Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 07:27 am GMT

PDB ID	:	5O80
Title	:	Crystal Structure of R67A Mutant of alpha-L-arabinofuranosidase Ara51 from Clostridium thermocellum in complex with L-Arabinofuranose
Authors	:	Lafite, P.; Daniellou, R.
Deposited on	:	2017-06-12
Resolution	:	2.92 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 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:

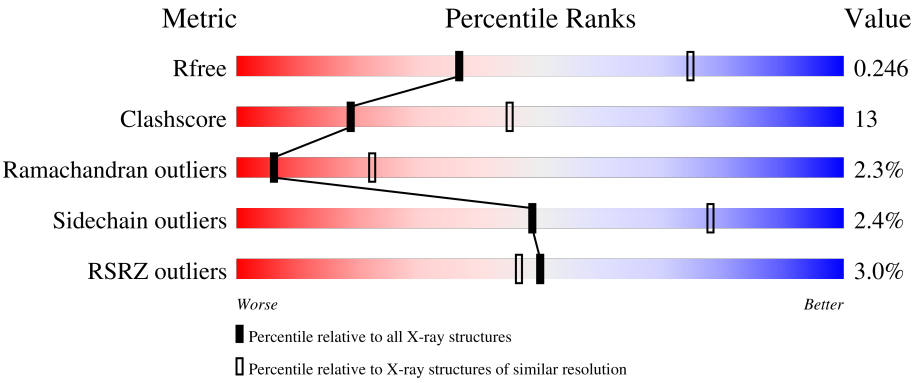
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	501	2% 72% 25%
1	B	501	4% 72% 25%
1	C	501	2% 71% 26%
1	D	501	5% 69% 27%
1	E	501	% 71% 26%

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Mol	Chain	Length	Quality of chain
1	F	501	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DIO	A	601	-	-	X	-
3	DIO	B	601	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23944 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.

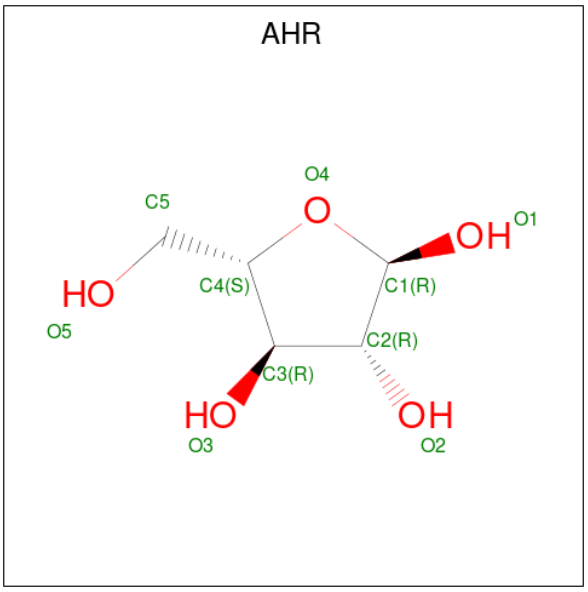
- Molecule 1 is a protein called Intracellular exo-alpha-(1->5)-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	1	0
			3978	2527	675	754	22			
1	B	496	Total	C	N	O	S	0	1	0
			3978	2527	674	755	22			
1	C	496	Total	C	N	O	S	0	1	0
			3962	2518	669	752	23			
1	D	496	Total	C	N	O	S	0	1	0
			3978	2527	674	755	22			
1	E	496	Total	C	N	O	S	0	0	0
			3963	2519	670	752	22			
1	F	496	Total	C	N	O	S	0	1	0
			3977	2527	674	754	22			

There are 6 discrepancies between the modelled and reference sequences:

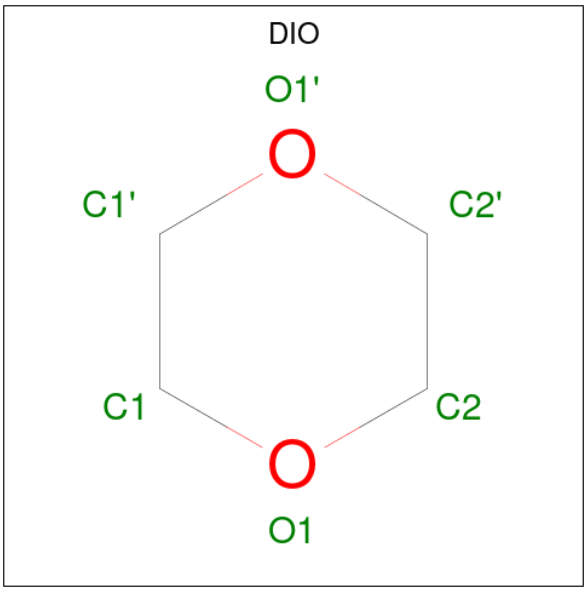
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	ARG	engineered mutation	UNP A3DIH0
B	67	ALA	ARG	engineered mutation	UNP A3DIH0
C	67	ALA	ARG	engineered mutation	UNP A3DIH0
D	67	ALA	ARG	engineered mutation	UNP A3DIH0
E	67	ALA	ARG	engineered mutation	UNP A3DIH0
F	67	ALA	ARG	engineered mutation	UNP A3DIH0

- Molecule 2 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	D	1	Total C O 10 5 5	0	0
2	E	1	Total C O 10 5 5	0	0
2	F	1	Total C O 10 5 5	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	B	1	Total C O 6 4 2	0	0
3	C	1	Total C O 6 4 2	0	0
3	D	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 water.

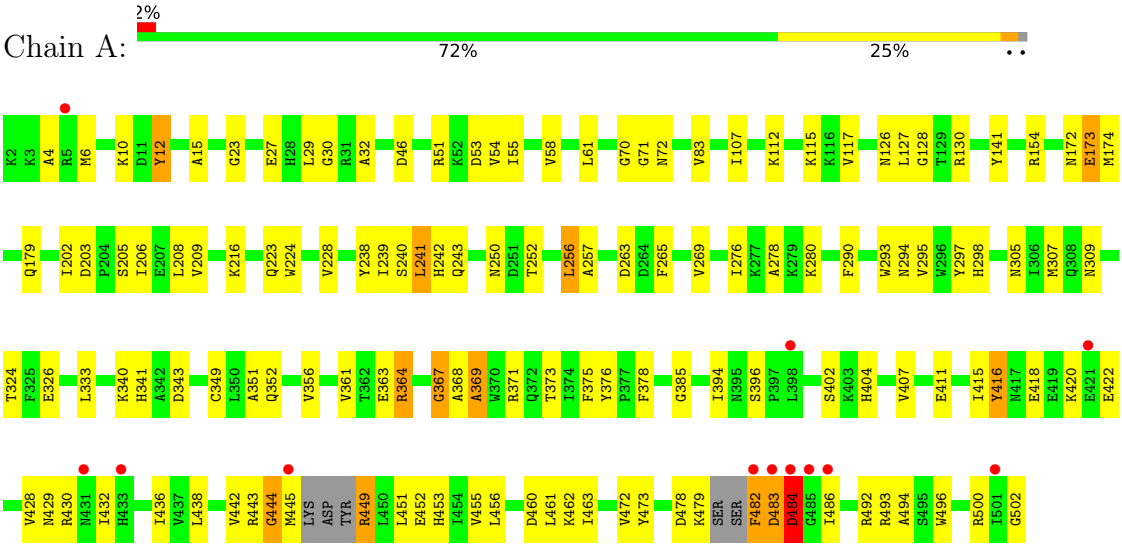
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0
4	D	2	Total O 2 2	0	0
4	E	3	Total O 3 3	0	0
4	F	2	Total O 2 2	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

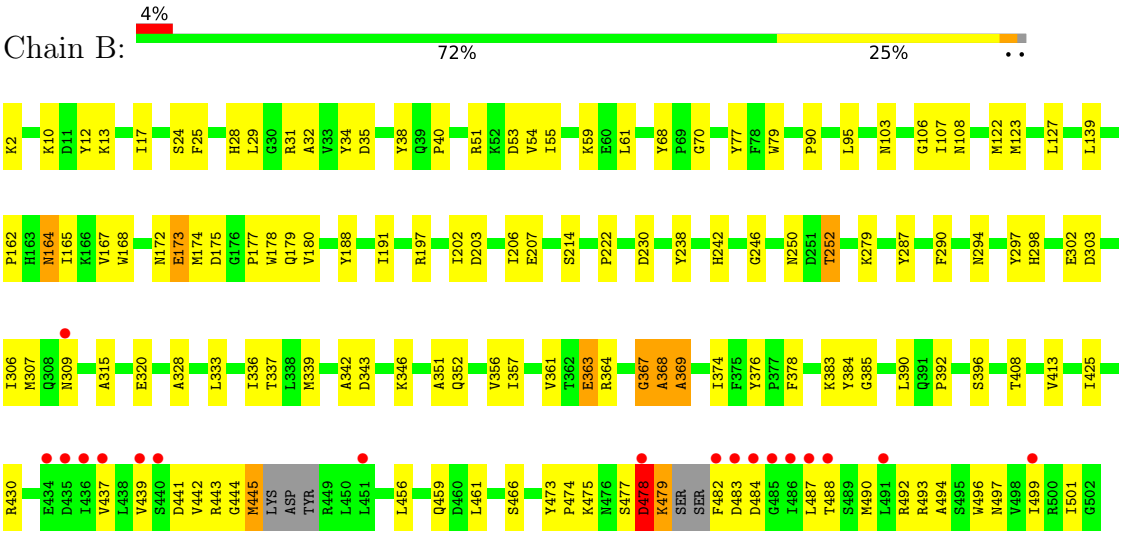
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

Chain A:



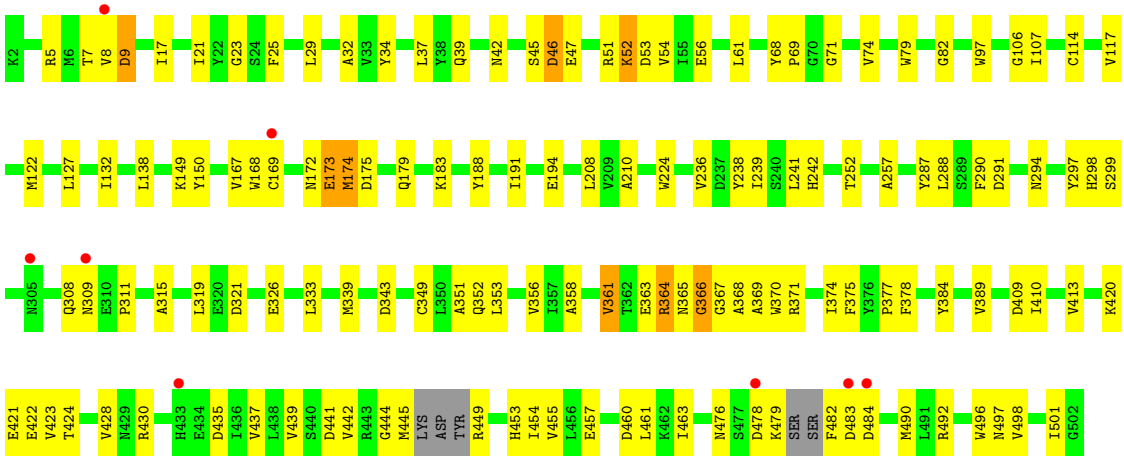
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

