	4	1
5	C	122	0	0	5	1
5	D	165	0	0	5	0
5	E	225	0	0	7	1
5	F	105	0	0	2	1
All	All	15045	0	13644	415	2

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 (415) 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:B:275:ARG:HH22	1:E:216:ARG:NH1	1.45	1.13
1:D:67:VAL:HG12	1:D:74:LEU:HD21	1.32	1.12
1:B:275:ARG:HH22	1:E:216:ARG:HH11	1.09	1.00
1:E:217:TRP:HB3	3:E:2001:DIO:H2'2	1.43	0.98
1:C:220:THR:HG23	1:C:222:THR:H	1.23	0.97
3:C:2009:DIO:H1'2	1:D:2:GLY:H	1.27	0.97
1:D:185:GLU:H	1:D:191:GLN:NE2	1.65	0.94
1:D:185:GLU:N	1:D:191:GLN:HE22	1.66	0.94
1:F:61:ARG:HG2	1:F:61:ARG:HH11	1.34	0.92
3:E:2001:DIO:H2'1	5:E:4063:HOH:O	1.68	0.92
1:C:297:TYR:HB2	1:C:299:VAL:HG23	1.51	0.92
1:F:216:ARG:HG3	1:F:217:TRP:H	1.34	0.90
1:B:275:ARG:NH2	1:E:216:ARG:HH11	1.69	0.89
1:F:248:SER:HB2	1:F:249:MET:HE2	1.54	0.87
1:F:220:THR:HB	1:F:267:ARG:HH22	1.39	0.87
1:C:136:LYS:HZ1	3:C:2009:DIO:H1'1	1.39	0.86
1:B:275:ARG:HG2	1:E:221:ASN:HD22	1.40	0.86
1:A:222:THR:HB	1:A:263:ASP:OD1	1.77	0.85
1:A:230:ASN:HD21	1:A:241:LEU:H	1.22	0.85
1:D:300:ASN:C	1:D:300:ASN:HD22	1.81	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:SER:N	5:B:4105:HOH:O	2.03	0.84
1:B:162:HIS:NE2	3:B:2007:DIO:H1'1	1.93	0.84
1:D:164:LEU:HD22	1:D:172:VAL:HB	1.60	0.84
1:F:91:ASN:ND2	1:F:92:GLN:HG3	1.93	0.83
1:D:74:LEU:HD12	1:D:90:VAL:HG21	1.59	0.82
1:C:95:PRO:HG2	1:C:96:ASN:ND2	1.94	0.82
1:C:136:LYS:HZ1	3:C:2009:DIO:C1'	1.93	0.81
1:E:294:ARG:HG2	1:E:294:ARG:HH11	1.45	0.81
1:D:57:MET:O	1:D:60:VAL:HG12	1.80	0.79
1:B:273:GLY:HA2	3:E:2001:DIO:H21	1.65	0.79
3:C:2009:DIO:H2'2	5:C:4124:HOH:O	1.83	0.78
1:C:155:ILE:HD11	1:C:157:TYR:OH	1.83	0.78
1:F:216:ARG:O	1:F:219:VAL:HG23	1.82	0.77
1:B:275:ARG:NH2	1:E:216:ARG:NH1	2.26	0.76
1:F:241:LEU:HD22	1:F:262:LEU:HD21	1.67	0.76
1:C:31:TRP:HZ2	1:C:92:GLN:HG2	1.50	0.76
1:E:75:GLY:H	1:E:91:ASN:ND2	1.83	0.75
1:C:43:ILE:HD11	1:C:81:TYR:OH	1.86	0.75
1:D:67:VAL:CG1	1:D:74:LEU:HD21	2.14	0.75
1:D:61:ARG:HG3	1:D:64:ASN:HB2	1.66	0.75
1:E:61:ARG:HB3	1:E:63:HIS:CE1	2.21	0.74
1:A:188:PRO:HB3	4:A:4001:MRD:H1C1	1.69	0.74
1:D:67:VAL:O	1:D:74:LEU:HD23	1.88	0.74
1:A:230:ASN:ND2	1:A:241:LEU:H	1.86	0.74
1:F:249:MET:H	1:F:249:MET:CE	2.00	0.73
1:B:186:ASP:C	4:B:4002:MRD:H5C2	2.09	0.73
1:D:74:LEU:H	1:D:74:LEU:HD23	1.51	0.73
1:A:260:LYS:HE3	5:A:4097:HOH:O	1.90	0.72
1:D:94:ASN:HB3	1:D:97:THR:OG1	1.89	0.72
1:A:69:LYS:HE2	5:A:4104:HOH:O	1.89	0.72
1:F:220:THR:HG22	1:F:267:ARG:HH12	1.55	0.72
1:E:294:ARG:CG	1:E:294:ARG:HH11	2.02	0.71
1:A:136:LYS:HE2	5:A:4096:HOH:O	1.91	0.71
1:C:96:ASN:N	1:C:96:ASN:HD22	1.89	0.71
1:F:70:ASN:O	1:F:71:ASN:HB2	1.88	0.71
1:B:227:GLU:O	1:B:231:THR:HG23	1.89	0.71
1:F:230:ASN:O	1:F:234:LYS:HG3	1.91	0.69
1:F:220:THR:HG21	1:F:264:SER:HA	1.73	0.69
1:B:294:ARG:HG2	1:B:300:ASN:HA	1.75	0.69
1:F:275:ARG:HA	3:F:2003:DIO:H1'1	1.75	0.69
1:F:210:ALA:HB1	1:F:215:GLU:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2009:DIO:H1'2	1:D:2:GLY:N	2.06	0.68
1:C:95:PRO:HG2	1:C:96:ASN:HD22	1.55	0.68
1:C:225:SER:H	3:C:2008:DIO:C1'	2.07	0.68
