Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:05 PM EDT

PDB ID	:	5O7Z
Title	:	Crystal Structure of R67A Mutant of alpha-L-arabinofuranosidase Ara51 from Clostridium thermocellum
Authors	:	Lafite, P.; Daniellou, R.
Deposited on	:	2017-06-12
Resolution	:	2.64 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

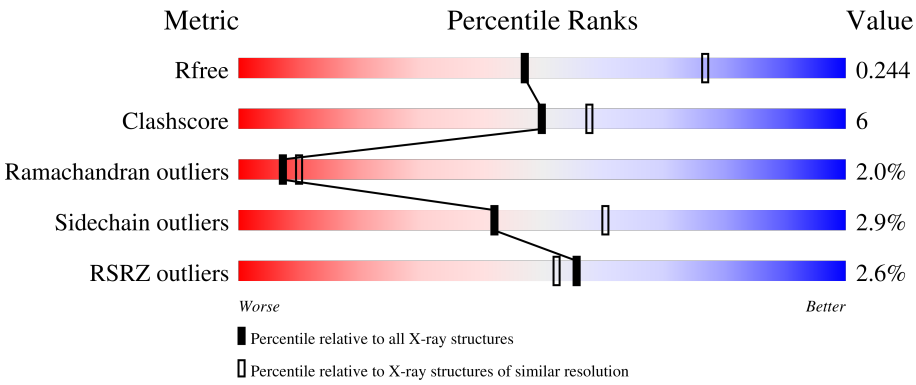
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	1%, 81%, 17%
1	B	501	2%, 83%, 14%
1	C	501	3%, 80%, 17%
1	D	501	4%, 85%, 13%
1	E	501	3%, 82%, 16%

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Mol	Chain	Length	Quality of chain
1	F	501	3% 81% 16%

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	DIO	C	601	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24186 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.

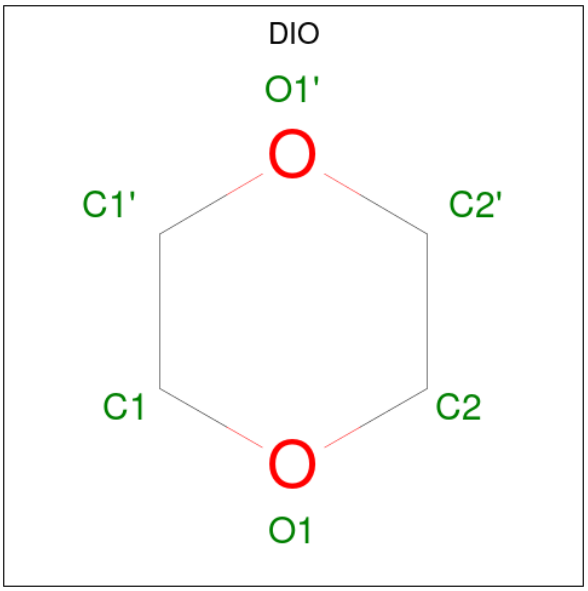
- Molecule 1 is a protein called Intracellular exo-alpha-(1->5)-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	3977	2525	674	756	22	0	0	0
1	B	496	3974	2524	673	755	22	0	1	0
1	C	498	3975	2525	674	754	22	0	0	0
1	D	498	3972	2522	673	755	22	0	0	0
1	E	496	3974	2524	673	755	22	0	1	0
1	F	496	3974	2524	673	755	22	0	1	0

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



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

- Molecule 3 is water.

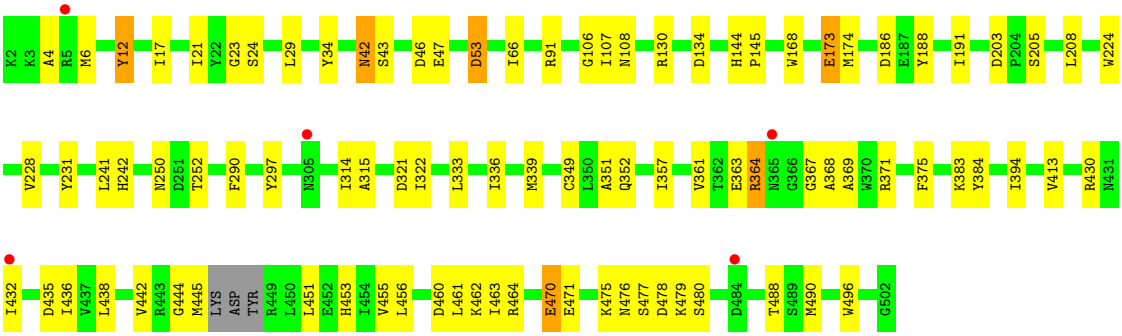
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	48	48	48	0	0
3	B	68	68	68	0	0
3	C	45	45	45	0	0
3	D	60	60	60	0	0
3	E	50	50	50	0	0
3	F	45	45	45	0	0

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.