Chain B:

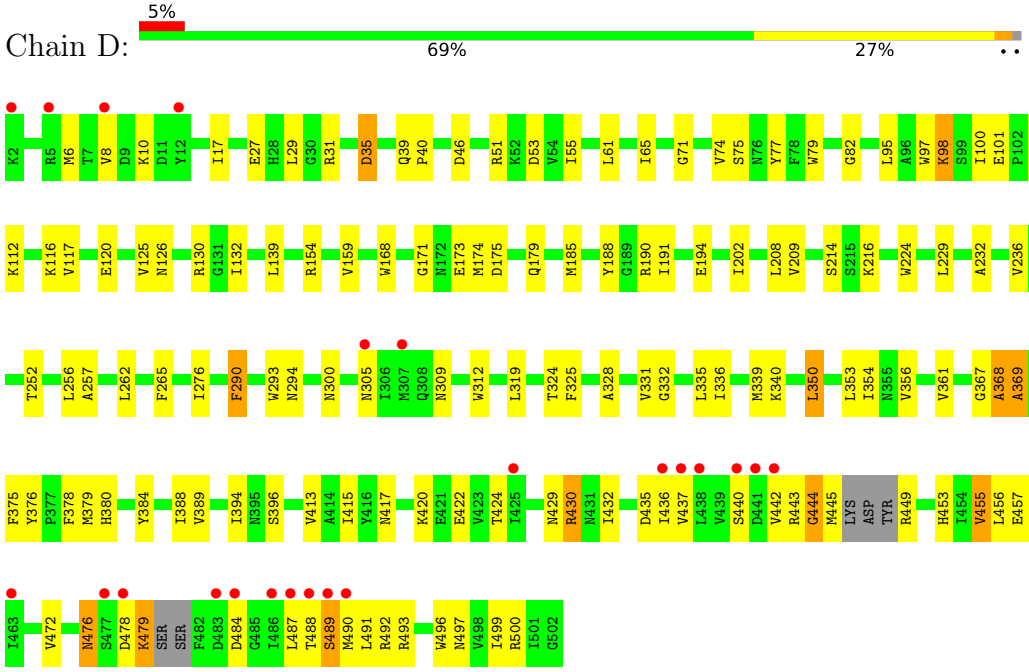


• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

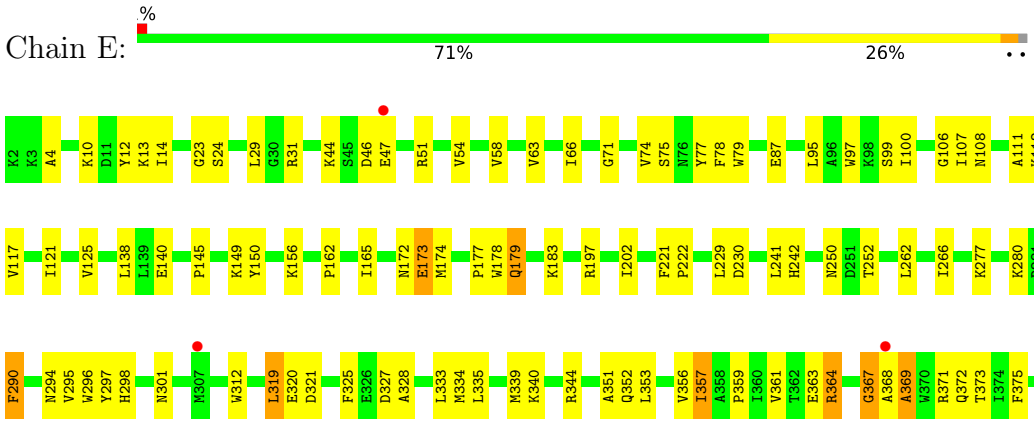
Chain C:

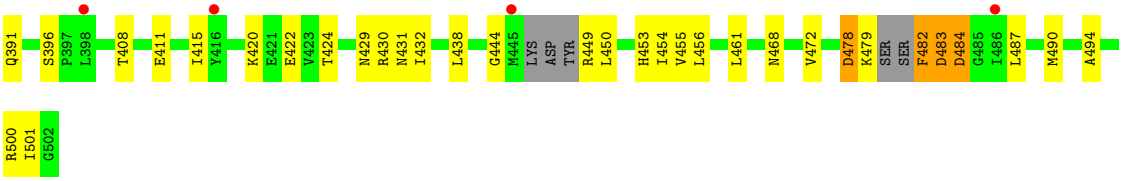


• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

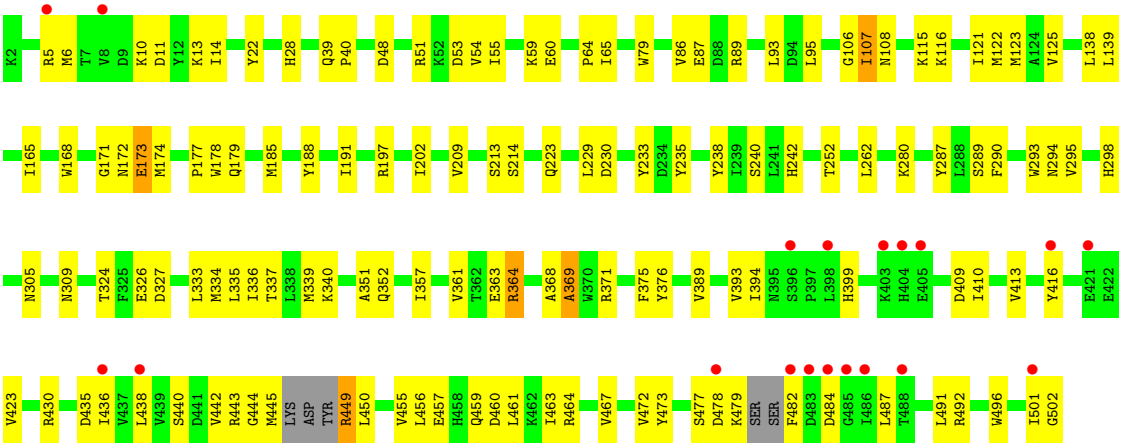


• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase





• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	173.74Å 173.74Å 271.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.92 48.76 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.76-2.92) 99.9 (48.76-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.246 0.179 , 0.246	Depositor DCC
R_{free} test set	4538 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	63.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23944	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.55	0/4068	0.69	0/5509
1	B	0.49	0/4068	0.66	0/5509
1	C	0.54	0/4055	0.67	0/5494
1	D	0.49	0/4068	0.68	0/5509
1	E	0.48	0/4053	0.64	0/5490
1	F	0.50	0/4067	0.64	0/5508
All	All	0.51	0/24379	0.66	0/33019

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3978	0	3869	128	0
1	B	3978	0	3867	102	0
1	C	3962	0	3845	102	0
1	D	3978	0	3867	124	0
1	E	3963	0	3851	93	0
1	F	3977	0	3864	86	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	6	0	8	4	0
3	B	6	0	8	4	0
3	C	6	0	8	2	0
3	D	6	0	8	2	0
3	E	6	0	8	1	0
3	F	6	0	8	3	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
All	All	23944	0	23211	619	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 13.