1:D:300:ASN:C	1:D:300:ASN:ND2	2.44	0.68
1:C:220:THR:HG23	1:C:222:THR:N	2.05	0.67
1:D:63:HIS:HB2	5:D:4167:HOH:O	1.95	0.67
1:C:136:LYS:NZ	3:C:2009:DIO:H1'1	2.09	0.67
1:C:155:ILE:HG13	1:C:157:TYR:CE1	2.30	0.67
1:D:185:GLU:H	1:D:191:GLN:HE22	0.82	0.66
1:F:220:THR:HB	1:F:267:ARG:NH2	2.10	0.66
1:D:91:ASN:HD22	1:D:91:ASN:C	1.97	0.66
1:F:199:SER:O	1:F:203:VAL:HG23	1.96	0.66
1:F:256:GLN:HA	1:F:256:GLN:HE21	1.60	0.66
1:F:288:THR:OG1	1:F:291:GLU:HG3	1.96	0.66
1:F:220:THR:CB	1:F:267:ARG:HH22	2.08	0.65
1:E:91:ASN:ND2	5:E:4192:HOH:O	2.25	0.64
1:E:164:LEU:HD22	1:E:172:VAL:HB	1.80	0.64
1:B:226:LEU:C	1:B:226:LEU:HD23	2.18	0.64
1:F:240:GLU:O	1:F:242:SER:N	2.31	0.64
1:A:208:TYR:CE1	1:A:261:LEU:HD12	2.31	0.64
1:C:256:GLN:OE1	1:C:260:LYS:HG2	1.97	0.64
1:F:21:SER:OG	1:F:66:SER:HB3	1.97	0.64
1:F:192:LEU:HD22	2:F:3010:SO4:O4	1.98	0.64
1:F:205:ALA:HB1	1:F:292:VAL:HG21	1.81	0.63
1:B:295:GLN:HG3	5:B:4211:HOH:O	1.99	0.63
1:A:91:ASN:C	1:A:91:ASN:HD22	2.01	0.63
1:B:226:LEU:O	1:B:226:LEU:HD23	1.99	0.63
1:A:106:LYS:NZ	5:A:4148:HOH:O	2.31	0.63
1:A:138:SER:OG	1:B:4:ARG:HD2	1.99	0.63
1:C:297:TYR:HB2	1:C:299:VAL:CG2	2.28	0.63
1:C:96:ASN:N	1:C:96:ASN:ND2	2.44	0.63
1:F:130:ARG:NH1	1:F:136:LYS:HE3	2.14	0.63
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.64	0.62
1:F:268:LEU:HB3	1:F:272:PHE:HE1	1.63	0.62
1:C:292:VAL:O	1:C:296:MET:HG2	2.00	0.62
1:B:186:ASP:HB2	4:B:4002:MRD:C5	2.30	0.62
1:E:6:MET:CE	1:F:138:SER:HB3	2.30	0.62
1:A:41:HIS:HD2	5:A:4007:HOH:O	1.83	0.62
1:C:57:MET:HA	1:C:57:MET:HE3	1.81	0.61
1:B:226:LEU:CD2	1:B:230:ASN:ND2	2.63	0.61
1:E:249:MET:HE1	1:E:293:ILE:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:THR:CG2	1:F:267:ARG:HH12	2.14	0.61
1:B:275:ARG:HG2	1:E:221:ASN:ND2	2.14	0.61
1:C:216:ARG:HG3	1:C:216:ARG:HH11	1.65	0.61
1:C:209:ALA:HA	1:C:296:MET:HE2	1.83	0.60
1:F:204:VAL:HB	1:F:247:PHE:CE2	2.37	0.60
1:E:41:HIS:HD2	5:E:4042:HOH:O	1.85	0.60
1:B:231:THR:HA	1:B:234:LYS:NZ	2.16	0.59
1:F:216:ARG:HG3	1:F:217:TRP:N	2.13	0.59
1:E:6:MET:HE1	1:F:138:SER:HB3	1.84	0.59
1:A:61:ARG:HD2	1:A:63:HIS:HE1	1.67	0.59
1:B:41:HIS:HB3	4:B:4002:MRD:H5C1	1.85	0.59
1:A:220:THR:OG1	1:A:267:ARG:NH2	2.35	0.59
1:F:207:LEU:O	1:F:210:ALA:HB3	2.02	0.59
1:D:52:ASN:CG	1:D:55:ASN:HD22	2.06	0.59
1:B:186:ASP:O	4:B:4002:MRD:H5C2	2.01	0.59
1:F:61:ARG:HG2	1:F:61:ARG:NH1	2.06	0.59
1:E:294:ARG:CG	1:E:294:ARG:NH1	2.64	0.59
1:A:40:ARG:O	1:A:43:ILE:HG22	2.03	0.58
1:B:226:LEU:HD23	1:B:230:ASN:ND2	2.18	0.58
1:D:301:LEU:HD13	1:D:301:LEU:O	2.04	0.58
1:F:256:GLN:HA	1:F:256:GLN:NE2	2.17	0.58
1:A:221:ASN:ND2	1:F:275:ARG:HD3	2.19	0.58
1:C:103:LYS:HG2	1:C:157:TYR:CD2	2.39	0.58
1:D:33:GLY:HA2	1:D:93:VAL:HG13	1.85	0.58
1:E:218:PHE:O	1:E:267:ARG:NH2	2.36	0.58
1:F:220:THR:OG1	1:F:264:SER:HB3	2.03	0.58
1:C:155:ILE:HD11	1:C:157:TYR:CZ	2.38	0.58
1:C:51:ILE:CD1	4:C:4003:MRD:H5C3	2.34	0.58
1:F:244:THR:HG22	1:F:258:VAL:HG11	1.86	0.58
1:C:155:ILE:CG1	1:C:157:TYR:CE1	2.88	0.57
1:D:91:ASN:ND2	1:D:91:ASN:C	2.58	0.57