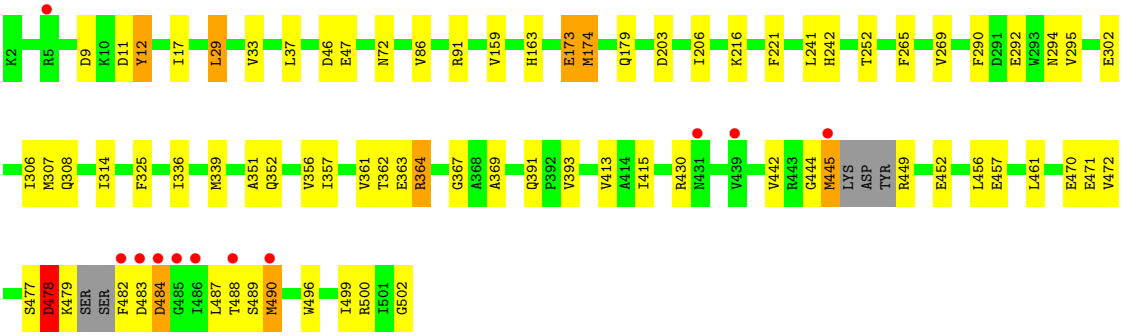
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

Chain A:



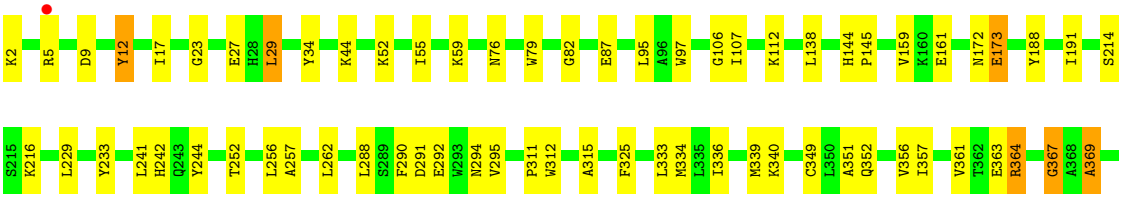
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

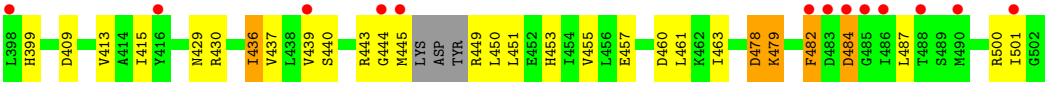
Chain B:



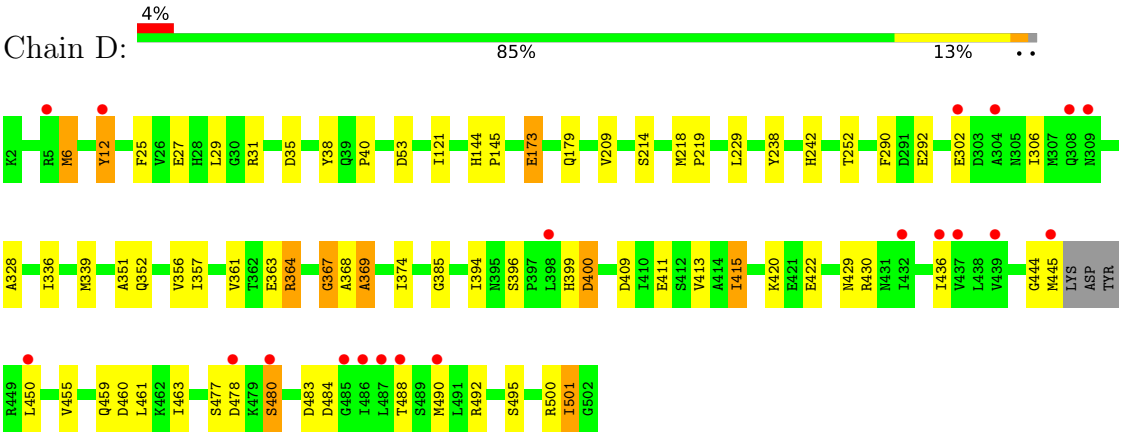
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

Chain C:

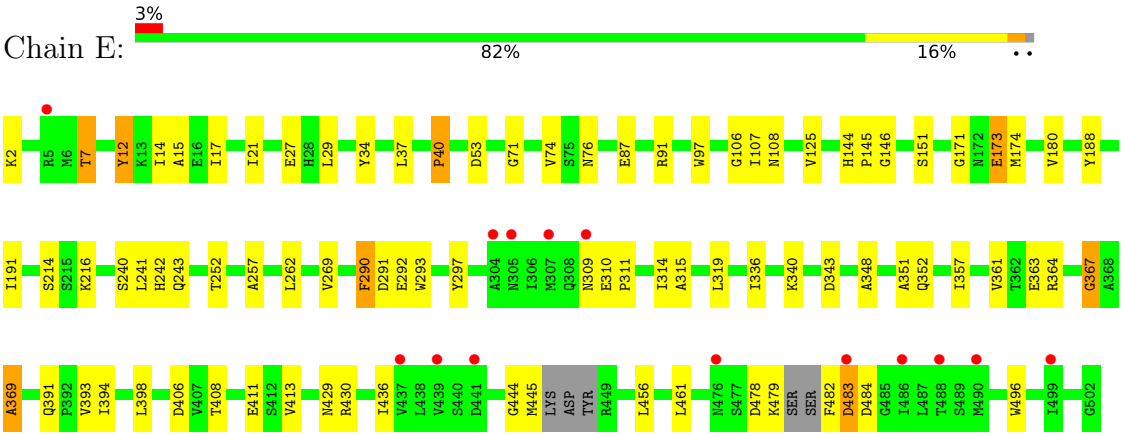




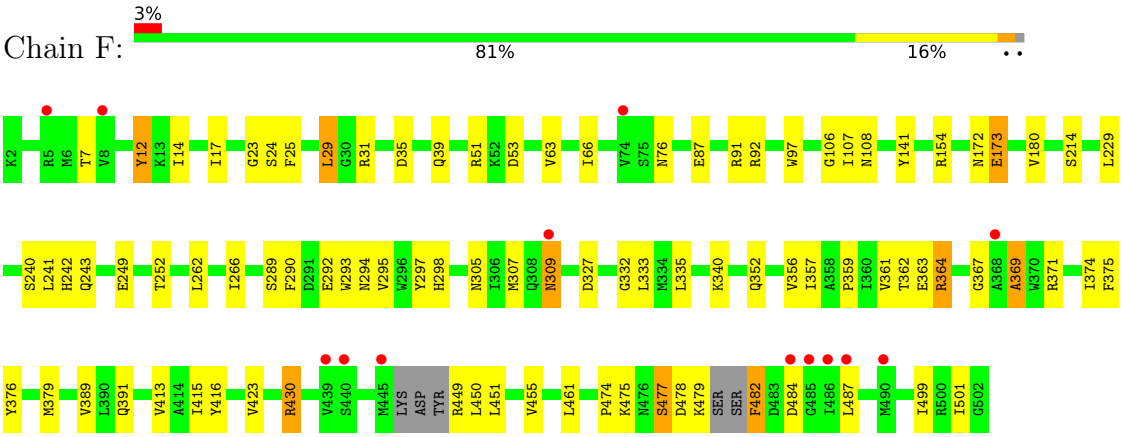
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase



• 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	173.75Å 173.75Å 272.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.64 48.81 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.81-2.64) 99.8 (48.81-2.64)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.244 0.193 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24186	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.45% 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 (i)

5.1 Standard geometry (i)

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

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	0.43	0/4068	0.60	0/5512
1	B	0.44	0/4064	0.61	0/5505
1	C	0.42	0/4066	0.60	0/5510
1	D	0.43	0/4063	0.61	0/5507
1	E	0.41	0/4064	0.59	0/5505
1	F	0.42	0/4064	0.59	0/5505
All	All	0.43	0/24389	0.60	0/33044

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 (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	3977	0	3862	44	0
1	B	3974	0	3856	46	0
1	C	3975	0	3856	54	0
1	D	3972	0	3848	40	0
1	E	3974	0	3856	44	0
1	F	3974	0	3856	50	0
2	C	6	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	0	8	1	0
2	E	6	0	8	2	0
2	F	6	0	8	1	0
3	A	48	0	0	0	0
3	B	68	0	0	1	0
3	C	45	0	0	0	0
3	D	60	0	0	0	0
3	E	50	0	0	2	0
3	F	45	0	0	0	0
All	All	24186	0	23166	274	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 6.