All (619) 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:240:SER:C	1:A:241:LEU:HD23	1.66	1.15
1:A:240:SER:C	1:A:241:LEU:CD2	2.16	1.14
1:D:256:LEU:O	1:D:430:ARG:NH2	1.83	1.11
1:A:240:SER:O	1:A:241:LEU:HD22	1.51	1.10
1:A:241:LEU:HD11	1:A:269:VAL:HG11	1.13	1.09
1:C:257:ALA:HA	1:C:430:ARG:HH21	1.00	1.08
1:A:223:GLN:NE2	1:B:279:LYS:HE2	1.73	1.03
1:A:241:LEU:HD23	1:A:241:LEU:N	1.77	0.99
1:A:173:GLU:O	1:A:179[B]:GLN:NE2	1.94	0.98
1:A:241:LEU:HD13	1:A:269:VAL:HG21	1.47	0.97
1:A:241:LEU:CD1	1:A:269:VAL:HG21	1.96	0.96
1:E:44:LYS:HD2	1:E:51:ARG:NH2	1.80	0.96
1:A:241:LEU:HD11	1:A:269:VAL:CG1	1.95	0.95
1:A:241:LEU:CD1	1:A:269:VAL:HG11	1.98	0.93
1:C:257:ALA:HA	1:C:430:ARG:NH2	1.83	0.93
1:B:363:GLU:HB2	1:B:367:GLY:HA3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:VAL:O	1:D:335:LEU:HD22	1.72	0.89
1:A:241:LEU:CD2	1:A:241:LEU:N	2.35	0.89
1:B:478:ASP:HA	1:B:479:LYS:HG3	1.58	0.86
1:E:479:LYS:HE2	1:E:490:MET:HG2	1.59	0.85
1:E:385:GLY:HA2	1:E:415:ILE:HD11	1.59	0.84
1:E:478:ASP:HA	1:E:479:LYS:HB3	1.59	0.84
1:C:252:THR:HG21	1:C:461:LEU:HD13	1.58	0.84
1:E:44:LYS:HD2	1:E:51:ARG:HH21	1.43	0.84
1:A:240:SER:O	1:A:241:LEU:CD2	2.23	0.83
1:A:478:ASP:HA	1:A:479:LYS:HB3	1.61	0.82
1:A:240:SER:C	1:A:241:LEU:HD22	1.91	0.82
1:A:263:ASP:OD1	1:A:341:HIS:NE2	2.13	0.82
1:A:223:GLN:HE22	1:B:279:LYS:HE2	1.44	0.81
1:A:452:GLU:OE2	1:A:500:ARG:NH1	2.14	0.81
1:E:432:ILE:HG22	1:E:494:ALA:HB2	1.61	0.80
1:C:435:ASP:HB3	1:C:490:MET:HE3	1.62	0.79
1:D:380:HIS:HD2	1:D:496:TRP:HE1	1.29	0.79
1:E:75:SER:OG	1:E:179:GLN:OE1	1.98	0.79
1:C:363:GLU:O	1:C:364:ARG:CB	2.32	0.78
1:D:39:GLN:OE1	1:D:51:ARG:NH1	2.16	0.78
1:D:51:ARG:HH12	1:D:367:GLY:HA3	1.47	0.78
1:D:75:SER:OG	1:D:179:GLN:NE2	2.16	0.78
1:F:252:THR:HG21	1:F:461:LEU:HD13	1.65	0.78
1:F:14:ILE:HB	1:F:389:VAL:HG23	1.65	0.76
1:C:435:ASP:HB3	1:C:490:MET:CE	2.14	0.76
1:D:437:VAL:HG12	1:D:490:MET:HG2	1.68	0.76
1:F:242:HIS:CE1	3:F:601:DIO:H2'2	2.20	0.76
1:A:407:VAL:HG13	1:A:430:ARG:HH21	1.50	0.76
1:F:340:LYS:HG3	1:F:413:VAL:HG21	1.68	0.76
1:D:325:PHE:HE1	1:D:456:LEU:CD2	2.00	0.75
1:C:420:LYS:HB2	1:C:422:GLU:HG3	1.66	0.75
1:F:361:VAL:O	1:F:369:ALA:HA	1.87	0.75
1:D:340:LYS:HG2	1:D:413:VAL:HG11	1.67	0.75
1:A:172:ASN:OD1	3:A:601:DIO:H1'2	1.87	0.74
1:B:408:THR:HG23	1:B:430:ARG:HH21	1.53	0.74
1:E:325:PHE:HA	1:E:373:THR:HG21	1.67	0.73
1:D:432:ILE:HD12	1:D:432:ILE:H	1.54	0.73
1:C:257:ALA:CA	1:C:430:ARG:HH21	1.92	0.73
1:D:35:ASP:HA	1:D:39:GLN:HG2	1.71	0.72
1:E:252:THR:HG21	1:E:461:LEU:HD13	1.70	0.72
1:B:252:THR:HG21	1:B:461:LEU:HD13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASN:O	1:B:174:MET:HG3	1.89	0.72
1:E:363:GLU:O	1:E:364:ARG:HB2	1.89	0.72
1:A:29:LEU:HD13	1:A:356:VAL:HG11	1.72	0.71
1:D:479:LYS:CD	1:D:489:SER:HA	2.20	0.71
1:A:128:GLY:HA2	1:A:174:MET:CE	2.21	0.71
1:D:252:THR:O	1:D:256:LEU:HD12	1.89	0.71
1:D:336:ILE:HA	1:D:339:MET:HE2	1.73	0.71
1:D:324:THR:O	1:D:373:THR:HG21	1.90	0.70
1:D:51:ARG:HH22	1:D:368:ALA:H	1.39	0.70
1:A:385:GLY:HA2	1:A:415:ILE:HD11	1.73	0.70
1:D:29:LEU:HD13	1:D:356:VAL:HG11	1.74	0.70
1:A:71:GLY:H	3:A:601:DIO:H1'2	1.56	0.70
1:A:128:GLY:HA2	1:A:174:MET:HE2	1.72	0.69
1:F:363:GLU:O	1:F:364:ARG:HB2	1.92	0.69
1:B:51:ARG:NH2	1:B:367:GLY:O	2.26	0.69
1:D:185:MET:HG2	1:D:224:TRP:HA	1.75	0.68
1:A:12:TYR:HH	1:B:12:TYR:HE2	1.39	0.68
1:E:100:ILE:HD11	1:E:312:TRP:HB3	1.76	0.67
1:F:399:HIS:ND1	1:F:409:ASP:OD1	2.24	0.67
1:D:376:TYR:HD1	1:D:379:MET:HE2	1.60	0.67
1:F:449:ARG:N	1:F:482:PHE:HE2	1.92	0.67
1:B:444:GLY:HA3	1:B:445:MET:HB3	1.76	0.67
1:C:361:VAL:HG21	1:C:370:TRP:CZ2	2.29	0.67
1:A:324:THR:HG23	1:A:462:LYS:HA	1.77	0.66
1:F:172:ASN:O	1:F:174:MET:HG3	1.96	0.66
1:D:35:ASP:HB2	1:D:39:GLN:HE21	1.59	0.66
1:D:444:GLY:HA3	1:D:445:MET:C	2.15	0.66
1:C:361:VAL:CG2	1:C:370:TRP:CE2	2.79	0.66
1:A:361:VAL:O	1:A:369:ALA:HA	1.95	0.66
1:E:31:ARG:NH1	1:E:320:GLU:OE2	2.26	0.66
1:A:172:ASN:OD1	3:A:601:DIO:C1'	2.44	0.65
1:F:337:THR:HA	1:F:340:LYS:HE3	1.79	0.65
1:D:305:ASN:N	1:D:305:ASN:OD1	2.29	0.65
1:F:449:ARG:NH2	1:F:502:GLY:HA2	2.11	0.65
1:A:240:SER:CA	1:A:241:LEU:HD23	2.27	0.65
1:D:168:TRP:HB2	1:D:208:LEU:HD23	1.78	0.64
1:D:331:VAL:HG12	1:D:335:LEU:HD21	1.77	0.64
1:F:444:GLY:HA3	1:F:445:MET:C	2.17	0.64
1:D:46:ASP:OD2	1:D:116:LYS:NZ	2.29	0.64
1:A:6:MET:HB3	1:A:394:ILE:HD13	1.78	0.64
1:E:361:VAL:O	1:E:369:ALA:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LYS:HA	1:E:390:LEU:HD22	1.80	0.63
1:F:48:ASP:OD2	1:F:116:LYS:NZ	2.31	0.63
1:E:77:TYR:CE2	1:E:79:TRP:HA	2.34	0.63
1:A:445:MET:HB3	1:A:449:ARG:NH1	2.14	0.63
1:D:456:LEU:HD23	1:D:456:LEU:C	2.18	0.63
1:B:53:ASP:N	1:B:53:ASP:OD1	2.32	0.62
1:D:173[B]:GLU:HG3	1:D:242:HIS:CE1	2.34	0.62
1:D:332:GLY:HA2	1:D:335:LEU:HD23	1.81	0.62
1:B:478:ASP:HA	1:B:479:LYS:CG	2.27	0.62
1:A:252:THR:OG1	1:A:326:GLU:OE1	2.18	0.62
1:D:331:VAL:O	1:D:335:LEU:CD2	2.45	0.62
1:A:451:LEU:HD11	1:A:502:GLY:HA3	1.81	0.62
1:C:5:ARG:HA	1:C:439:VAL:HG23	1.81	0.62
1:D:458:HIS:ND1	1:D:459:GLN:N	2.48	0.61
1:A:445:MET:HB3	1:A:449:ARG:HH12	1.64	0.61
1:C:172:ASN:ND2	1:C:179:GLN:OE1	2.33	0.61
1:C:478:ASP:HA	1:C:479:LYS:HB3	1.82	0.61
1:C:188:TYR:HA	1:C:191:ILE:HG22	1.82	0.61
1:A:241:LEU:CD1	1:A:269:VAL:CG2	2.77	0.61
1:F:106:GLY:O	1:F:108:ASN:N	2.34	0.61
1:C:34:TYR:HB2	1:C:315:ALA:HB2	1.83	0.61
1:B:328:ALA:HA	1:B:374:ILE:HG22	1.80	0.61
1:E:173:GLU:OE2	1:E:173:GLU:N	2.31	0.61
1:B:459:GLN:HG3	1:B:492:ARG:NH2	2.16	0.61
1:E:449:ARG:O	1:E:449:ARG:HG2	2.00	0.60
1:C:291:ASP:OD2	3:C:601:DIO:H2'1	2.01	0.60
1:D:242:HIS:CE1	3:D:601:DIO:H11	2.36	0.60
1:F:340:LYS:HG3	1:F:413:VAL:CG2	2.30	0.60
1:D:476:ASN:C	1:D:476:ASN:HD22	2.04	0.60
1:E:125:VAL:HG12	1:E:138:LEU:HD23	1.83	0.60
1:D:340:LYS:HG2	1:D:413:VAL:CG1	2.32	0.60
1:A:478:ASP:CA	1:A:479:LYS:HB3	2.32	0.60
1:B:172:ASN:ND2	3:B:601:DIO:H21	2.17	0.60
1:A:12:TYR:OH	1:B:12:TYR:HE2	1.85	0.60
1:B:51:ARG:O	1:B:54:VAL:HG22	2.02	0.60
1:D:455:VAL:HG13	1:D:457:GLU:HG2	1.83	0.60
1:F:298:HIS:HE1	1:F:327:ASP:OD2	1.85	0.60
1:F:305:ASN:O	1:F:309:ASN:HB2	2.02	0.59
1:B:482:PHE:HB2	1:B:487:LEU:HD12	1.84	0.59
1:A:10:LYS:HG3	1:A:416:TYR:HE2	1.67	0.59
1:A:340:LYS:NZ	1:A:411:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:SER:HB2	1:D:487:LEU:HB3	1.85	0.59
1:E:242:HIS:NE2	3:E:601:DIO:H2'2	2.18	0.59
1:F:209:VAL:HG13	1:F:238:TYR:HB2	1.84	0.59
1:D:257:ALA:HA	1:D:430:ARG:NH2	2.18	0.58
1:A:252:THR:HG21	1:A:461:LEU:HD13	1.83	0.58
1:C:483:ASP:OD1	1:C:484:ASP:N	2.35	0.58
1:D:479:LYS:HD3	1:D:489:SER:HA	1.85	0.58
1:C:51:ARG:HH12	1:C:367:GLY:HA2	1.68	0.58
1:C:23:GLY:O	1:C:349:CYS:HA	2.03	0.58
1:F:335:LEU:O	1:F:339:MET:HG2	2.04	0.58
1:D:458:HIS:CE1	1:D:460:ASP:H	2.22	0.58
1:E:277:LYS:NZ	1:E:282:SER:O	2.37	0.58
1:E:456:LEU:HD22	1:E:472:VAL:HG12	1.86	0.58
1:F:185:MET:SD	1:F:223:GLN:HG2	2.44	0.58
1:B:302:GLU:O	1:B:306:ILE:HG13	2.04	0.58
1:F:294:ASN:OD1	1:F:295:VAL:N	2.36	0.57