1:F:220:THR:HG23	5:F:4103:HOH:O	2.05	0.57
1:E:249:MET:HE1	1:E:293:ILE:CG2	2.34	0.57
1:E:249:MET:HE1	1:E:293:ILE:HG23	1.86	0.57
1:F:41:HIS:HB2	4:F:4006:MRD:HMC3	1.86	0.57
1:C:92:GLN:HG3	1:C:93:VAL:N	2.20	0.56
1:A:138:SER:HA	1:B:1:SER:HB3	1.88	0.56
1:C:47:THR:HB	4:C:4003:MRD:H3C2	1.87	0.56
1:F:272:PHE:O	1:F:275:ARG:HB2	2.04	0.56
1:F:130:ARG:HB3	1:F:196:ASN:HD21	1.70	0.56
1:F:268:LEU:HD22	1:F:272:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:ARG:CA	3:F:2003:DIO:H1'1	2.36	0.56
1:F:235:THR:O	1:F:236:ASN:ND2	2.37	0.56
1:D:185:GLU:HG2	1:D:191:GLN:NE2	2.21	0.56
1:D:234:LYS:HE3	1:D:234:LYS:CA	2.36	0.56
1:F:226:LEU:HD12	1:F:262:LEU:HD11	1.88	0.56
1:F:275:ARG:HA	3:F:2003:DIO:C1'	2.35	0.56
1:B:112:ASN:O	1:B:148:GLY:HA2	2.06	0.56
1:D:41:HIS:HD2	5:D:4076:HOH:O	1.88	0.56
1:D:19:ARG:NH1	1:D:21:SER:HB2	2.21	0.56
1:E:22:TYR:CE1	1:E:64:ASN:HB3	2.42	0.56
1:F:233:ALA:O	1:F:235:THR:N	2.38	0.55
1:F:234:LYS:HE3	1:F:240:GLU:OE2	2.05	0.55
1:A:91:ASN:ND2	1:A:91:ASN:C	2.60	0.55
3:E:2001:DIO:H2'1	5:E:4229:HOH:O	2.06	0.55
1:F:249:MET:HE2	1:F:249:MET:H	1.72	0.55
1:A:226:LEU:HD21	1:A:241:LEU:HD12	1.89	0.55
1:C:209:ALA:HA	1:C:296:MET:CE	2.35	0.54
1:C:208:TYR:CE1	1:C:261:LEU:HD12	2.42	0.54
1:C:225:SER:H	3:C:2008:DIO:H1'1	1.73	0.54
1:E:132:GLN:NE2	5:E:4087:HOH:O	2.22	0.54
1:E:6:MET:CE	1:F:138:SER:CB	2.86	0.54
1:D:74:LEU:HD12	1:D:90:VAL:CG2	2.33	0.54
1:C:41:HIS:HD2	5:C:4009:HOH:O	1.91	0.54
3:E:2002:DIO:H2'2	5:E:4185:HOH:O	2.08	0.54
1:A:267:ARG:NH1	1:A:267:ARG:HB2	2.23	0.53
1:A:61:ARG:HD2	1:A:63:HIS:CE1	2.42	0.53
1:B:1:SER:HB2	5:B:4220:HOH:O	2.07	0.53
1:B:223:SER:HB2	1:B:259:GLU:HB3	1.89	0.53
1:F:106:LYS:O	1:F:109:GLU:HG3	2.07	0.53
1:A:35:GLU:OE2	1:A:89:LYS:HE2	2.08	0.53
1:C:31:TRP:CZ2	1:C:92:GLN:HG2	2.39	0.53
1:C:34:ASP:O	1:C:90:VAL:HG22	2.08	0.53
1:A:21:SER:OG	1:A:66:SER:HB3	2.08	0.53
1:A:217:TRP:HB3	2:A:3011:SO4:O1	2.08	0.53
1:C:224:MET:HA	3:C:2008:DIO:H11	1.90	0.53
1:D:295:GLN:OE1	5:D:4051:HOH:O	2.18	0.53
1:F:262:LEU:N	1:F:262:LEU:HD23	2.22	0.53
1:E:292:VAL:O	1:E:296:MET:HG2	2.09	0.53
1:E:112:ASN:O	1:E:148:GLY:HA2	2.09	0.53
1:E:8:GLN:NE2	1:E:151:LEU:HB2	2.24	0.53
1:A:224:MET:SD	1:A:266:VAL:HG21	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:ARG:NH1	1:F:136:LYS:HG3	2.23	0.53
1:C:51:ILE:HD11	4:C:4003:MRD:H5C3	1.90	0.53
1:A:10:SER:HB3	1:A:124:VAL:HG11	1.91	0.52
1:E:91:ASN:N	1:E:91:ASN:HD22	2.08	0.52
1:C:19:ARG:HH11	1:C:19:ARG:HG2	1.73	0.52
1:F:204:VAL:HB	1:F:247:PHE:CZ	2.44	0.52
1:F:61:ARG:CG	1:F:61:ARG:HH11	2.14	0.52
1:A:188:PRO:HB3	4:A:4001:MRD:C1	2.40	0.52
1:A:91:ASN:HD22	1:A:92:GLN:N	2.08	0.52
1:D:278:LEU:O	1:D:279:SER:HB2	2.10	0.52
1:F:227:GLU:O	1:F:231:THR:HB	2.09	0.52
1:F:233:ALA:O	1:F:236:ASN:N	2.41	0.52
1:F:217:TRP:CG	1:F:218:PHE:N	2.78	0.52
1:B:226:LEU:HD21	1:B:230:ASN:ND2	2.25	0.52
1:F:130:ARG:NH1	1:F:136:LYS:CE	2.72	0.52
1:F:227:GLU:N	1:F:227:GLU:OE2	2.40	0.52
1:B:216:ARG:O	1:B:219:VAL:HB	2.10	0.51
1:C:294:ARG:HH11	1:C:294:ARG:HG2	1.75	0.51
1:F:163:HIS:HB3	1:F:164:LEU:HD12	1.91	0.51