All (274) 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:478:ASP:HB3	1:B:479:LYS:HA	1.51	0.91
1:B:241:LEU:HD21	1:B:269:VAL:HG21	1.59	0.84
1:B:336:ILE:HA	1:B:339:MET:HE2	1.60	0.81
1:C:444:GLY:HA3	1:C:445:MET:HB2	1.65	0.78
1:B:252:THR:HG21	1:B:461:LEU:HD13	1.68	0.76
1:E:340:LYS:NZ	1:E:411:GLU:OE2	2.20	0.74
1:C:478:ASP:HA	1:C:479:LYS:HB2	1.69	0.74
1:E:252:THR:HG21	1:E:461:LEU:HD13	1.69	0.73
1:A:322:ILE:HG21	1:A:464:ARG:HH11	1.52	0.73
1:B:363:GLU:HB2	1:B:367:GLY:HA3	1.70	0.72
1:E:478:ASP:HA	1:E:479:LYS:HB3	1.68	0.72
1:C:487:LEU:HD13	1:C:501:ILE:HD11	1.73	0.70
1:D:420:LYS:HB3	1:D:422:GLU:HG3	1.75	0.69
1:F:305:ASN:O	1:F:309:ASN:HB2	1.93	0.69
1:B:470:GLU:O	1:B:472:VAL:N	2.26	0.68
1:C:482:PHE:HB2	1:C:487:LEU:HD12	1.76	0.68
1:C:252:THR:HG21	1:C:461:LEU:HD13	1.75	0.67
1:F:361:VAL:O	1:F:369:ALA:HA	1.95	0.67
1:D:252:THR:HG21	1:D:461:LEU:HD13	1.77	0.66
1:A:336:ILE:HA	1:A:339:MET:HE2	1.77	0.66
1:F:252:THR:HG21	1:F:461:LEU:HD13	1.76	0.66
1:F:333:LEU:HD21	1:F:430:ARG:HG2	1.79	0.65
1:A:371:ARG:NH1	1:A:470:GLU:OE2	2.29	0.65
1:A:250:ASN:OD1	1:A:462:LYS:NZ	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:GLU:OE1	2:E:601:DIO:H21	1.97	0.64
1:F:17:ILE:HG13	1:F:389:VAL:HG23	1.80	0.64
1:A:6:MET:HB2	1:A:394:ILE:HG12	1.79	0.63
1:D:363:GLU:HB2	1:D:367:GLY:HA2	1.79	0.63
1:B:336:ILE:HG23	1:B:413:VAL:HG23	1.81	0.63
1:C:399:HIS:ND1	1:C:409:ASP:OD1	2.23	0.63
1:D:450:LEU:HD21	1:D:480:SER:HB3	1.81	0.62
1:F:29:LEU:HD13	1:F:356:VAL:HG11	1.81	0.62
1:D:459:GLN:HG2	1:D:492:ARG:HH22	1.63	0.62
1:B:29:LEU:HD13	1:B:356:VAL:HG11	1.80	0.61
1:C:97:TRP:HZ2	2:C:601:DIO:H2'2	1.65	0.61
1:C:363:GLU:HB2	1:C:367:GLY:HA2	1.83	0.61
1:E:257:ALA:HA	1:E:430:ARG:HH21	1.65	0.60
1:B:452:GLU:OE2	1:B:500:ARG:NH1	2.33	0.60
1:A:444:GLY:HA3	1:A:445:MET:HB2	1.83	0.60
1:C:440:SER:HB2	1:C:487:LEU:HB3	1.83	0.60
1:C:9:ASP:HB3	1:C:12:TYR:HB2	1.84	0.59
1:C:97:TRP:CZ2	2:C:601:DIO:H2'2	2.37	0.59
1:C:336:ILE:HG23	1:C:413:VAL:HG23	1.83	0.59
1:C:429:ASN:HD21	1:C:436:ILE:HG13	1.67	0.59
1:C:336:ILE:HA	1:C:339:MET:HE2	1.85	0.58
1:C:29:LEU:HD13	1:C:356:VAL:HG11	1.86	0.58
1:D:492:ARG:O	1:D:495:SER:OG	2.18	0.58
1:A:53:ASP:OD1	1:A:53:ASP:N	2.36	0.58
1:D:385:GLY:HA2	1:D:415:ILE:HG12	1.85	0.57
1:C:262:LEU:HD22	1:C:334:MET:HG2	1.85	0.57
1:D:429:ASN:HD21	1:D:436:ILE:HG12	1.70	0.57
1:A:168:TRP:HB2	1:A:208:LEU:HD23	1.87	0.56
1:A:252:THR:HG21	1:A:461:LEU:HD13	1.87	0.56
1:A:363:GLU:H	1:A:367:GLY:HA2	1.70	0.56
1:A:106:GLY:O	1:A:108:ASN:N	2.39	0.56
1:B:47:GLU:CD	1:B:47:GLU:H	2.10	0.56
1:E:240:SER:O	1:E:241:LEU:HD23	2.06	0.56
1:B:91:ARG:NH2	1:B:314:ILE:HD11	2.20	0.55
1:A:361:VAL:O	1:A:369:ALA:HA	2.06	0.55
1:D:361:VAL:O	1:D:369:ALA:HA	2.05	0.55
1:B:449:ARG:O	1:B:502:GLY:N	2.26	0.55
1:B:487:LEU:HD21	1:B:499:ILE:HG21	1.89	0.55
1:F:363:GLU:HB2	1:F:367:GLY:HA2	1.89	0.55
1:D:336:ILE:HA	1:D:339:MET:HE2	1.89	0.55
1:C:478:ASP:CA	1:C:479:LYS:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:TYR:HA	1:C:191:ILE:HG22	1.88	0.54
1:E:361:VAL:O	1:E:369:ALA:HA	2.06	0.54
1:E:2:LYS:N	3:E:701:HOH:O	2.39	0.54
1:E:15:ALA:HB2	1:E:343:ASP:HB3	1.90	0.54
1:F:172:ASN:ND2	1:F:173[B]:GLU:HG2	2.23	0.53
1:A:12:TYR:HH	1:F:12:TYR:HH	1.53	0.53
1:B:72:ASN:HA	1:B:179:GLN:HE22	1.74	0.53
1:B:242:HIS:CD2	1:B:292:GLU:HB2	2.43	0.53
1:C:5:ARG:HG2	1:C:439:VAL:HB	1.90	0.53
1:E:429:ASN:HD21	1:E:436:ILE:HG12	1.74	0.53
1:D:214:SER:O	1:D:242:HIS:HB2	2.09	0.53
1:D:363:GLU:O	1:D:364:ARG:HB2	2.10	0.52
1:F:450:LEU:HD12	1:F:451:LEU:H	1.74	0.52
1:F:214:SER:O	1:F:242:HIS:HB2	2.09	0.52
1:A:17:ILE:HD12	1:A:21:ILE:HD11	1.91	0.52
1:F:478:ASP:HA	1:F:479:LYS:CB	2.39	0.52
1:C:2:LYS:O	1:C:437:VAL:HG12	2.10	0.52
1:A:363:GLU:N	1:A:367:GLY:HA2	2.23	0.52
1:A:34:TYR:HB2	1:A:315:ALA:HB2	1.92	0.51
1:A:336:ILE:HG23	1:A:413:VAL:HG23	1.91	0.51
1:B:336:ILE:HG23	1:B:413:VAL:CG2	2.41	0.51
1:C:333:LEU:HD11	1:C:430:ARG:HG2	1.93	0.51
1:A:478:ASP:HA	1:A:479:LYS:HB3	1.93	0.51
1:F:362:THR:HG22	1:F:369:ALA:HB2	1.93	0.51
1:F:416:TYR:HB2	1:F:423:VAL:HG22	1.92	0.51
1:B:483:ASP:OD1	1:B:484:ASP:N	2.38	0.50
1:C:449:ARG:N	1:C:482:PHE:HE2	2.10	0.50
1:E:456:LEU:HB3	1:E:496:TRP:HB3	1.92	0.50