1:A:202:ILE:HG12	1:D:95:LEU:HD22	1.86	0.57
1:D:325:PHE:HE1	1:D:456:LEU:HD22	1.70	0.57
1:C:168:TRP:HB2	1:C:208:LEU:HD23	1.86	0.57
1:C:361:VAL:HG22	1:C:370:TRP:CE2	2.40	0.57
1:A:173:GLU:O	1:A:179[B]:GLN:HG2	2.05	0.57
1:A:324:THR:HG22	1:A:326:GLU:H	1.69	0.57
1:C:52:LYS:HD2	1:C:52:LYS:O	2.03	0.57
1:A:173:GLU:CD	1:A:173:GLU:H	2.07	0.56
1:A:444:GLY:HA2	1:A:445:MET:HB2	1.87	0.56
1:B:483:ASP:OD1	1:B:484:ASP:N	2.36	0.56
1:C:363:GLU:O	1:C:364:ARG:HB3	2.05	0.56
1:E:87:GLU:CD	1:E:87:GLU:H	2.09	0.56
1:C:454:ILE:HB	1:C:498:VAL:HG22	1.86	0.56
1:C:333:LEU:HG	1:C:428:VAL:HG21	1.87	0.56
1:E:58:VAL:HG22	1:E:353:LEU:HD11	1.88	0.56
1:F:455:VAL:HG12	1:F:457:GLU:HG2	1.87	0.56
1:B:197:ARG:HD3	1:E:177:PRO:O	2.06	0.56
1:C:361:VAL:HG21	1:C:370:TRP:CE2	2.41	0.56
1:A:127:LEU:O	1:A:174:MET:HE2	2.06	0.55
1:C:82:GLY:O	1:C:106:GLY:HA3	2.06	0.55
1:B:106:GLY:O	1:B:108:ASN:N	2.39	0.55
1:C:437:VAL:HG22	1:C:490:MET:SD	2.47	0.55
1:E:328:ALA:HB2	1:E:373:THR:HG22	1.89	0.55
1:F:409:ASP:O	1:F:410:ILE:HD12	2.07	0.55
1:D:479:LYS:HD2	1:D:489:SER:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:GLN:OE1	1:F:51:ARG:NH1	2.40	0.55
1:F:442:VAL:O	1:F:444:GLY:N	2.40	0.55
1:C:17:ILE:HD12	1:C:21:ILE:HD11	1.89	0.55
1:A:128:GLY:CA	1:A:174:MET:CE	2.85	0.55
1:A:206:ILE:HD12	1:A:208:LEU:HD21	1.89	0.55
1:C:51:ARG:O	1:C:54:VAL:HG22	2.07	0.55
1:D:8:VAL:HG22	1:D:442:VAL:HA	1.89	0.55
1:D:188:TYR:HA	1:D:191:ILE:HG22	1.89	0.54
1:E:23:GLY:HA2	1:E:63:VAL:HG13	1.89	0.54
1:D:479:LYS:NZ	1:D:479:LYS:HB3	2.22	0.54
1:E:106:GLY:O	1:E:108:ASN:N	2.40	0.54
1:A:252:THR:O	1:A:256:LEU:HD12	2.07	0.54
1:B:333:LEU:O	1:B:337:THR:HG23	2.07	0.54
1:B:392:PRO:HG3	1:B:413:VAL:HG23	1.90	0.54
1:F:376:TYR:CE2	1:F:473:TYR:HA	2.42	0.54
1:A:10:LYS:HG3	1:A:416:TYR:CE2	2.42	0.54
1:C:363:GLU:O	1:C:364:ARG:HB2	2.07	0.54
1:B:17:ILE:HD13	1:B:385:GLY:O	2.08	0.54
1:B:175:ASP:OD1	1:B:214:SER:OG	2.23	0.54
1:C:308:GLN:O	1:C:309:ASN:ND2	2.41	0.54
1:A:83:VAL:HG13	1:A:107:ILE:HD13	1.89	0.54
1:B:336:ILE:HA	1:B:339:MET:HE2	1.90	0.54
1:B:437:VAL:HG23	1:B:490:MET:HB2	1.90	0.54
1:D:417:ASN:HD22	1:D:420:LYS:HE2	1.71	0.54
1:E:262:LEU:HD22	1:E:334:MET:HG2	1.90	0.54
1:A:429:ASN:HD21	1:A:436:ILE:HG13	1.72	0.53
1:C:479:LYS:HE3	1:C:490:MET:HG2	1.89	0.53
1:D:82:GLY:O	1:D:106:GLY:HA3	2.07	0.53
1:D:429:ASN:ND2	1:D:436:ILE:HG22	2.23	0.53
1:D:478:ASP:HB3	1:D:479:LYS:HG3	1.89	0.53
1:F:450:LEU:HD12	1:F:501:ILE:HG22	1.90	0.53
1:B:202:ILE:HG12	1:E:95:LEU:HD22	1.90	0.53
1:E:29:LEU:HD13	1:E:356:VAL:HG11	1.90	0.53
1:A:278:ALA:HB3	1:B:222:PRO:HG3	1.90	0.53
1:E:478:ASP:HB3	1:E:479:LYS:C	2.28	0.53
1:F:242:HIS:HE1	3:F:601:DIO:H2'2	1.73	0.53
1:A:112:LYS:HA	1:A:115:LYS:HG3	1.91	0.53
1:E:335:LEU:O	1:E:339:MET:HG2	2.08	0.53
1:C:210:ALA:HB2	1:C:236:VAL:HG11	1.91	0.53
1:B:487:LEU:HD13	1:B:501:ILE:HD11	1.90	0.53
1:B:361:VAL:O	1:B:369:ALA:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASP:HB3	1:D:224:TRP:CZ3	2.44	0.52
1:E:298:HIS:HE1	1:E:327:ASP:OD2	1.93	0.52
1:E:97:TRP:O	1:E:99:SER:OG	2.23	0.52
1:E:408:THR:OG1	1:E:430:ARG:NH2	2.41	0.52
1:E:411:GLU:OE1	1:E:430:ARG:NH2	2.42	0.52
1:A:12:TYR:HE2	1:B:12:TYR:HD2	1.58	0.52
1:B:167:VAL:HG22	1:B:207:GLU:HB2	1.91	0.52
1:B:51:ARG:NH2	1:B:368:ALA:O	2.37	0.52
1:C:51:ARG:NH2	1:C:53:ASP:OD2	2.26	0.52
1:B:302:GLU:O	1:B:302:GLU:HG3	2.10	0.52
1:D:6:MET:SD	1:D:394:ILE:HD11	2.50	0.52
1:D:479:LYS:NZ	1:D:479:LYS:CB	2.73	0.52
1:B:473:TYR:CZ	1:B:475:LYS:HE3	2.44	0.52
1:C:127:LEU:O	1:C:183:LYS:HE2	2.10	0.52
1:A:241:LEU:HD11	1:A:269:VAL:CB	2.39	0.52
1:E:149:LYS:HG2	1:E:150:TYR:CD1	2.45	0.52
1:F:177:PRO:HD2	1:F:178:TRP:CZ3	2.45	0.52
1:A:141:TYR:O	1:A:154:ARG:HD3	2.10	0.52
1:A:172:ASN:OD1	3:A:601:DIO:O1'	2.28	0.52
1:D:61:LEU:HD22	1:D:378:PHE:HD2	1.74	0.52
1:E:71:GLY:O	1:E:74:VAL:HG12	2.10	0.52
1:A:250:ASN:OD1	1:A:462:LYS:NZ	2.28	0.51
1:D:242:HIS:HE1	3:D:601:DIO:H11	1.76	0.51
1:A:61:LEU:HD22	1:A:378:PHE:HD1	1.74	0.51
1:D:100:ILE:HD12	1:D:312:TRP:HB3	1.92	0.51
1:D:55:ILE:HG23	1:D:117:VAL:HG12	1.91	0.51
1:E:424:THR:HG23	1:E:500:ARG:HG2	1.92	0.51
1:B:28:HIS:NE2	1:B:68:TYR:OH	2.33	0.51
1:B:29:LEU:HD13	1:B:356:VAL:HG11	1.92	0.51
1:B:439:VAL:HG12	1:B:488:THR:HG23	1.93	0.51
1:C:444:GLY:HA3	1:C:445:MET:HB3	1.93	0.51
1:F:79:TRP:CG	1:F:138:LEU:HD13	2.44	0.51
1:E:450:LEU:HB2	1:E:482:PHE:HB2	1.93	0.51
1:F:438:LEU:HB2	1:F:491:LEU:HD11	1.92	0.51
1:F:479:LYS:HZ1	1:F:482:PHE:N	2.08	0.51
1:A:324:THR:HG22	1:A:326:GLU:N	2.25	0.51
1:E:328:ALA:CB	1:E:373:THR:HG22	2.40	0.51
1:A:492:ARG:HG2	1:A:493:ARG:O	2.11	0.51
1:F:121:ILE:HG21	1:F:123:MET:HE1	1.93	0.51
1:C:7:THR:HG22	1:C:441:ASP:HB3	1.93	0.51
1:E:449:ARG:N	1:E:482:PHE:CE2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ILE:HD12	1:D:437:VAL:H	1.76	0.51
1:D:17:ILE:HG13	1:D:389:VAL:HG23	1.92	0.50
1:D:107:ILE:H	1:D:107:ILE:HD12	1.76	0.50
1:E:262:LEU:O	1:E:266:ILE:HG13	2.10	0.50
1:A:478:ASP:HB3	1:A:479:LYS:C	2.31	0.50
1:E:422:GLU:HA	1:E:501:ILE:O	2.12	0.50
1:E:296:TRP:CZ2	1:E:319:LEU:HD21	2.46	0.50
1:D:361:VAL:O	1:D:369:ALA:HA	2.11	0.50
1:F:87:GLU:H	1:F:87:GLU:CD	2.12	0.50
1:D:139:LEU:HD23	1:D:202:ILE:HB	1.94	0.50
1:E:51:ARG:O	1:E:54:VAL:HG22	2.12	0.49
1:F:6:MET:HB2	1:F:394:ILE:HD12	1.93	0.49
1:B:376:TYR:CE2	1:B:474:PRO:HD3	2.47	0.49
1:C:39:GLN:HG3	1:C:51:ARG:HG2	1.93	0.49
1:D:77:TYR:CE2	1:D:79:TRP:HA	2.47	0.49
1:D:492:ARG:HG3	1:D:493:ARG:N	2.27	0.49
1:A:15:ALA:HB2	1:A:343:ASP:HB3	1.94	0.49
1:C:361:VAL:CG2	1:C:370:TRP:NE1	2.75	0.49
1:B:174:MET:HE1	1:B:188:TYR:CE1	2.47	0.49
1:C:241:LEU:O	1:C:242:HIS:HD2	1.95	0.49
1:B:139:LEU:HD23	1:B:202:ILE:HB	1.92	0.49
1:C:53:ASP:OD1	1:C:53:ASP:N	2.44	0.49
1:F:6:MET:O	1:F:440:SER:HA	2.13	0.49
1:F:393:VAL:C	1:F:394:ILE:HD13	2.32	0.49
1:F:449:ARG:N	1:F:482:PHE:CE2	2.77	0.49
1:A:12:TYR:HE2	1:B:12:TYR:CD2	2.29	0.49
1:B:70:GLY:O	3:B:601:DIO:H2'2	2.12	0.49
1:C:29:LEU:HG	1:C:97:TRP:CE2	2.48	0.49
1:F:371:ARG:HG2	1:F:375:PHE:CG	2.47	0.49
1:A:107:ILE:HD12	1:A:107:ILE:H	1.78	0.49
1:C:435:ASP:HB3	1:C:490:MET:HE1	1.93	0.49
1:E:389:VAL:HA	1:E:415:ILE:HG22	1.95	0.49
1:C:132:ILE:HD11	1:C:194:GLU:HB3	1.95	0.49
1:C:455:VAL:HG11	1:C:457:GLU:OE1	2.12	0.49
1:A:453:HIS:CD2	1:A:455:VAL:HG23	2.48	0.48
1:C:29:LEU:HD13	1:C:356:VAL:HG11	1.95	0.48
1:D:29:LEU:HD21	1:D:319:LEU:HD13	1.95	0.48
1:D:331:VAL:HG12	1:D:335:LEU:CD2	2.41	0.48
1:E:145:PRO:HA	1:E:162:PRO:HG3	1.96	0.48
1:A:442:VAL:O	1:A:444:GLY:N	2.47	0.48
1:B:383:LYS:HD3	1:B:384:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169[B]:CYS:SG	3:C:601:DIO:H22	2.53	0.48
1:C:298:HIS:HB2	1:C:321:ASP:CG	2.34	0.48
1:C:175:ASP:HB3	1:C:224:TRP:CZ3	2.47	0.48
1:E:241:LEU:O	1:E:242:HIS:HD2	1.97	0.48
1:E:298:HIS:HB2	1:E:321:ASP:CG	2.33	0.48
1:D:125:VAL:O	1:D:171:GLY:HA2	2.14	0.48
1:E:450:LEU:C	1:E:450:LEU:HD23	2.34	0.48
1:E:483:ASP:OD1	1:E:484:ASP:N	2.46	0.48
1:F:376:TYR:HB3	1:F:456:LEU:HD11	1.96	0.48
1:F:60:GLU:OE1	1:F:371:ARG:NH2	2.46	0.48