1:A:133:GLY:HA2	3:A:2005:DIO:H21	1.93	0.51
1:A:8:GLN:HB3	1:A:151:LEU:HD12	1.92	0.51
1:D:52:ASN:ND2	1:D:55:ASN:HD22	2.08	0.51
1:F:130:ARG:HH12	1:F:136:LYS:CE	2.24	0.51
1:F:187:GLN:C	4:F:4006:MRD:H1C2	2.30	0.51
1:A:222:THR:CB	1:A:263:ASP:OD1	2.55	0.51
1:C:151:LEU:HD23	1:C:156:LEU:HA	1.93	0.51
1:F:268:LEU:HB3	1:F:272:PHE:CE1	2.43	0.51
1:C:175:ASN:HB2	5:C:4068:HOH:O	2.11	0.51
1:C:78:SER:HB3	1:C:89:LYS:HB2	1.91	0.51
1:D:227:GLU:HG3	5:D:4123:HOH:O	2.10	0.51
1:F:130:ARG:HH11	1:F:136:LYS:HG3	1.76	0.51
1:A:116:CYS:O	1:A:143:THR:HA	2.11	0.51
1:B:220:THR:HG23	1:B:222:THR:H	1.75	0.51
1:C:225:SER:HB2	3:C:2008:DIO:H1'1	1.93	0.50
1:F:217:TRP:CD2	1:F:218:PHE:N	2.79	0.50
1:F:80:ARG:HG2	1:F:80:ARG:HH11	1.75	0.50
1:A:267:ARG:CB	1:A:267:ARG:HH11	2.24	0.50
1:C:220:THR:HG22	5:C:4041:HOH:O	2.11	0.50
1:F:222:THR:HG22	1:F:263:ASP:OD2	2.12	0.50
1:F:40:ARG:HG3	1:F:53:TYR:CE2	2.47	0.50
1:E:6:MET:HE3	1:F:138:SER:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:GLY:H	1:E:91:ASN:HD21	1.57	0.50
1:C:14:GLU:N	1:C:15:PRO:HD2	2.27	0.50
1:C:40:ARG:HA	1:C:86:LEU:HB2	1.93	0.50
1:D:74:LEU:N	1:D:74:LEU:HD23	2.23	0.50
1:B:231:THR:HA	1:B:234:LYS:HZ2	1.77	0.49
1:D:112:ASN:O	1:D:148:GLY:HA2	2.13	0.49
1:F:203:VAL:HG11	1:F:283:LEU:HD13	1.94	0.49
1:A:230:ASN:HD21	1:A:241:LEU:N	2.02	0.49
1:F:216:ARG:NH1	1:F:217:TRP:HB3	2.28	0.49
1:C:34:ASP:HA	1:C:92:GLN:O	2.13	0.49
1:F:216:ARG:CG	1:F:217:TRP:H	2.11	0.49
2:F:3019:SO4:O4	3:F:2003:DIO:H1'2	2.13	0.49
1:C:220:THR:O	1:C:260:LYS:HE2	2.13	0.49
1:F:210:ALA:HB1	1:F:215:GLU:CG	2.42	0.49
1:B:196:ASN:OD1	5:B:4131:HOH:O	2.20	0.48
1:C:57:MET:HA	1:C:57:MET:CE	2.42	0.48
1:D:16:CYS:SG	1:D:98:PRO:HD3	2.53	0.48
1:F:249:MET:H	1:F:249:MET:HE3	1.78	0.48
1:F:91:ASN:HD22	1:F:91:ASN:N	2.11	0.48
1:A:296:MET:O	1:A:297:TYR:C	2.51	0.48
1:B:226:LEU:HD21	1:B:230:ASN:HD21	1.78	0.48
1:C:225:SER:H	3:C:2008:DIO:H11	1.78	0.48
1:C:299:VAL:HG12	1:C:300:ASN:N	2.27	0.48
1:F:212:ILE:HD11	1:F:250:LEU:HD22	1.95	0.48
1:C:225:SER:H	3:C:2008:DIO:C1	2.26	0.48
1:E:164:LEU:CB	4:E:4005:MRD:HMC2	2.44	0.48
1:F:220:THR:HG21	1:F:264:SER:CA	2.43	0.48
1:F:232:TRP:CZ2	1:F:266:VAL:HG13	2.48	0.48
1:F:40:ARG:O	1:F:43:ILE:HG22	2.13	0.48
1:E:35:GLU:HG2	1:E:89:LYS:HD2	1.95	0.47
1:F:203:VAL:O	1:F:206:PHE:HB3	2.13	0.47
1:C:18:VAL:HG12	1:C:69:LYS:HG2	1.96	0.47
1:F:112:ASN:O	1:F:148:GLY:HA2	2.15	0.47
1:A:213:ASN:O	1:A:213:ASN:CG	2.53	0.47
1:D:35:GLU:OE2	1:D:89:LYS:NZ	2.37	0.47
1:B:113:ILE:O	1:B:124:VAL:HA	2.14	0.47
1:B:294:ARG:CD	1:B:300:ASN:HA	2.44	0.47
1:F:216:ARG:O	1:F:219:VAL:CG2	2.60	0.47
1:B:294:ARG:CG	1:B:300:ASN:HA	2.42	0.47
1:F:294:ARG:HG2	1:F:299:VAL:HB	1.97	0.47
1:E:148:GLY:HA3	1:E:160:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:ARG:CB	3:F:2003:DIO:H1'1	2.44	0.47
1:A:40:ARG:HA	1:A:86:LEU:HB2	1.97	0.47
1:D:235:THR:HG22	1:D:236:ASN:ND2	2.30	0.47
1:D:148:GLY:HA3	1:D:160:TYR:HB3	1.97	0.47
1:D:57:MET:HG2	5:D:4114:HOH:O	2.14	0.47
1:D:70:ASN:HD22	1:D:70:ASN:N	2.13	0.47
1:C:112:ASN:O	1:C:148:GLY:HA2	2.15	0.46