1:D:29:LEU:HD13	1:D:356:VAL:HG11	1.94	0.50
1:A:456:LEU:HB2	1:A:496:TRP:HD1	1.75	0.50
1:E:173[A]:GLU:HG2	1:E:214:SER:OG	2.10	0.50
1:D:53:ASP:OD1	1:D:53:ASP:N	2.44	0.50
1:B:294:ASN:OD1	1:B:295:VAL:N	2.40	0.50
1:C:244:TYR:OH	2:C:601:DIO:H12	2.11	0.50
1:E:214:SER:O	1:E:242:HIS:HB2	2.11	0.50
1:F:242:HIS:CD2	1:F:292:GLU:HB2	2.47	0.49
1:A:479:LYS:HD3	1:A:490:MET:HB2	1.94	0.49
1:D:302:GLU:O	1:D:306:ILE:HG13	2.13	0.49
1:B:444:GLY:HA3	1:B:445:MET:C	2.33	0.49
1:F:371:ARG:HD3	1:F:375:PHE:CE1	2.48	0.49
1:B:456:LEU:HB2	1:B:496:TRP:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:VAL:O	1:C:369:ALA:HA	2.13	0.49
1:C:241:LEU:HD11	1:C:288:LEU:HG	1.94	0.49
1:E:336:ILE:HG23	1:E:413:VAL:HG22	1.95	0.49
1:C:460:ASP:HB3	1:C:463:ILE:HB	1.94	0.48
1:D:328:ALA:HA	1:D:374:ILE:HG22	1.95	0.48
1:E:108:ASN:HB2	3:E:716:HOH:O	2.13	0.48
1:E:188:TYR:HA	1:E:191:ILE:HG22	1.94	0.48
1:A:241:LEU:O	1:A:242:HIS:HD2	1.96	0.48
1:D:444:GLY:HA3	1:D:445:MET:HB2	1.95	0.48
1:E:408:THR:O	1:E:430:ARG:HD3	2.13	0.48
1:B:393:VAL:HB	1:D:12:TYR:CD2	2.48	0.48
1:A:460:ASP:HB3	1:A:463:ILE:HB	1.95	0.48
1:D:460:ASP:HB3	1:D:463:ILE:HB	1.96	0.48
1:F:332:GLY:HA2	1:F:335:LEU:HD12	1.95	0.48
1:B:362:THR:HG22	1:B:369:ALA:HB2	1.95	0.48
1:E:398:LEU:HD13	1:E:406:ASP:HB3	1.96	0.48
1:A:475:LYS:O	1:A:477:SER:N	2.46	0.48
1:B:490:MET:SD	1:B:490:MET:N	2.86	0.48
1:F:340:LYS:HG3	1:F:413:VAL:HG21	1.96	0.48
1:B:221:PHE:CE1	1:B:265:PHE:HE1	2.32	0.47
1:E:241:LEU:HD21	1:E:269:VAL:HG21	1.95	0.47
1:B:361:VAL:O	1:B:369:ALA:HA	2.14	0.47
1:F:262:LEU:O	1:F:266:ILE:HG13	2.14	0.47
1:E:351:ALA:HA	1:E:352:GLN:HA	1.65	0.47
1:A:453:HIS:HB2	1:A:480:SER:HB3	1.97	0.47
1:B:216:LYS:HB3	1:B:265:PHE:CE1	2.49	0.47
1:C:214:SER:O	1:C:242:HIS:HB2	2.14	0.47
1:D:38:TYR:CZ	1:D:40:PRO:HG3	2.49	0.47
1:E:478:ASP:HB3	1:E:479:LYS:C	2.35	0.47
1:F:173[A]:GLU:OE1	1:F:173[A]:GLU:N	2.47	0.47
1:C:351:ALA:HA	1:C:352:GLN:HA	1.69	0.47
1:E:76:ASN:HB2	1:E:180:VAL:HG21	1.96	0.47
1:B:351:ALA:HA	1:B:352:GLN:HA	1.68	0.47
1:D:25:PHE:HE2	2:D:601:DIO:H2'2	1.79	0.47
1:E:216:LYS:HE3	1:E:216:LYS:HB2	1.79	0.47
1:B:241:LEU:HD23	3:B:601:HOH:O	2.15	0.47
1:D:27:GLU:HG2	1:D:29:LEU:HB2	1.96	0.47
1:C:340:LYS:HG3	1:C:413:VAL:CG2	2.44	0.47
1:E:71:GLY:O	1:E:74:VAL:HG12	2.14	0.47
1:D:336:ILE:HG21	1:D:411:GLU:HG3	1.97	0.47
1:A:91:ARG:NH2	1:A:314:ILE:HD11	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:OD1	1:A:231:TYR:OH	2.22	0.46
1:E:146:GLY:HA2	1:E:151:SER:HB2	1.97	0.46
1:B:477:SER:O	1:B:478:ASP:HB2	2.16	0.46
1:D:399:HIS:ND1	1:D:409:ASP:OD1	2.42	0.46
1:D:422:GLU:OE1	1:D:500:ARG:NH2	2.37	0.46
1:E:106:GLY:O	1:E:108:ASN:N	2.48	0.46
1:A:363:GLU:O	1:A:364:ARG:HB2	2.16	0.46
1:E:14:ILE:HG13	1:E:391:GLN:HG2	1.98	0.46
1:A:371:ARG:HD3	1:A:375:PHE:CE1	2.51	0.46
1:E:12:TYR:CE1	1:E:391:GLN:HG3	2.51	0.46
1:C:55:ILE:HG22	1:C:59:LYS:HE2	1.98	0.46
1:F:39:GLN:OE1	1:F:51:ARG:NH1	2.34	0.46
1:B:444:GLY:HA3	1:B:445:MET:HG2	1.97	0.45
1:D:351:ALA:HA	1:D:352:GLN:HA	1.62	0.45
1:A:188:TYR:HA	1:A:191:ILE:HG22	1.99	0.45
1:B:159:VAL:HG11	1:B:163:HIS:CE1	2.51	0.45
1:B:393:VAL:HB	1:D:12:TYR:HD2	1.81	0.45
1:C:292:GLU:OE1	2:C:601:DIO:H1'2	2.17	0.45
1:F:12:TYR:CE1	1:F:391:GLN:HG3	2.52	0.45
1:A:203:ASP:OD1	1:A:205:SER:OG	2.32	0.45
1:D:173:GLU:HB2	1:D:214:SER:OG	2.17	0.45
1:D:500:ARG:O	1:D:501:ILE:HG13	2.17	0.45
1:F:363:GLU:O	1:F:364:ARG:HB2	2.15	0.45
1:E:7:THR:HG23	1:E:393:VAL:HB	1.98	0.45
1:F:455:VAL:HG12	1:F:475:LYS:O	2.17	0.45
1:C:229:LEU:O	1:C:233:TYR:HB2	2.17	0.45
1:C:340:LYS:HG3	1:C:413:VAL:HG22	1.97	0.45
1:D:422:GLU:HA	1:D:501:ILE:O	2.17	0.45
1:F:241:LEU:O	1:F:242:HIS:HD2	2.00	0.45
1:C:23:GLY:O	1:C:349:CYS:HA	2.17	0.45
1:A:435:ASP:OD1	1:A:436:ILE:N	2.50	0.45
1:C:82:GLY:O	1:C:106:GLY:HA3	2.17	0.44
1:F:53:ASP:OD1	1:F:53:ASP:N	2.41	0.44
1:C:144:HIS:HA	1:C:145:PRO:HD3	1.88	0.44
1:E:21:ILE:HA	1:E:348:ALA:H	1.82	0.44
1:C:44:LYS:O	1:C:52:LYS:HB2	2.18	0.44
1:C:294:ASN:OD1	1:C:295:VAL:N	2.46	0.44
1:D:218:MET:HA	1:D:219:PRO:HD3	1.89	0.44
1:A:224:TRP:O	1:A:228:VAL:HG23	2.18	0.44
1:C:79:TRP:CD2	1:C:138:LEU:HD13	2.53	0.44
1:A:333:LEU:HD11	1:A:430:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:HIS:CD2	1:D:292:GLU:HB2	2.53	0.44