1:B:203:ASP:O	1:B:206:ILE:HG12	2.13	0.48
1:D:457:GLU:OE2	1:D:492:ARG:HB3	2.14	0.48
1:F:467:VAL:HG22	1:F:467:VAL:O	2.13	0.48
1:A:371:ARG:HD3	1:A:375:PHE:CD1	2.49	0.48
1:D:214:SER:O	1:D:242:HIS:HB2	2.14	0.48
1:E:241:LEU:HD11	1:E:288:LEU:HG	1.96	0.48
1:A:239:ILE:HG23	1:A:241:LEU:HD21	1.95	0.47
1:C:241:LEU:HD11	1:C:288:LEU:HG	1.95	0.47
1:C:371:ARG:HD3	1:C:375:PHE:CD1	2.49	0.47
1:E:4:ALA:O	1:E:438:LEU:HD12	2.14	0.47
1:A:239:ILE:HG23	1:A:239:ILE:O	2.14	0.47
1:D:256:LEU:O	1:D:430:ARG:CZ	2.58	0.47
1:A:483:ASP:CG	1:A:484:ASP:N	2.67	0.47
1:B:408:THR:HG23	1:B:430:ARG:NH2	2.27	0.47
1:D:35:ASP:CB	1:D:39:GLN:HE21	2.27	0.47
1:D:491:LEU:HD22	1:D:497:ASN:CG	2.34	0.47
1:F:333:LEU:HD22	1:F:430:ARG:HH11	1.78	0.47
1:B:34:TYR:HB2	1:B:315:ALA:HB2	1.96	0.47
1:C:122:MET:HG3	1:C:167:VAL:HG23	1.96	0.47
1:A:449:ARG:N	1:A:482:PHE:CD2	2.83	0.47
1:B:376:TYR:CZ	1:B:474:PRO:HD3	2.49	0.47
1:C:51:ARG:HH12	1:C:367:GLY:CA	2.27	0.47
1:D:112:LYS:HE3	1:D:112:LYS:HB2	1.60	0.47
1:E:420:LYS:O	1:E:422:GLU:HG3	2.14	0.47
1:F:336:ILE:HG22	1:F:340:LYS:HE2	1.96	0.47
1:A:243:GLN:O	1:A:293:TRP:HA	2.15	0.47
1:B:351:ALA:HA	1:B:352:GLN:HA	1.60	0.47
1:C:8:VAL:HG22	1:C:442:VAL:HA	1.97	0.47
1:C:333:LEU:HD11	1:C:430:ARG:HG2	1.96	0.47
1:C:8:VAL:O	1:C:9:ASP:HB2	2.15	0.47
1:E:172:ASN:O	1:E:174:MET:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ILE:HD13	1:F:436:ILE:HD12	1.97	0.47
1:F:460:ASP:HB3	1:F:463:ILE:HB	1.96	0.47
1:C:17:ILE:HG12	1:C:389:VAL:HG23	1.97	0.47
1:E:487:LEU:HD13	1:E:501:ILE:HD11	1.97	0.47
1:B:51:ARG:NH1	1:B:53:ASP:OD2	2.35	0.47
1:B:230:ASP:OD2	1:B:279:LYS:HE3	2.15	0.47
1:E:24:SER:O	1:E:66:ILE:HA	2.16	0.46
1:F:293:TRP:O	1:F:294:ASN:HB2	2.14	0.46
1:B:51:ARG:NH1	1:B:53:ASP:OD1	2.48	0.46
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.77	0.46
1:A:460:ASP:HB3	1:A:463:ILE:HB	1.96	0.46
1:D:336:ILE:O	1:D:340:LYS:HG3	2.15	0.46
1:E:140:GLU:HG3	1:F:93:LEU:HD11	1.97	0.46
1:F:22:TYR:O	1:F:64:PRO:HD2	2.16	0.46
1:F:86:VAL:HA	1:F:89:ARG:HG3	1.97	0.46
1:F:197:ARG:NH1	1:F:235:TYR:OH	2.48	0.46
1:A:363:GLU:O	1:A:364:ARG:HB2	2.16	0.46
1:C:173:GLU:CD	1:C:173:GLU:H	2.19	0.46
1:A:224:TRP:O	1:A:228:VAL:HG23	2.15	0.46
1:B:459:GLN:HG3	1:B:492:ARG:HH22	1.81	0.46
1:D:458:HIS:ND1	1:D:460:ASP:N	2.54	0.46
1:F:55:ILE:O	1:F:59:LYS:HG3	2.16	0.46
1:F:123:MET:HE2	1:F:165:ILE:HD13	1.98	0.46
1:D:262:LEU:HD11	1:D:290:PHE:CE2	2.51	0.46
1:D:380:HIS:CD2	1:D:496:TRP:HE1	2.20	0.46
1:D:442:VAL:O	1:D:444:GLY:N	2.44	0.46
1:E:371:ARG:HD3	1:E:375:PHE:CD1	2.51	0.46
1:F:53:ASP:OD1	1:F:53:ASP:N	2.49	0.46
1:D:27:GLU:HG2	1:D:29:LEU:HB2	1.97	0.46
1:D:154:ARG:HD2	1:D:159:VAL:O	2.16	0.46
1:C:384:TYR:HB3	1:C:424:THR:HG21	1.98	0.46
1:D:243:GLN:O	1:D:293:TRP:HA	2.16	0.46
1:D:417:ASN:ND2	1:D:420:LYS:HE2	2.31	0.46
1:A:324:THR:CG2	1:A:462:LYS:HA	2.46	0.45
1:E:351:ALA:HA	1:E:352:GLN:HA	1.56	0.45
1:A:29:LEU:HD23	1:A:30:GLY:N	2.31	0.45
1:B:90:PRO:O	1:B:103:ASN:ND2	2.46	0.45
1:B:174:MET:CE	1:B:188:TYR:CD1	2.99	0.45
1:A:209:VAL:HG13	1:A:238:TYR:HB2	1.98	0.45
1:A:371:ARG:HD3	1:A:375:PHE:CE1	2.51	0.45
1:C:453:HIS:ND1	1:C:453:HIS:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:CYS:HA	1:C:117:VAL:HG22	1.99	0.45
1:C:299:SER:OG	1:C:321:ASP:OD1	2.30	0.45
1:E:51:ARG:NH1	1:E:367:GLY:O	2.50	0.45
1:B:343:ASP:OD1	1:B:343:ASP:N	2.50	0.45
1:C:29:LEU:HD21	1:C:319:LEU:HD13	1.97	0.45
1:F:336:ILE:HG23	1:F:413:VAL:HG23	1.98	0.45
1:A:373:THR:HG22	1:A:472:VAL:HB	1.99	0.45
1:C:449:ARG:N	1:C:482:PHE:HE2	2.13	0.45
1:D:132:ILE:HD11	1:D:194:GLU:HB3	1.98	0.45
1:D:216:LYS:HB3	1:D:265:PHE:CE1	2.52	0.45
1:F:188:TYR:HA	1:F:191:ILE:HG22	1.99	0.45
1:B:461:LEU:HD21	1:B:494:ALA:HB1	1.99	0.45
1:B:492:ARG:HG3	1:B:493:ARG:N	2.30	0.45
1:B:425:ILE:HG23	1:B:499:ILE:HB	1.99	0.45
1:C:68:TYR:CD1	1:C:69:PRO:HA	2.52	0.45
1:D:53:ASP:OD1	1:D:53:ASP:N	2.50	0.45
1:B:174:MET:HE3	1:B:188:TYR:CD1	2.52	0.45
1:B:294:ASN:ND2	1:B:357:ILE:O	2.50	0.45
1:E:51:ARG:HB2	1:E:54:VAL:HG22	1.98	0.45
1:A:58:VAL:CG2	1:A:117:VAL:HB	2.47	0.44
1:B:172:ASN:O	1:B:173[A]:GLU:C	2.55	0.44
1:B:383:LYS:HD3	1:B:384:TYR:CZ	2.52	0.44
1:C:498:VAL:HG23	1:C:498:VAL:O	2.16	0.44
1:E:359:PRO:HA	1:E:372:GLN:HB2	1.99	0.44
1:F:351:ALA:HA	1:F:352:GLN:HA	1.63	0.44
1:A:53:ASP:OD1	1:A:53:ASP:N	2.47	0.44
1:B:24:SER:OG	1:B:25:PHE:N	2.49	0.44
1:F:238:TYR:HA	1:F:287:TYR:O	2.17	0.44
1:C:423:VAL:HG12	1:C:423:VAL:O	2.17	0.44
1:F:242:HIS:NE2	3:F:601:DIO:H2'2	2.31	0.44
1:F:455:VAL:HG21	1:F:478:ASP:OD2	2.18	0.44
1:A:4:ALA:O	1:A:438:LEU:HA	2.18	0.44
1:A:51:ARG:HB2	1:A:54:VAL:HG12	2.00	0.44
1:C:42:ASN:HB3	1:C:45:SER:OG	2.16	0.44
1:D:35:ASP:HB2	1:D:39:GLN:NE2	2.31	0.44
1:D:65:ILE:HA	1:D:120:GLU:O	2.18	0.44
1:E:344:ARG:HA	1:E:344:ARG:HD2	1.72	0.44
1:B:162:PRO:HG2	1:B:164:ASN:OD1	2.17	0.44
1:B:477:SER:O	1:B:478:ASP:HB2	2.17	0.44
1:D:71:GLY:O	1:D:74:VAL:HG12	2.17	0.44
1:D:293:TRP:O	1:D:294:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:GLU:CD	1:F:371:ARG:HH21	2.21	0.44
1:F:368:ALA:O	1:F:369:ALA:HB3	2.18	0.44
1:E:368:ALA:O	1:E:369:ALA:HB3	2.17	0.44
1:E:371:ARG:HD3	1:E:375:PHE:CE1	2.52	0.44
1:F:65:ILE:HD11	1:F:122:MET:HB2	2.00	0.44
1:F:262:LEU:HD22	1:F:334:MET:HG2	2.00	0.44
1:A:416:TYR:CE1	1:A:418:GLU:HA	2.52	0.44
1:A:432:ILE:HG22	1:A:494:ALA:HB2	1.99	0.44
1:D:328:ALA:HB2	1:D:373:THR:HG23	2.00	0.44
1:F:139:LEU:HA	1:F:168:TRP:CH2	2.53	0.44
1:A:12:TYR:CZ	1:B:12:TYR:HE2	2.36	0.43
1:A:32:ALA:HB2	1:A:356:VAL:HG23	2.00	0.43
1:A:449:ARG:N	1:A:482:PHE:HD2	2.16	0.43
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.85	0.43
1:D:456:LEU:CD2	1:D:456:LEU:C	2.86	0.43
1:A:351:ALA:HA	1:A:352:GLN:HA	1.67	0.43
1:A:407:VAL:CG1	1:A:430:ARG:HH21	2.25	0.43
1:C:32:ALA:O	1:C:37:LEU:HD23	2.17	0.43
1:C:353:LEU:O	1:C:358:ALA:HB1	2.18	0.43
1:A:363:GLU:HB2	1:A:367:GLY:HA2	2.00	0.43
1:B:303:ASP:O	1:B:307:MET:HG2	2.18	0.43
1:D:126:ASN:ND2	1:D:130:ARG:HG3	2.34	0.43
1:F:107:ILE:CD1	1:F:138:LEU:HD11	2.48	0.43
1:A:257:ALA:CB	1:A:404:HIS:HD2	2.32	0.43
1:C:52:LYS:NZ	1:C:56:GLU:OE1	2.47	0.43
1:E:230:ASP:O	1:E:280:LYS:HE3	2.18	0.43
1:F:459:GLN:CD	1:F:459:GLN:H	2.22	0.43
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.86	0.43
1:B:55:ILE:HG22	1:B:59:LYS:HE2	2.00	0.43
1:E:356:VAL:O	1:E:357:ILE:C	2.56	0.43
1:B:188:TYR:HA	1:B:191:ILE:HG22	2.01	0.43
1:D:190:ARG:HA	1:D:190:ARG:HD2	1.77	0.43
1:D:388:ILE:O	1:D:415:ILE:HA	2.19	0.43
1:D:453:HIS:ND1	1:D:499:ILE:HG12	2.34	0.43
1:F:125:VAL:O	1:F:171:GLY:HA2	2.19	0.43
1:A:55:ILE:HG23	1:A:117:VAL:HG12	2.00	0.43
1:B:95:LEU:CD2	1:F:202:ILE:HG12	2.49	0.43
1:C:460:ASP:O	1:C:463:ILE:HG22	2.19	0.43
1:C:478:ASP:HA	1:C:479:LYS:CB	2.49	0.43
1:D:174:MET:HA	1:D:179:GLN:HG2	2.01	0.43
1:F:214:SER:O	1:F:242:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ASP:O	1:F:280:LYS:NZ	2.51	0.43
1:A:72:ASN:ND2	1:A:179[A]:GLN:OE1	2.51	0.43
1:A:257:ALA:HB2	1:A:407:VAL:HG11	2.00	0.43