1:A:278:LEU:O	1:A:279:SER:HB2	2.15	0.46
1:C:4:ARG:HG2	1:C:4:ARG:HH11	1.80	0.46
1:F:229:TYR:O	1:F:233:ALA:N	2.40	0.46
1:B:153:ASN:O	1:B:153:ASN:OD1	2.33	0.46
1:B:40:ARG:HG3	1:B:53:TYR:CE2	2.51	0.46
1:C:236:ASN:O	1:C:237:SER:HB2	2.16	0.46
1:C:94:ASN:OD1	5:C:4017:HOH:O	2.21	0.46
1:E:206:PHE:CE1	1:E:278:LEU:HD12	2.50	0.46
1:F:241:LEU:O	1:F:243:SER:N	2.49	0.46
1:A:188:PRO:CA	4:A:4001:MRD:C1	2.93	0.46
1:E:249:MET:O	1:E:253:LYS:HD2	2.16	0.46
1:E:21:SER:OG	1:E:66:SER:HB3	2.16	0.46
1:C:69:LYS:C	1:C:70:ASN:O	2.52	0.46
1:D:116:CYS:O	1:D:143:THR:HA	2.14	0.46
1:A:294:ARG:HA	1:A:299:VAL:HG23	1.98	0.46
1:B:43:ILE:HD11	1:B:81:TYR:OH	2.16	0.46
1:A:188:PRO:HA	4:A:4001:MRD:H1C2	1.98	0.46
1:C:90:VAL:HG23	1:C:92:GLN:O	2.15	0.46
1:F:204:VAL:HG21	1:F:241:LEU:HD11	1.97	0.45
1:F:116:CYS:O	1:F:143:THR:HA	2.17	0.45
1:D:41:HIS:ND1	4:D:4004:MRD:HMC2	2.31	0.45
1:C:70:ASN:HD22	1:C:70:ASN:N	2.13	0.45
1:E:164:LEU:HB3	4:E:4005:MRD:HMC2	1.98	0.45
1:F:247:PHE:O	1:F:248:SER:C	2.54	0.45
1:F:77:VAL:HG23	1:F:89:LYS:HB2	1.97	0.45
1:C:103:LYS:NZ	1:C:152:GLU:OE1	2.42	0.45
1:A:138:SER:HA	1:B:1:SER:CB	2.47	0.45
1:C:217:TRP:N	2:C:3023:SO4:O1	2.50	0.45
1:F:244:THR:HG22	1:F:258:VAL:CG1	2.47	0.45
1:F:193:GLU:N	2:F:3010:SO4:O1	2.45	0.45
1:A:188:PRO:N	4:A:4001:MRD:H1C3	2.32	0.45
1:A:298:GLY:HA3	1:B:140:ILE:HD12	1.97	0.45
1:A:296:MET:O	1:A:298:GLY:N	2.50	0.45
1:B:130:ARG:HB3	1:B:196:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:LYS:HA	1:D:234:LYS:HE3	1.98	0.45
1:D:300:ASN:O	1:D:300:ASN:ND2	2.49	0.45
1:F:241:LEU:HD22	1:F:262:LEU:CD2	2.42	0.45
1:F:248:SER:CB	1:F:249:MET:HE2	2.38	0.45
1:A:57:MET:HB2	1:A:81:TYR:CE1	2.52	0.44
1:F:16:CYS:SG	1:F:98:PRO:HD2	2.57	0.44
1:C:21:SER:HA	1:C:25:ASN:O	2.17	0.44
1:D:272:PHE:CD1	1:D:272:PHE:N	2.86	0.44
1:E:249:MET:HE1	1:E:293:ILE:CG1	2.46	0.44
1:F:94:ASN:HB3	1:F:97:THR:OG1	2.16	0.44
1:C:139:PHE:HB3	1:C:143:THR:OG1	2.18	0.44
1:C:260:LYS:HZ2	1:C:260:LYS:HG2	1.57	0.44
1:C:40:ARG:HG2	1:C:84:VAL:O	2.17	0.44
1:F:210:ALA:O	1:F:215:GLU:HG2	2.18	0.44
1:F:204:VAL:HG12	1:F:208:TYR:CE1	2.53	0.44
1:A:199:SER:O	1:A:203:VAL:HG23	2.17	0.44
1:C:202:ASN:OD1	1:C:288:THR:HA	2.17	0.44
1:C:61:ARG:HD2	1:C:64:ASN:ND2	2.32	0.44
1:E:21:SER:HA	1:E:25:ASN:O	2.18	0.44
1:F:168:ASN:HD21	1:F:193:GLU:HB2	1.83	0.44
1:B:290:THR:O	1:B:294:ARG:HG3	2.18	0.44
1:D:21:SER:OG	1:D:26:VAL:HG22	2.18	0.44
1:D:33:GLY:CA	1:D:93:VAL:HG13	2.48	0.43
1:F:61:ARG:HD2	5:F:4021:HOH:O	2.18	0.43
1:E:27:LEU:HD21	1:E:42:VAL:HB	2.00	0.43
1:F:241:LEU:CD2	1:F:262:LEU:HD21	2.44	0.43
1:C:253:LYS:HD3	1:C:297:TYR:CZ	2.53	0.43
1:F:233:ALA:O	1:F:234:LYS:C	2.57	0.43
1:A:105:ILE:HG12	1:A:159:VAL:HB	2.01	0.43
1:C:212:ILE:HB	1:C:296:MET:HE3	2.00	0.43
1:C:221:ASN:HA	1:C:221:ASN:HD22	1.62	0.43
1:C:294:ARG:HG2	1:C:294:ARG:NH1	2.33	0.43
1:F:222:THR:HG22	1:F:223:SER:N	2.34	0.43
1:B:57:MET:O	1:B:60:VAL:HB	2.19	0.43
1:E:31:TRP:CE2	1:E:94:ASN:HB2	2.52	0.43
1:B:220:THR:HG21	1:B:263:ASP:OD1	2.18	0.43
1:C:8:GLN:NE2	1:C:151:LEU:HB2	2.34	0.43