1:B:216:LYS:HB3	1:B:265:PHE:CD1	2.53	0.43
1:C:450:LEU:HD12	1:C:500:ARG:O	2.17	0.43
1:B:479:LYS:HZ2	1:B:482:PHE:N	2.16	0.43
1:C:172:ASN:O	1:C:173:GLU:C	2.56	0.43
1:D:336:ILE:HG23	1:D:413:VAL:CG2	2.48	0.43
1:E:291:ASP:O	1:E:292:GLU:HG3	2.18	0.43
1:B:9:ASP:OD2	1:B:11:ASP:HB2	2.18	0.43
1:B:241:LEU:O	1:B:242:HIS:HD2	2.01	0.43
1:F:243:GLN:O	1:F:293:TRP:HA	2.18	0.43
1:F:294:ASN:OD1	1:F:295:VAL:N	2.49	0.43
1:E:243:GLN:O	1:E:293:TRP:HA	2.18	0.43
1:A:4:ALA:HB3	1:A:438:LEU:HA	2.00	0.43
1:A:383:LYS:HD3	1:A:384:TYR:CE1	2.54	0.43
1:A:24:SER:O	1:A:66:ILE:HA	2.18	0.43
1:B:12:TYR:CE1	1:B:391:GLN:HG3	2.54	0.43
1:B:363:GLU:O	1:B:364:ARG:HB2	2.19	0.43
1:C:325:PHE:CZ	1:C:457:GLU:HA	2.53	0.43
1:E:363:GLU:HB2	1:E:367:GLY:HA2	2.00	0.43
1:A:478:ASP:HA	1:A:479:LYS:CB	2.49	0.43
1:E:310:GLU:N	1:E:311:PRO:HD3	2.34	0.43
1:B:33:VAL:HA	1:B:37:LEU:HG	2.01	0.42
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.80	0.42
1:F:376:TYR:CG	1:F:474:PRO:HD3	2.54	0.42
1:A:322:ILE:HG22	1:A:464:ARG:HD2	2.01	0.42
1:F:240:SER:HA	1:F:289:SER:O	2.18	0.42
1:B:325:PHE:CZ	1:B:457:GLU:HA	2.54	0.42
1:C:76:ASN:HD22	1:C:95:LEU:HG	1.83	0.42
1:E:97:TRP:HZ2	2:E:601:DIO:H22	1.83	0.42
1:A:130:ARG:HB3	1:A:134:ASP:OD2	2.19	0.42
1:E:91:ARG:NH2	1:E:314:ILE:HD11	2.34	0.42
1:F:141:TYR:O	1:F:154:ARG:HD3	2.18	0.42
1:F:359:PRO:HB3	1:F:374:ILE:HG13	2.00	0.42
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.73	0.42
1:D:6:MET:HB2	1:D:394:ILE:HB	2.01	0.42
1:C:34:TYR:HB2	1:C:315:ALA:HB2	2.01	0.42
1:E:144:HIS:HA	1:E:145:PRO:HD3	1.90	0.42
1:F:106:GLY:O	1:F:108:ASN:N	2.53	0.42
1:F:478:ASP:HA	1:F:479:LYS:HB3	2.01	0.42
1:A:23:GLY:O	1:A:349:CYS:HA	2.20	0.42
1:E:444:GLY:HA3	1:E:445:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:TRP:HZ2	2:F:601:DIO:H22	1.85	0.42
1:F:449:ARG:N	1:F:482:PHE:HE2	2.18	0.42
1:C:159:VAL:HG12	1:C:161:GLU:O	2.20	0.42
1:C:257:ALA:HA	1:C:430:ARG:HH21	1.84	0.42
1:E:29:LEU:HD21	1:E:319:LEU:HD13	2.02	0.41
1:E:125:VAL:O	1:E:171:GLY:HA2	2.19	0.41
1:B:302:GLU:O	1:B:306:ILE:HG13	2.20	0.41
1:D:173:GLU:O	1:D:179:GLN:HG3	2.20	0.41
1:D:400:ASP:OD1	1:D:400:ASP:N	2.54	0.41
1:F:76:ASN:HB2	1:F:180:VAL:HG21	2.02	0.41
1:B:456:LEU:HB2	1:B:496:TRP:CD1	2.56	0.41
1:C:291:ASP:O	1:C:292:GLU:HG3	2.21	0.41
1:E:262:LEU:HD11	1:E:290:PHE:CZ	2.56	0.41
1:A:351:ALA:HA	1:A:352:GLN:HA	1.76	0.41
1:B:174:MET:HE3	1:B:174:MET:HB2	1.88	0.41
1:C:12:TYR:CZ	1:E:12:TYR:CE2	3.08	0.41
1:C:216:LYS:HB2	1:C:216:LYS:HE3	1.82	0.41
1:F:298:HIS:HE1	1:F:327:ASP:OD2	2.04	0.41
1:C:87:GLU:H	1:C:87:GLU:CD	2.23	0.41
1:F:91:ARG:O	1:F:92:ARG:HD2	2.21	0.41
1:F:430:ARG:H	1:F:430:ARG:HG3	1.52	0.41
1:F:475:LYS:C	1:F:477:SER:H	2.24	0.41
1:F:487:LEU:HD21	1:F:499:ILE:HG21	2.03	0.41
1:A:144:HIS:HA	1:A:145:PRO:HD3	1.79	0.41
1:D:144:HIS:HA	1:D:145:PRO:HD3	1.94	0.41
1:F:23:GLY:HA2	1:F:63:VAL:HG13	2.03	0.41
1:F:24:SER:O	1:F:66:ILE:HA	2.21	0.41
1:F:229:LEU:HD23	1:F:229:LEU:HA	1.88	0.41
1:B:173[B]:GLU:CD	1:B:173[B]:GLU:H	2.24	0.41
1:B:203:ASP:O	1:B:206:ILE:HG12	2.21	0.41
1:F:478:ASP:HB3	1:F:479:LYS:C	2.41	0.41
1:A:42:ASN:OD1	1:A:43:SER:N	2.53	0.40
1:B:241:LEU:CD2	1:B:269:VAL:HG21	2.42	0.40
1:E:53:ASP:OD1	1:E:53:ASP:N	2.54	0.40
1:F:450:LEU:HD12	1:F:451:LEU:N	2.35	0.40
1:A:173:GLU:H	1:A:173:GLU:CD	2.25	0.40
1:E:34:TYR:HB2	1:E:315:ALA:HB2	2.03	0.40
1:F:31:ARG:HD2	1:F:35:ASP:OD2	2.22	0.40
1:C:27:GLU:HG2	1:C:29:LEU:HB2	2.03	0.40
1:D:31:ARG:HD2	1:D:35:ASP:OD2	2.21	0.40
1:F:25:PHE:O	1:F:352:GLN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:TYR:HD1	1:F:379:MET:HE2	1.86	0.40
1:C:311:PRO:HB2	1:C:312:TRP:CD1	2.56	0.40
1:C:363:GLU:O	1:C:364:ARG:HB2	2.22	0.40
1:D:209:VAL:HG22	1:D:238:TYR:HB2	2.04	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	494/501 (99%)	455 (92%)	28 (6%)	11 (2%)	6 9
1	B	491/501 (98%)	456 (93%)	26 (5%)	9 (2%)	8 11
1	C	494/501 (99%)	449 (91%)	35 (7%)	10 (2%)	7 10
1	D	494/501 (99%)	450 (91%)	33 (7%)	11 (2%)	6 9
1	E	491/501 (98%)	451 (92%)	28 (6%)	12 (2%)	6 7
1	F	491/501 (98%)	447 (91%)	35 (7%)	9 (2%)	8 11
All	All	2955/3006 (98%)	2708 (92%)	185 (6%)	62 (2%)	7 9