1:A:305:ASN:O	1:A:309:ASN:HB2	2.18	0.43
1:C:238:TYR:HA	1:C:287:TYR:O	2.19	0.43
1:D:479:LYS:HB3	1:D:479:LYS:HZ2	1.84	0.43
1:E:114:CYS:HA	1:E:117:VAL:HG22	2.01	0.43
1:E:202:ILE:HG12	1:F:95:LEU:HD22	2.00	0.43
1:A:241:LEU:CD1	1:A:269:VAL:CB	2.97	0.43
1:B:177:PRO:HD2	1:B:178:TRP:CZ3	2.54	0.43
1:B:456:LEU:HD12	1:B:456:LEU:HA	1.72	0.43
1:C:339:MET:HE3	1:C:413:VAL:HG11	2.00	0.43
1:C:374:ILE:O	1:C:377:PRO:HD2	2.18	0.43
1:C:478:ASP:HB3	1:C:479:LYS:C	2.39	0.43
1:E:333:LEU:HD21	1:E:430:ARG:HD3	2.01	0.43
1:E:456:LEU:HD23	1:E:456:LEU:HA	1.94	0.43
1:A:456:LEU:HB2	1:A:496:TRP:HD1	1.83	0.43
1:B:31:ARG:NE	1:B:320:GLU:OE2	2.41	0.43
1:C:39:GLN:HG3	1:C:51:ARG:CG	2.49	0.43
1:E:112:LYS:HB2	1:E:112:LYS:HE2	1.74	0.43
1:F:440:SER:HB2	1:F:487:LEU:HB3	1.99	0.43
1:A:27:GLU:HG3	1:A:70:GLY:HA2	2.01	0.42
1:B:2:LYS:HB3	1:B:2:LYS:HE2	1.73	0.42
1:F:123:MET:HE2	1:F:123:MET:HB2	1.76	0.42
1:B:172:ASN:HD22	3:B:601:DIO:H21	1.84	0.42
1:D:479:LYS:HD3	1:D:489:SER:OG	2.18	0.42
1:F:463:ILE:HD12	1:F:464:ARG:H	1.84	0.42
1:B:32:ALA:HB2	1:B:356:VAL:HG23	2.01	0.42
1:B:342:ALA:O	1:B:346:LYS:HE2	2.18	0.42
1:C:25:PHE:O	1:C:352:GLN:HB3	2.19	0.42
1:C:343:ASP:N	1:C:343:ASP:OD1	2.50	0.42
1:C:422:GLU:HA	1:C:501:ILE:O	2.19	0.42
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.92	0.42
1:D:442:VAL:O	1:D:442:VAL:HG23	2.19	0.42
1:E:221:PHE:HA	1:E:222:PRO:HA	1.76	0.42
1:E:429:ASN:OD1	1:E:431:ASN:N	2.50	0.42
1:F:324:THR:OG1	1:F:326:GLU:HG2	2.19	0.42
1:A:126:ASN:ND2	1:A:130:ARG:HG3	2.34	0.42
1:C:52:LYS:NZ	1:C:56:GLU:HG2	2.34	0.42
1:C:52:LYS:HZ2	1:C:56:GLU:HG2	1.84	0.42
1:C:149:LYS:HD3	1:C:150:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLY:HA2	1:B:297:TYR:CD1	2.55	0.42
1:B:478:ASP:HA	1:B:479:LYS:CB	2.50	0.42
1:C:61:LEU:HD22	1:C:378:PHE:HD1	1.84	0.42
1:C:351:ALA:HA	1:C:352:GLN:HA	1.59	0.42
1:D:232:ALA:O	1:D:236:VAL:HG22	2.19	0.42
1:D:257:ALA:CA	1:D:430:ARG:NH2	2.82	0.42
1:E:177:PRO:HD2	1:E:178:TRP:CZ3	2.54	0.42
1:F:376:TYR:CB	1:F:456:LEU:HD11	2.49	0.42
1:C:428:VAL:HG12	1:C:496:TRP:HA	2.01	0.42
1:B:61:LEU:HD22	1:B:378:PHE:HD2	1.85	0.42
1:B:442:VAL:O	1:B:444:GLY:N	2.53	0.42
1:D:453:HIS:CE1	1:D:499:ILE:HG12	2.55	0.42
1:A:58:VAL:HG23	1:A:117:VAL:HB	2.02	0.42
1:A:376:TYR:CD2	1:A:473:TYR:HA	2.54	0.42
1:B:123:MET:HE2	1:B:165:ILE:HD13	2.01	0.42
1:D:185:MET:HE2	1:D:185:MET:HB2	1.77	0.42
1:D:209:VAL:HG13	1:D:238:TYR:HB2	2.00	0.42
1:D:276:ILE:HD13	1:D:276:ILE:HA	1.89	0.42
1:D:476:ASN:C	1:D:476:ASN:ND2	2.72	0.42
1:A:453:HIS:HD2	1:A:455:VAL:HG23	1.83	0.42
1:B:408:THR:CG2	1:B:430:ARG:HH21	2.28	0.42
1:C:79:TRP:CD2	1:C:138:LEU:HD13	2.55	0.42
1:D:432:ILE:H	1:D:432:ILE:CD1	2.24	0.42
1:D:487:LEU:HD21	1:D:499:ILE:HG21	2.01	0.42
1:E:156:LYS:O	1:E:156:LYS:HG2	2.20	0.42
1:E:478:ASP:HA	1:E:479:LYS:CB	2.36	0.42
1:A:203:ASP:OD1	1:A:205:SER:OG	2.33	0.42
1:A:444:GLY:HA2	1:A:445:MET:CB	2.48	0.42
1:B:38:TYR:CE1	1:B:40:PRO:HG3	2.54	0.42
1:C:46:ASP:HB2	1:C:47:GLU:H	1.68	0.42
1:B:10:LYS:HA	1:B:390:LEU:HD22	2.02	0.41
1:B:95:LEU:HB2	1:B:180:VAL:HG21	2.02	0.41
1:B:376:TYR:CE2	1:B:473:TYR:HA	2.55	0.41
1:D:479:LYS:HE2	1:D:488:THR:O	2.20	0.41
1:E:363:GLU:HB2	1:E:367:GLY:HA3	2.02	0.41
1:F:456:LEU:HD22	1:F:472:VAL:HG13	2.02	0.41
1:D:216:LYS:HE3	1:D:216:LYS:HB2	1.60	0.41
1:E:14:ILE:HG13	1:E:391:GLN:HA	2.01	0.41
1:A:420:LYS:O	1:A:422:GLU:HG3	2.20	0.41
1:B:238:TYR:HA	1:B:287:TYR:O	2.20	0.41
1:C:210:ALA:O	1:C:239:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:C	1:C:242:HIS:HD2	2.24	0.41
1:C:252:THR:HG23	1:C:326:GLU:OE1	2.20	0.41
1:D:97:TRP:O	1:D:98:LYS:C	2.59	0.41
1:D:436:ILE:HD12	1:D:437:VAL:N	2.35	0.41
1:A:12:TYR:CE2	1:B:12:TYR:CD2	3.08	0.41
1:A:451:LEU:HD12	1:A:451:LEU:N	2.35	0.41
1:B:77:TYR:CE2	1:B:79:TRP:HA	2.55	0.41
1:B:297:TYR:CZ	1:B:298:HIS:CE1	3.08	0.41
1:C:174:MET:HE2	1:C:174:MET:HB2	1.81	0.41
1:D:31:ARG:HD2	1:D:35:ASP:OD1	2.20	0.41
1:B:31:ARG:HD2	1:B:35:ASP:OD2	2.21	0.41
1:D:293:TRP:CH2	1:D:350:LEU:HD12	2.55	0.41
1:D:371:ARG:HD3	1:D:375:PHE:CD1	2.55	0.41
1:F:173[A]:GLU:HG2	1:F:242:HIS:CE1	2.55	0.41
1:A:297:TYR:CZ	1:A:298:HIS:CE1	3.09	0.41
1:F:229:LEU:O	1:F:233:TYR:HB2	2.19	0.41
1:A:294:ASN:OD1	1:A:295:VAL:N	2.49	0.41
1:A:385:GLY:CA	1:A:415:ILE:HD11	2.48	0.41
1:B:172:ASN:HD22	3:B:601:DIO:H12	1.86	0.41
1:D:35:ASP:CA	1:D:39:GLN:HE21	2.34	0.41
1:E:111:ALA:HA	1:E:121:ILE:HD11	2.02	0.41
1:E:454:ILE:HG22	1:E:455:VAL:H	1.85	0.41
1:F:423:VAL:HG22	1:F:501:ILE:HG12	2.01	0.41
1:A:23:GLY:O	1:A:349:CYS:HA	2.21	0.41
1:A:276:ILE:HD13	1:A:276:ILE:HA	1.89	0.41
1:A:368:ALA:O	1:A:369:ALA:HB3	2.20	0.41
1:C:319:LEU:HB2	1:C:356:VAL:HG13	2.03	0.41
1:C:364:ARG:O	1:C:366:GLY:N	2.54	0.41
1:D:100:ILE:CD1	1:D:312:TRP:HB3	2.50	0.41
1:A:324:THR:CG2	1:A:326:GLU:HG2	2.49	0.41
1:A:376:TYR:CE2	1:A:473:TYR:HA	2.55	0.41
1:A:482:PHE:HA	1:A:486:ILE:O	2.21	0.41
1:B:139:LEU:HD12	1:B:168:TRP:CZ2	2.55	0.41
1:C:409:ASP:O	1:C:410:ILE:HD13	2.21	0.41
1:D:325:PHE:CE1	1:D:456:LEU:CD2	2.90	0.41
1:D:456:LEU:HD21	1:D:472:VAL:HG13	2.02	0.41
1:E:121:ILE:HB	1:E:165:ILE:HD13	2.01	0.41
1:E:229:LEU:HD23	1:E:229:LEU:HA	1.89	0.41
1:E:294:ASN:OD1	1:E:295:VAL:N	2.50	0.41
1:F:363:GLU:O	1:F:364:ARG:CB	2.65	0.41
1:B:173[B]:GLU:OE2	1:B:214:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLN:HE21	1:C:51:ARG:HG3	1.86	0.41
1:C:309:ASN:C	1:C:311:PRO:HD3	2.41	0.41
1:D:101:GLU:HG3	1:D:103:ASN:ND2	2.36	0.41
1:D:422:GLU:OE1	1:D:500:ARG:NH2	2.31	0.41
1:E:262:LEU:HD11	1:E:290:PHE:CZ	2.56	0.41
1:F:240:SER:HA	1:F:289:SER:O	2.21	0.41
1:A:173:GLU:CD	1:A:173:GLU:N	2.69	0.40
1:A:333:LEU:HG	1:A:428:VAL:HG11	2.03	0.40
1:B:307:MET:HG3	1:B:307:MET:O	2.21	0.40
1:B:483:ASP:CG	1:B:484:ASP:N	2.74	0.40
1:D:353:LEU:O	1:D:354:ILE:HD13	2.21	0.40
1:F:51:ARG:O	1:F:54:VAL:HG22	2.21	0.40
1:A:72:ASN:HD22	1:A:179[A]:GLN:CD	2.24	0.40
1:A:216:LYS:HB3	1:A:265:PHE:CE1	2.56	0.40
1:B:456:LEU:HB2	1:B:496:TRP:HD1	1.87	0.40
1:E:13:LYS:HB2	1:E:13:LYS:HE2	1.81	0.40
1:E:174:MET:HB3	1:E:183:LYS:H	1.86	0.40
1:E:197:ARG:HD3	1:F:177:PRO:O	2.21	0.40
1:F:10:LYS:O	1:F:13:LYS:HD3	2.20	0.40
1:C:239:ILE:HD12	1:C:239:ILE:HA	1.85	0.40
1:D:328:ALA:HA	1:D:374:ILE:HG22	2.04	0.40
1:D:384:TYR:HB2	1:D:424:THR:HG21	2.03	0.40
1:E:78:PHE:CD1	1:E:78:PHE:N	2.89	0.40
1:E:340:LYS:HB3	1:E:340:LYS:HE2	1.95	0.40
1:C:71:GLY:O	1:C:74:VAL:HG12	2.22	0.40
1:C:455:VAL:HG22	1:C:497:ASN:HD22	1.86	0.40
1:E:453:HIS:CD2	1:E:453:HIS:C	2.95	0.40
1:A:307:MET:O	1:A:307:MET:HG3	2.21	0.40
1:D:389:VAL:HG22	1:D:415:ILE:HD11	2.03	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	491/501 (98%)	447 (91%)	36 (7%)	8 (2%)	9 31
1	B	491/501 (98%)	436 (89%)	42 (9%)	13 (3%)	5 19
1	C	491/501 (98%)	438 (89%)	40 (8%)	13 (3%)	5 19
1	D	491/501 (98%)	427 (87%)	55 (11%)	9 (2%)	8 28
1	E	490/501 (98%)	438 (89%)	39 (8%)	13 (3%)	5 18
1	F	491/501 (98%)	441 (90%)	38 (8%)	12 (2%)	6 21
All	All	2945/3006 (98%)	2627 (89%)	250 (8%)	68 (2%)	6 22