1:F:5:LYS:NZ	1:F:291:GLU:OE1	2.48	0.43
1:C:205:ALA:HB1	1:C:292:VAL:HG21	2.00	0.43
1:D:234:LYS:HA	1:D:234:LYS:CE	2.48	0.43
1:D:84:VAL:O	1:D:163:HIS:HE1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:PHE:O	1:F:220:THR:N	2.52	0.43
1:A:247:PHE:O	1:A:248:SER:C	2.57	0.43
1:B:152:GLU:O	1:B:153:ASN:CG	2.58	0.43
1:B:46:ASP:OD2	1:B:49:ARG:HD2	2.18	0.43
1:B:220:THR:OG1	1:B:222:THR:HB	2.19	0.42
1:D:69:LYS:O	1:D:70:ASN:HB2	2.19	0.42
1:F:247:PHE:CD1	1:F:247:PHE:N	2.86	0.42
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.64	0.42
3:A:2006:DIO:H1'1	5:A:4112:HOH:O	2.20	0.42
1:A:27:LEU:HD21	1:A:42:VAL:HB	2.00	0.42
1:C:207:LEU:HD23	1:C:207:LEU:HA	1.83	0.42
1:F:50:VAL:O	1:F:50:VAL:HG13	2.18	0.42
1:C:94:ASN:HB3	1:C:97:THR:OG1	2.20	0.42
1:E:116:CYS:O	1:E:143:THR:HA	2.19	0.42
1:F:261:LEU:O	1:F:262:LEU:C	2.58	0.42
1:D:272:PHE:N	1:D:272:PHE:HD1	2.18	0.42
1:F:105:ILE:HG23	1:F:109:GLU:HB2	2.01	0.42
1:D:185:GLU:HG2	1:D:191:GLN:HE22	1.84	0.42
1:D:22:TYR:CD2	1:D:43:ILE:HA	2.54	0.42
1:E:8:GLN:HB3	1:E:151:LEU:HD12	2.00	0.42
1:F:77:VAL:HG22	1:F:89:LYS:O	2.19	0.42
1:A:130:ARG:NH1	2:A:3004:SO4:S	2.90	0.42
1:D:235:THR:CG2	1:D:235:THR:O	2.67	0.42
1:C:75:GLY:O	1:C:91:ASN:N	2.53	0.42
1:E:31:TRP:CD2	1:E:94:ASN:HB2	2.55	0.42
1:F:130:ARG:CZ	1:F:136:LYS:HE3	2.49	0.42
1:D:73:PHE:CD2	1:D:73:PHE:N	2.87	0.41
1:E:91:ASN:H	1:E:91:ASN:HD22	1.67	0.41
1:D:74:LEU:CD1	1:D:90:VAL:HG21	2.40	0.41
1:E:82:LYS:HG3	5:E:4226:HOH:O	2.20	0.41
1:A:267:ARG:NH1	1:A:267:ARG:CB	2.83	0.41
1:B:164:LEU:HB2	4:B:4002:MRD:H1C1	2.02	0.41
1:C:155:ILE:HD11	1:C:157:TYR:CE1	2.54	0.41
1:F:226:LEU:CD1	1:F:262:LEU:HD11	2.50	0.41
1:C:61:ARG:HD2	1:C:64:ASN:HD22	1.85	0.41
1:D:299:VAL:HG12	1:D:300:ASN:N	2.34	0.41
1:F:202:ASN:HB3	1:F:287:PHE:O	2.19	0.41
1:A:6:MET:CE	1:B:138:SER:HB3	2.50	0.41
1:B:294:ARG:HD2	1:B:300:ASN:HB3	2.02	0.41
1:E:57:MET:O	1:E:60:VAL:HG12	2.19	0.41
1:F:257:SER:OG	1:F:260:LYS:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD13	1:A:90:VAL:HG21	2.03	0.41
1:C:4:ARG:HG2	1:C:4:ARG:NH1	2.36	0.41
1:D:175:ASN:C	1:D:175:ASN:OD1	2.58	0.41
1:D:299:VAL:CG1	1:D:300:ASN:N	2.83	0.41
1:F:160:TYR:CE1	1:F:173:GLY:HA3	2.56	0.41
1:F:232:TRP:CE2	1:F:236:ASN:OD1	2.73	0.41
1:F:264:SER:O	1:F:268:LEU:HD12	2.21	0.41
1:F:130:ARG:HH12	1:F:136:LYS:HE2	1.86	0.41
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.33	0.41
1:E:27:LEU:C	1:E:27:LEU:HD12	2.41	0.41
1:F:190:MET:HG3	1:F:190:MET:H	1.59	0.41
1:F:229:TYR:CD2	1:F:262:LEU:HD13	2.56	0.41
1:A:73:PHE:N	1:A:73:PHE:CD2	2.88	0.41
1:F:130:ARG:NH1	1:F:136:LYS:CG	2.84	0.41
1:F:287:PHE:N	1:F:287:PHE:CD1	2.89	0.41
1:A:222:THR:HG22	1:A:223:SER:N	2.36	0.40
1:A:94:ASN:HB3	1:A:97:THR:OG1	2.22	0.40
1:C:211:LEU:HD11	1:C:261:LEU:HD21	2.03	0.40
1:C:38:CYS:HA	1:C:161:MET:SD	2.61	0.40
1:D:19:ARG:HB2	1:D:119:GLY:HA3	2.03	0.40
1:F:265:ILE:O	1:F:268:LEU:N	2.40	0.40
1:D:199:SER:O	1:D:203:VAL:HG23	2.22	0.40
1:F:47:THR:HG23	4:F:4006:MRD:H3C2	2.02	0.40
1:B:219:VAL:O	1:B:219:VAL:HG12	2.21	0.40
1:D:57:MET:O	1:D:59:SER:N	2.55	0.40