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	364	ARG
1	A	470	GLU
1	A	471	GLU
1	B	364	ARG
1	C	364	ARG
1	C	479	LYS
1	D	173	GLU

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Mol	Chain	Res	Type
1	D	364	ARG
1	D	478	ASP
1	D	484	ASP
1	E	173[A]	GLU
1	E	173[B]	GLU
1	E	364	ARG
1	F	364	ARG
1	A	46	ASP
1	A	297	TYR
1	A	368	ALA
1	B	357	ILE
1	B	471	GLU
1	C	367	GLY
1	C	478	ASP
1	D	367	GLY
1	D	483	ASP
1	E	309	ASN
1	E	367	GLY
1	E	483	ASP
1	E	484	ASP
1	F	107	ILE
1	F	173[A]	GLU
1	F	173[B]	GLU
1	F	309	ASN
1	A	42	ASN
1	A	476	ASN
1	B	46	ASP
1	B	308	GLN
1	B	478	ASP
1	B	484	ASP
1	C	482	PHE
1	E	40	PRO
1	E	297	TYR
1	F	297	TYR
1	F	477	SER
1	A	173	GLU
1	B	173[A]	GLU
1	B	173[B]	GLU
1	C	443	ARG
1	C	484	ASP
1	D	480	SER
1	F	369	ALA