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLU
1	A	364	ARG
1	A	444	GLY
1	A	484	ASP
1	B	250	ASN
1	B	368	ALA
1	B	443	ARG
1	C	364	ARG
1	C	365	ASN
1	C	368	ALA
1	C	421	GLU
1	D	484	ASP
1	E	107	ILE
1	E	364	ARG
1	F	40	PRO
1	F	364	ARG
1	A	367	GLY
1	A	369	ALA
1	B	164	ASN
1	B	367	GLY
1	B	369	ALA
1	C	9	ASP
1	C	173	GLU
1	D	35	ASP
1	D	98	LYS
1	D	368	ALA
1	E	46	ASP
1	E	250	ASN
1	E	357	ILE
1	E	367	GLY

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Mol	Chain	Res	Type
1	F	28	HIS
1	F	173[A]	GLU
1	F	173[B]	GLU
1	F	443	ARG
1	A	443	ARG
1	B	252	THR
1	B	364	ARG
1	B	441	ASP
1	B	478	ASP
1	C	46	ASP
1	C	297	TYR
1	C	476	ASN
1	E	297	TYR
1	E	369	ALA
1	B	309	ASN
1	B	363	GLU
1	C	294	ASN
1	C	369	ALA
1	D	10	LYS
1	D	369	ALA
1	D	443	ARG
1	E	173	GLU
1	E	483	ASP
1	E	484	ASP
1	F	11	ASP
1	F	107	ILE
1	F	477	SER
1	F	484	ASP
1	A	483	ASP
1	B	107	ILE
1	E	478	ASP
1	F	369	ALA
1	C	366	GLY
1	E	444	GLY
1	F	357	ILE
1	C	107	ILE
1	D	444	GLY
1	D	40	PRO