1:F:217:TRP:CE3	1:F:218:PHE:HA	2.56	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
5:B:4062:HOH:O	5:E:4223:HOH:O[1_655]	2.14	0.06
5:C:4035:HOH:O	5:F:4086:HOH:O[2_657]	2.18	0.02

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	297/302 (98%)	279 (94%)	15 (5%)	3 (1%)	15 6
1	B	298/302 (99%)	288 (97%)	8 (3%)	2 (1%)	22 11
1	C	298/302 (99%)	281 (94%)	16 (5%)	1 (0%)	41 30
1	D	299/302 (99%)	283 (95%)	13 (4%)	3 (1%)	15 6
1	E	297/302 (98%)	285 (96%)	11 (4%)	1 (0%)	41 30
1	F	297/302 (98%)	263 (89%)	24 (8%)	10 (3%)	3 0
All	All	1786/1812 (99%)	1679 (94%)	87 (5%)	20 (1%)	14 5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	300	ASN
1	F	219	VAL
1	F	234	LYS
1	F	241	LEU
1	F	242	SER
1	B	2	GLY
1	D	2	GLY
1	E	298	GLY
1	F	298	GLY
1	A	221	ASN
1	B	242	SER
1	D	58	SER
1	F	265	ILE
1	A	217	TRP
1	A	296	MET
1	C	70	ASN
1	F	217	TRP
1	F	233	ALA
1	F	248	SER
1	F	266	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	255/258 (99%)	246 (96%)	9 (4%)	36 24
1	B	256/258 (99%)	242 (94%)	14 (6%)	21 9
1	C	256/258 (99%)	244 (95%)	12 (5%)	26 13
1	D	257/258 (100%)	244 (95%)	13 (5%)	24 11
1	E	255/258 (99%)	248 (97%)	7 (3%)	44 34
1	F	253/258 (98%)	236 (93%)	17 (7%)	16 5
All	All	1532/1548 (99%)	1460 (95%)	72 (5%)	26 13

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	91	ASN
1	A	130	ARG
1	A	136	LYS
1	A	216	ARG
1	A	226	LEU
1	A	228	SER
1	A	253	LYS
1	A	270	LYS
1	B	1	SER
1	B	27	LEU
1	B	60	VAL
1	B	89	LYS
1	B	91	ASN
1	B	151	LEU
1	B	190	MET
1	B	195	THR
1	B	196	ASN
1	B	201	ASP
1	B	219	VAL
1	B	226	LEU
1	B	241	LEU
1	B	300	ASN
1	C	37	ILE
1	C	57	MET
1	C	60	VAL

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Mol	Chain	Res	Type
1	C	69	LYS
1	C	77	VAL
1	C	92	GLN
1	C	96	ASN
1	C	199	SER
1	C	221	ASN
1	C	222	THR
1	C	242	SER
1	C	243	SER
1	D	4	ARG
1	D	56	GLU
1	D	61	ARG
1	D	64	ASN
1	D	69	LYS
1	D	91	ASN
1	D	99	GLU
1	D	150	VAL
1	D	164	LEU
1	D	195	THR
1	D	235	THR
1	D	249	MET
1	D	300	ASN
1	E	27	LEU
1	E	61	ARG
1	E	77	VAL
1	E	91	ASN
1	E	164	LEU
1	E	221	ASN
1	E	253	LYS
1	F	1	SER
1	F	27	LEU
1	F	47	THR
1	F	80	ARG
1	F	91	ASN
1	F	164	LEU
1	F	189	SER
1	F	198	MET
1	F	217	TRP
1	F	218	PHE
1	F	221	ASN
1	F	223	SER
1	F	231	THR

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Mol	Chain	Res	Type
1	F	249	MET
1	F	262	LEU
1	F	289	PRO
1	F	297	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	55	ASN
1	A	63	HIS
1	A	91	ASN
1	A	92	GLN
1	A	230	ASN
1	B	55	ASN
1	B	64	ASN
1	B	91	ASN
1	B	153	ASN
1	C	41	HIS
1	C	55	ASN
1	C	64	ASN
1	C	70	ASN
1	C	96	ASN
1	C	132	GLN
1	C	221	ASN
1	D	41	HIS
1	D	52	ASN
1	D	55	ASN
1	D	70	ASN
1	D	91	ASN
1	D	153	ASN
1	D	163	HIS
1	D	191	GLN
1	D	236	ASN
1	D	300	ASN
1	E	41	HIS
1	E	70	ASN
1	E	91	ASN
1	E	213	ASN
1	E	221	ASN
1	F	41	HIS
1	F	85	ASN

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Mol	Chain	Res	Type
1	F	91	ASN
1	F	92	GLN
1	F	196	ASN
1	F	221	ASN
1	F	230	ASN
1	F	236	ASN
1	F	256	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