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Mol	Chain	Res	Type
1	C	173	GLU
1	C	369	ALA
1	D	368	ALA
1	D	369	ALA
1	D	477	SER
1	E	369	ALA
1	A	357	ILE
1	E	107	ILE
1	C	357	ILE
1	D	357	ILE
1	F	357	ILE
1	E	357	ILE

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%)	417 (97%)	12 (3%)	43	61
1	B	428/439 (98%)	413 (96%)	15 (4%)	36	53
1	C	427/439 (97%)	415 (97%)	12 (3%)	43	61
1	D	427/439 (97%)	415 (97%)	12 (3%)	43	61
1	E	428/439 (98%)	417 (97%)	11 (3%)	46	65
1	F	428/439 (98%)	415 (97%)	13 (3%)	41	59
All	All	2567/2634 (98%)	2492 (97%)	75 (3%)	42	60

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	29	LEU
1	A	47	GLU
1	A	53	ASP
1	A	174	MET
1	A	290	PHE

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Mol	Chain	Res	Type
1	A	321	ASP
1	A	432	ILE
1	A	442	VAL
1	A	451	LEU
1	A	455	VAL
1	A	488	THR
1	B	12	TYR
1	B	17	ILE
1	B	29	LEU
1	B	86	VAL
1	B	174	MET
1	B	290	PHE
1	B	307	MET
1	B	415	ILE
1	B	430	ARG
1	B	442	VAL
1	B	445	MET
1	B	478	ASP
1	B	488	THR
1	B	489	SER
1	B	490	MET
1	C	12	TYR
1	C	17	ILE
1	C	29	LEU
1	C	107	ILE
1	C	112	LYS
1	C	290	PHE
1	C	415	ILE
1	C	436	ILE
1	C	451	LEU
1	C	453	HIS
1	C	455	VAL
1	C	484	ASP
1	D	6	MET
1	D	12	TYR
1	D	121	ILE
1	D	290	PHE
1	D	396	SER
1	D	400	ASP
1	D	415	ILE
1	D	430	ARG
1	D	455	VAL

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Mol	Chain	Res	Type
1	D	488	THR
1	D	490	MET
1	D	501	ILE
1	E	7	THR
1	E	12	TYR
1	E	17	ILE
1	E	37	LEU
1	E	40	PRO
1	E	87	GLU
1	E	174	MET
1	E	290	PHE
1	E	394	ILE
1	E	482	PHE
1	E	483	ASP
1	F	7	THR
1	F	12	TYR
1	F	14	ILE
1	F	29	LEU
1	F	87	GLU
1	F	249	GLU
1	F	290	PHE
1	F	307	MET
1	F	415	ILE
1	F	430	ARG
1	F	482	PHE
1	F	484	ASP
1	F	501	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	D	476	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DIO	D	601	-	6,6,6	0.58	0	6,6,6	0.97	0
2	DIO	C	601	-	6,6,6	0.58	0	6,6,6	0.80	0
2	DIO	F	601	-	6,6,6	0.51	0	6,6,6	0.72	0
2	DIO	E	601	-	6,6,6	0.56	0	6,6,6	1.08	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	DIO	D	601	-	-	-	0/1/1/1
2	DIO	C	601	-	-	-	0/1/1/1
2	DIO	F	601	-	-	-	0/1/1/1
2	DIO	E	601	-	-	-	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.

4 monomers are involved in 8 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	498/501 (99%)	-0.09	5 (1%)	82	81	19, 38, 79, 114	0
1	B	496/501 (99%)	-0.31	11 (2%)	62	58	17, 35, 68, 104	0
1	C	498/501 (99%)	-0.23	14 (2%)	53	49	18, 37, 76, 111	0
1	D	498/501 (99%)	-0.07	20 (4%)	38	35	19, 39, 72, 98	0
1	E	496/501 (99%)	-0.07	14 (2%)	53	49	20, 39, 81, 106	0
1	F	496/501 (99%)	-0.08	13 (2%)	56	52	19, 40, 84, 113	0
All	All	2982/3006 (99%)	-0.14	77 (2%)	56	52	17, 38, 78, 114	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	488	THR	4.8
1	C	501	ILE	4.5
1	E	437	VAL	4.4
1	F	487	LEU	4.3
1	B	484	ASP	4.1
1	B	482	PHE	4.0
1	F	490	MET	4.0
1	D	5	ARG	3.9
1	F	445	MET	3.9
1	D	12	TYR	3.9
1	D	487	LEU	3.8
1	C	483	ASP	3.7
1	F	485	GLY	3.6
1	C	484	ASP	3.6
1	C	482	PHE	3.5
1	C	486	ILE	3.5
1	C	445	MET	3.5
1	A	484	ASP	3.4
1	C	488	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	439	VAL	3.4
1	B	5	ARG	3.3
1	C	416	TYR	3.2
1	E	307	MET	3.2
1	E	486	ILE	3.2
1	A	305	ASN	3.1
1	D	488	THR	3.0
1	E	304	ALA	3.0
1	E	5	ARG	2.9
1	C	398	LEU	2.9
1	E	441	ASP	2.8
1	E	305	ASN	2.8
1	D	436	ILE	2.8
1	B	490	MET	2.8
1	C	5	ARG	2.8
1	D	450	LEU	2.8
1	D	309	ASN	2.8
1	F	309	ASN	2.8
1	B	439	VAL	2.7
1	E	490	MET	2.7
1	E	309	ASN	2.7
1	F	486	ILE	2.7
1	A	5	ARG	2.7
1	C	485	GLY	2.6
1	B	488	THR	2.6
1	D	486	ILE	2.6
1	F	5	ARG	2.6
1	D	439	VAL	2.6
1	D	432	ILE	2.6
1	F	368	ALA	2.6
1	B	483	ASP	2.5
1	D	398	LEU	2.5
1	E	483	ASP	2.5
1	A	432	ILE	2.5
1	F	8	VAL	2.5
1	C	444	GLY	2.4
1	D	485	GLY	2.4
1	E	499	ILE	2.3
1	F	439	VAL	2.3
1	B	486	ILE	2.3
1	C	490	MET	2.3
1	A	365	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	490	MET	2.3
1	D	437	VAL	2.3
1	F	484	ASP	2.3
1	D	480	SER	2.2
1	D	302	GLU	2.2
1	B	445	MET	2.2
1	E	476	ASN	2.2
1	B	431	ASN	2.1
1	D	478	ASP	2.1
1	C	439	VAL	2.1
1	F	74	VAL	2.1
1	B	485	GLY	2.1
1	F	440	SER	2.1
1	D	304	ALA	2.0
1	D	308	GLN	2.0
1	D	445	MET	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DIO	E	601	6/6	0.77	0.34	33,46,49,50	0
2	DIO	D	601	6/6	0.82	0.33	38,44,51,51	0
2	DIO	F	601	6/6	0.84	0.25	39,49,49,49	0
2	DIO	C	601	6/6	0.92	0.26	32,45,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.