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	429/439 (98%)	416 (97%)	13 (3%)	41	73
1	B	429/439 (98%)	416 (97%)	13 (3%)	41	73
1	C	427/439 (97%)	422 (99%)	5 (1%)	71	90
1	D	429/439 (98%)	417 (97%)	12 (3%)	43	75
1	E	427/439 (97%)	417 (98%)	10 (2%)	50	79
1	F	428/439 (98%)	418 (98%)	10 (2%)	50	79
All	All	2569/2634 (98%)	2506 (98%)	63 (2%)	49	77

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	46	ASP
1	A	241	LEU
1	A	242	HIS
1	A	256	LEU
1	A	280	LYS
1	A	290	PHE
1	A	396	SER
1	A	402	SER
1	A	416	TYR
1	A	449	ARG
1	A	482	PHE
1	A	484	ASP
1	B	13	LYS
1	B	122	MET
1	B	173[A]	GLU
1	B	173[B]	GLU
1	B	179	GLN
1	B	242	HIS
1	B	290	PHE
1	B	396	SER
1	B	445	MET

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Mol	Chain	Res	Type
1	B	466	SER
1	B	478	ASP
1	B	479	LYS
1	B	497	ASN
1	C	52	LYS
1	C	174	MET
1	C	290	PHE
1	C	361	VAL
1	C	492	ARG
1	D	290	PHE
1	D	300	ASN
1	D	309	ASN
1	D	350	LEU
1	D	396	SER
1	D	430	ARG
1	D	435	ASP
1	D	449	ARG
1	D	455	VAL
1	D	476	ASN
1	D	479	LYS
1	D	489	SER
1	E	12	TYR
1	E	47	GLU
1	E	115	LYS
1	E	179	GLN
1	E	290	PHE
1	E	301	ASN
1	E	319	LEU
1	E	396	SER
1	E	468	ASN
1	E	482	PHE
1	F	5	ARG
1	F	115	LYS
1	F	179	GLN
1	F	213	SER
1	F	290	PHE
1	F	416	TYR
1	F	435	ASP
1	F	449	ARG
1	F	492	ARG
1	F	496	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	223	GLN
1	A	497	ASN
1	B	172	ASN
1	B	459	GLN
1	C	39	GLN
1	C	172	ASN
1	C	179	GLN
1	C	242	HIS
1	C	309	ASN
1	C	497	ASN
1	D	72	ASN
1	D	172	ASN
1	D	179	GLN
1	D	242	HIS
1	D	380	HIS
1	D	417	ASN
1	D	453	HIS
1	D	476	ASN
1	E	242	HIS
1	E	250	ASN
1	F	242	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

12 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	$\#\|Z\| > 2$
3	DIO	C	601	-	6,6,6	0.41	0	6,6,6	0.40	0
3	DIO	E	601	-	6,6,6	0.54	0	6,6,6	0.72	0
3	DIO	D	601	-	6,6,6	0.54	0	6,6,6	0.61	0
2	AHR	F	600	-	10,10,10	1.64	3 (30%)	13,14,14	1.39	2 (15%)
3	DIO	A	601	-	6,6,6	0.52	0	6,6,6	0.36	0
3	DIO	B	601	-	6,6,6	0.44	0	6,6,6	0.57	0
2	AHR	B	600	-	10,10,10	1.95	2 (20%)	13,14,14	1.60	3 (23%)
3	DIO	F	601	-	6,6,6	0.48	0	6,6,6	0.71	0
2	AHR	D	600	-	10,10,10	1.63	2 (20%)	13,14,14	1.35	1 (7%)
2	AHR	E	600	-	10,10,10	1.94	4 (40%)	13,14,14	1.60	3 (23%)
2	AHR	A	600	-	10,10,10	1.66	2 (20%)	13,14,14	1.11	1 (7%)
2	AHR	C	600	-	10,10,10	1.71	2 (20%)	13,14,14	1.74	3 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	C	601	-	-	-	0/1/1/1
3	DIO	E	601	-	-	-	0/1/1/1
3	DIO	D	601	-	-	-	0/1/1/1
2	AHR	F	600	-	-	0/2/18/18	0/1/1/1
3	DIO	A	601	-	-	-	0/1/1/1
3	DIO	B	601	-	-	-	0/1/1/1
2	AHR	B	600	-	-	2/2/18/18	0/1/1/1
3	DIO	F	601	-	-	-	0/1/1/1
2	AHR	D	600	-	-	0/2/18/18	0/1/1/1
2	AHR	E	600	-	-	1/2/18/18	0/1/1/1
2	AHR	A	600	-	-	0/2/18/18	0/1/1/1
2	AHR	C	600	-	-	0/2/18/18	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	AHR	C2-C3	-3.70	1.43	1.53
2	B	600	AHR	C1-C2	-3.69	1.48	1.52
2	A	600	AHR	C2-C3	-3.62	1.43	1.53
2	C	600	AHR	C2-C3	-3.56	1.43	1.53
2	E	600	AHR	C2-C3	-3.37	1.44	1.53
2	E	600	AHR	C1-C2	-3.25	1.48	1.52
2	D	600	AHR	C2-C3	-3.11	1.44	1.53
2	F	600	AHR	C2-C3	-3.01	1.45	1.53
2	F	600	AHR	C1-C2	-2.54	1.49	1.52
2	D	600	AHR	C1-C2	-2.37	1.50	1.52
2	E	600	AHR	C3-C4	-2.33	1.47	1.53
2	F	600	AHR	C3-C4	-2.16	1.47	1.53
2	A	600	AHR	C1-C2	-2.16	1.50	1.52
2	E	600	AHR	O4-C1	2.09	1.45	1.43
2	C	600	AHR	C3-C4	-2.07	1.47	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	AHR	C1-C2-C3	4.28	107.66	102.30
2	C	600	AHR	C5-C4-C3	-4.10	105.20	115.09
2	E	600	AHR	C1-C2-C3	3.84	107.10	102.30
2	F	600	AHR	C1-C2-C3	3.52	106.70	102.30
2	B	600	AHR	C1-C2-C3	3.39	106.54	102.30
2	B	600	AHR	C5-C4-C3	-3.22	107.32	115.09
2	B	600	AHR	C2-C3-C4	2.69	107.86	102.64
2	F	600	AHR	O4-C4-C5	2.68	115.01	109.21
2	C	600	AHR	C1-C2-C3	2.65	105.62	102.30
2	A	600	AHR	C1-C2-C3	2.44	105.35	102.30
2	C	600	AHR	C2-C3-C4	2.36	107.22	102.64
2	E	600	AHR	C5-C4-C3	-2.24	109.69	115.09
2	E	600	AHR	O4-C4-C5	2.22	114.01	109.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	AHR	O4-C4-C5-O5
2	B	600	AHR	C3-C4-C5-O5
2	E	600	AHR	O4-C4-C5-O5

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	DIO	2	0
3	E	601	DIO	1	0
3	D	601	DIO	2	0
3	A	601	DIO	4	0
3	B	601	DIO	4	0
3	F	601	DIO	3	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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	496/501 (99%)	-0.11	12 (2%)	59	57	31, 51, 83, 116	0
1	B	496/501 (99%)	0.05	18 (3%)	42	39	31, 54, 89, 117	0
1	C	496/501 (99%)	0.01	8 (1%)	72	71	32, 54, 96, 120	0
1	D	496/501 (99%)	0.06	24 (4%)	30	27	34, 56, 100, 130	0
1	E	496/501 (99%)	0.01	7 (1%)	75	76	29, 56, 99, 125	0
1	F	496/501 (99%)	-0.10	19 (3%)	40	37	31, 53, 92, 118	0
All	All	2976/3006 (99%)	-0.01	88 (2%)	50	46	29, 54, 94, 130	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169[A]	CYS	4.8
1	F	501	ILE	4.3
1	E	368	ALA	4.2
1	A	483	ASP	4.0
1	A	484	ASP	3.7
1	D	488	THR	3.7
1	D	478	ASP	3.6
1	F	404	HIS	3.6
1	D	437	VAL	3.5
1	D	440	SER	3.5
1	B	440	SER	3.4
1	C	8	VAL	3.4
1	D	8	VAL	3.4
1	A	486	ILE	3.3
1	D	436	ILE	3.3
1	B	436	ILE	3.2
1	A	501	ILE	3.1
1	D	483	ASP	3.1
1	F	398	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	435	ASP	3.0
1	F	483	ASP	3.0
1	B	488	THR	3.0
1	B	499	ILE	3.0
1	F	485	GLY	2.9
1	A	485	GLY	2.9
1	F	486	ILE	2.9
1	D	441	ASP	2.9
1	F	478	ASP	2.9
1	B	439	VAL	2.8
1	C	305	ASN	2.8
1	F	436	ILE	2.8
1	B	487	LEU	2.8
1	F	438	LEU	2.8
1	D	442	VAL	2.8
1	B	484	ASP	2.7
1	F	396	SER	2.7
1	D	461	LEU	2.7
1	D	486	ILE	2.7
1	F	8	VAL	2.6
1	F	5	ARG	2.6
1	C	484	ASP	2.6
1	E	307	MET	2.6
1	D	489	SER	2.6
1	F	405	GLU	2.6
1	F	488	THR	2.5
1	B	437	VAL	2.5
1	B	478	ASP	2.5
1	C	309	ASN	2.5
1	D	484	ASP	2.5
1	B	482	PHE	2.5
1	F	482	PHE	2.5
1	C	433	HIS	2.5
1	B	485	GLY	2.4
1	D	425	ILE	2.4
1	B	486	ILE	2.4
1	C	478	ASP	2.4
1	E	445	MET	2.4
1	D	305	ASN	2.4
1	B	491	LEU	2.4
1	B	451	LEU	2.4
1	B	434	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	484	ASP	2.4
1	E	486	ILE	2.4
1	F	403	LYS	2.4
1	A	482	PHE	2.3
1	D	438	LEU	2.3
1	A	421	GLU	2.2
1	F	416	TYR	2.2
1	D	477	SER	2.2
1	D	5	ARG	2.2
1	D	487	LEU	2.2
1	D	463	ILE	2.2
1	D	490	MET	2.2
1	E	398	LEU	2.1
1	A	5	ARG	2.1
1	E	416	TYR	2.1
1	A	398	LEU	2.1
1	E	47	GLU	2.1
1	B	483	ASP	2.1
1	C	483	ASP	2.1
1	D	12	TYR	2.1
1	D	2	LYS	2.1
1	A	431	ASN	2.1
1	B	309	ASN	2.1
1	D	307	MET	2.0
1	A	445	MET	2.0
1	A	433	HIS	2.0
1	F	421	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DIO	C	601	6/6	0.85	0.32	71,74,75,87	0
3	DIO	D	601	6/6	0.85	0.32	67,71,71,74	0
3	DIO	B	601	6/6	0.87	0.27	67,69,71,75	0
2	AHR	C	600	10/10	0.89	0.28	49,54,63,66	0
2	AHR	D	600	10/10	0.90	0.24	47,56,61,66	0
3	DIO	E	601	6/6	0.90	0.24	64,67,69,73	0
3	DIO	A	601	6/6	0.91	0.25	65,67,74,77	0
3	DIO	F	601	6/6	0.91	0.29	64,70,74,76	0
2	AHR	A	600	10/10	0.92	0.20	38,49,58,59	0
2	AHR	E	600	10/10	0.92	0.20	43,56,61,62	0
2	AHR	B	600	10/10	0.95	0.20	46,57,67,70	0
2	AHR	F	600	10/10	0.96	0.21	46,54,61,62	0

6.5 Other polymers (i)

There are no such residues in this entry.