42 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	SO4	C	3001	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	B	3026	-	4,4,4	0.16	0	6,6,6	0.18	0
4	MRD	C	4003	-	7,7,7	0.60	0	9,10,10	0.44	0
3	DIO	E	2002	-	6,6,6	0.68	0	6,6,6	0.26	0
2	SO4	D	3008	-	4,4,4	0.36	0	6,6,6	0.24	0
2	SO4	C	3015	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	F	3019	-	4,4,4	0.30	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	3027	-	4,4,4	0.31	0	6,6,6	0.27	0
2	SO4	D	3017	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	A	3022	-	4,4,4	0.32	0	6,6,6	0.28	0
2	SO4	C	3005	-	4,4,4	0.37	0	6,6,6	0.23	0
2	SO4	A	3003	-	4,4,4	0.23	0	6,6,6	0.48	0
2	SO4	C	3002	-	4,4,4	0.28	0	6,6,6	0.26	0
3	DIO	A	2006	-	6,6,6	0.61	0	6,6,6	0.34	0
3	DIO	F	2003	-	6,6,6	0.67	0	6,6,6	0.26	0
3	DIO	E	2001	-	6,6,6	0.70	0	6,6,6	0.22	0
4	MRD	E	4005	-	7,7,7	0.84	0	9,10,10	0.44	0
4	MRD	B	4002	-	7,7,7	0.60	0	9,10,10	0.48	0
2	SO4	D	3016	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	E	3013	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SO4	B	3014	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	3023	-	4,4,4	0.21	0	6,6,6	0.12	0
3	DIO	B	2007	-	6,6,6	0.68	0	6,6,6	0.27	0
3	DIO	A	2005	-	6,6,6	0.69	0	6,6,6	0.27	0
2	SO4	E	3007	-	4,4,4	0.34	0	6,6,6	0.23	0
2	SO4	E	3018	-	4,4,4	0.23	0	6,6,6	0.23	0
2	SO4	B	3006	-	4,4,4	0.28	0	6,6,6	0.33	0
2	SO4	F	3024	-	4,4,4	0.29	0	6,6,6	0.16	0
2	SO4	A	3004	-	4,4,4	0.23	0	6,6,6	0.32	0
4	MRD	A	4001	-	7,7,7	0.59	0	9,10,10	0.58	0
2	SO4	F	3025	-	4,4,4	0.28	0	6,6,6	0.06	0
4	MRD	F	4006	-	7,7,7	0.73	0	9,10,10	0.58	0
2	SO4	D	3021	-	4,4,4	0.27	0	6,6,6	0.13	0
3	DIO	C	2008	-	6,6,6	0.53	0	6,6,6	0.29	0
2	SO4	F	3010	-	4,4,4	0.21	0	6,6,6	0.27	0
2	SO4	A	3011	-	4,4,4	0.24	0	6,6,6	0.13	0
3	DIO	A	2004	-	6,6,6	0.74	0	6,6,6	0.21	0
2	SO4	E	3009	-	4,4,4	0.29	0	6,6,6	0.19	0
2	SO4	D	3012	-	4,4,4	0.47	0	6,6,6	0.32	0
4	MRD	D	4004	-	7,7,7	0.63	0	9,10,10	0.57	0
2	SO4	B	3020	-	4,4,4	0.24	0	6,6,6	0.21	0
3	DIO	C	2009	-	6,6,6	0.64	0	6,6,6	0.25	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
4	MRD	C	4003	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	F	2003	-	-	-	0/1/1/1
3	DIO	E	2002	-	-	-	0/1/1/1
4	MRD	E	4005	-	-	0/5/5/5	-
4	MRD	B	4002	-	-	0/5/5/5	-
3	DIO	B	2007	-	-	-	0/1/1/1
3	DIO	A	2005	-	-	-	0/1/1/1
3	DIO	C	2008	-	-	-	0/1/1/1
3	DIO	A	2006	-	-	-	0/1/1/1
4	MRD	A	4001	-	-	0/5/5/5	-
3	DIO	E	2001	-	-	-	0/1/1/1
4	MRD	F	4006	-	-	0/5/5/5	-
4	MRD	D	4004	-	-	0/5/5/5	-
3	DIO	A	2004	-	-	-	0/1/1/1
3	DIO	C	2009	-	-	-	0/1/1/1

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.

19 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4003	MRD	3	0
3	E	2002	DIO	1	0
2	F	3019	SO4	1	0
3	A	2006	DIO	1	0
3	F	2003	DIO	5	0
3	E	2001	DIO	4	0
4	E	4005	MRD	2	0
4	B	4002	MRD	5	0
2	C	3023	SO4	1	0
3	B	2007	DIO	1	0
3	A	2005	DIO	1	0
2	A	3004	SO4	1	0
4	A	4001	MRD	5	0
4	F	4006	MRD	3	0
3	C	2008	DIO	6	0
2	F	3010	SO4	2	0
2	A	3011	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4004	MRD	1	0
3	C	2009	DIO	6	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.