Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 06:08 PM JST

PDB ID	:	9JFL
Title	:	Molecular basis of the phosphorothioation-sensing antiphage defence system DndBCDE-DndI
Authors	:	Dan, W.
Deposited on	:	2024-09-04
Resolution	:	3.00 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:

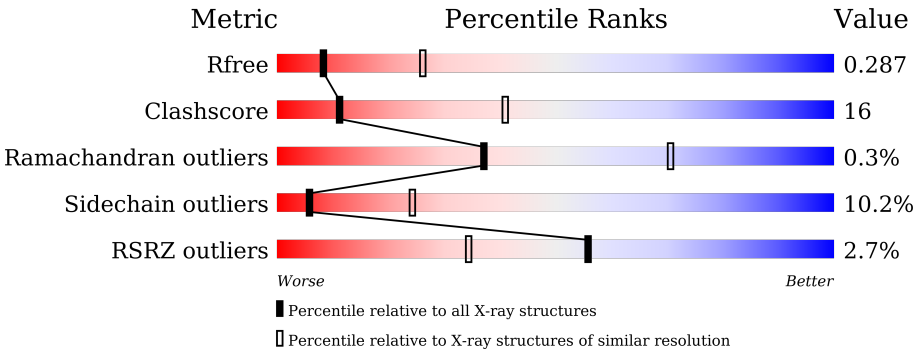
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	596	2% 71% 24% 5%
1	B	596	3% 66% 30% . .

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	EDO	B	602	-	-	X	-

2 Entry composition

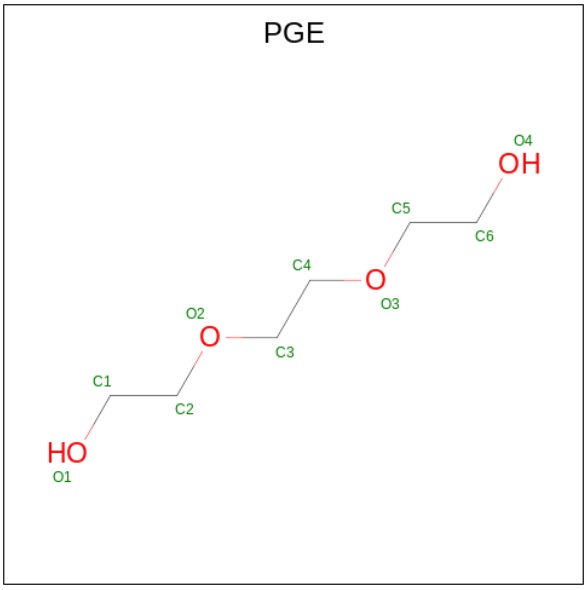
There are 4 unique types of molecules in this entry. The entry contains 9861 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DUF262 domain-containing protein.

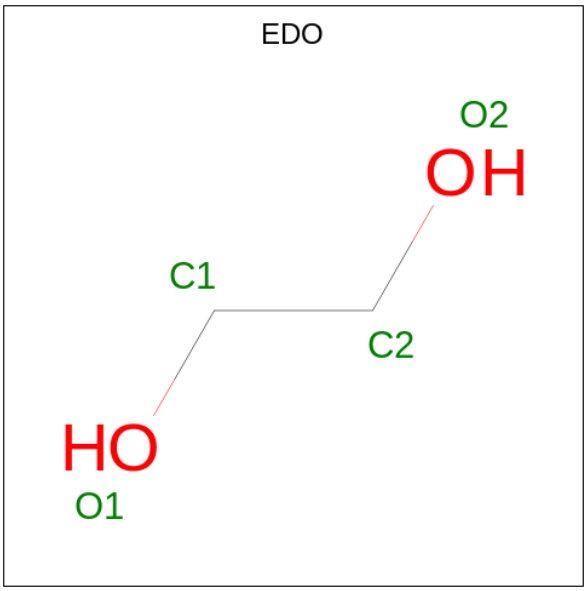
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	588	Total	C	N	O	S	0	0	0
			4860	3096	829	915	20			
1	A	594	Total	C	N	O	S	0	0	0
			4909	3126	839	924	20			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

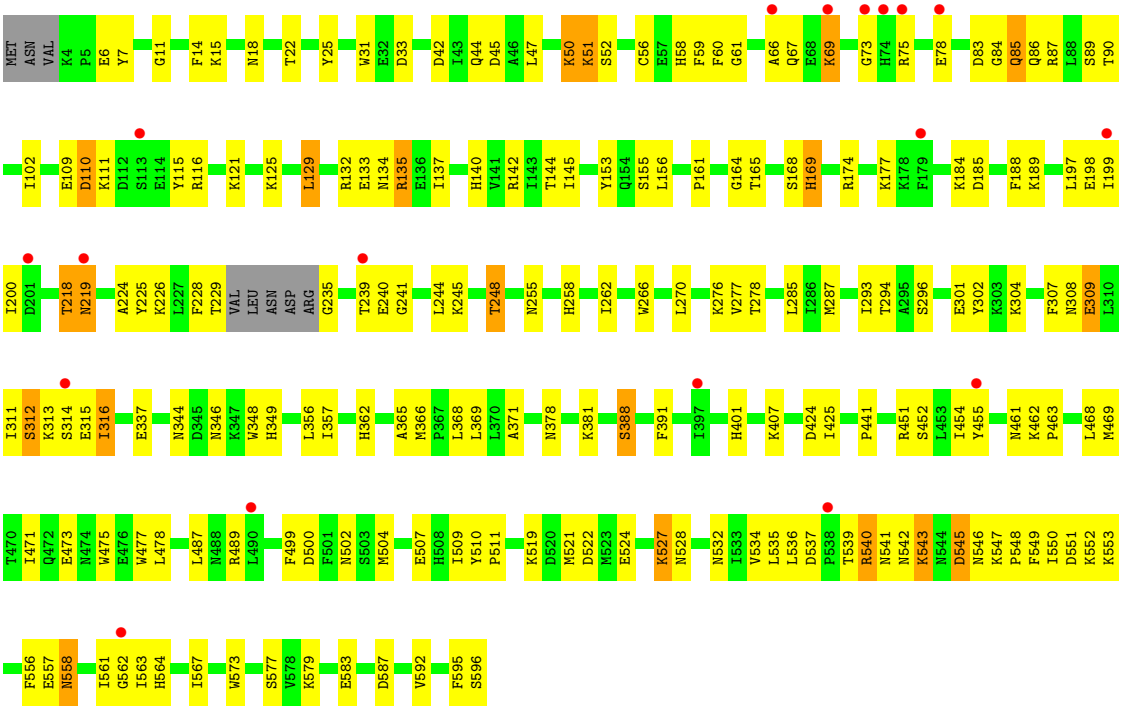
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	30	Total O 30 30	0	0
4	A	40	Total O 40 40	0	0

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.

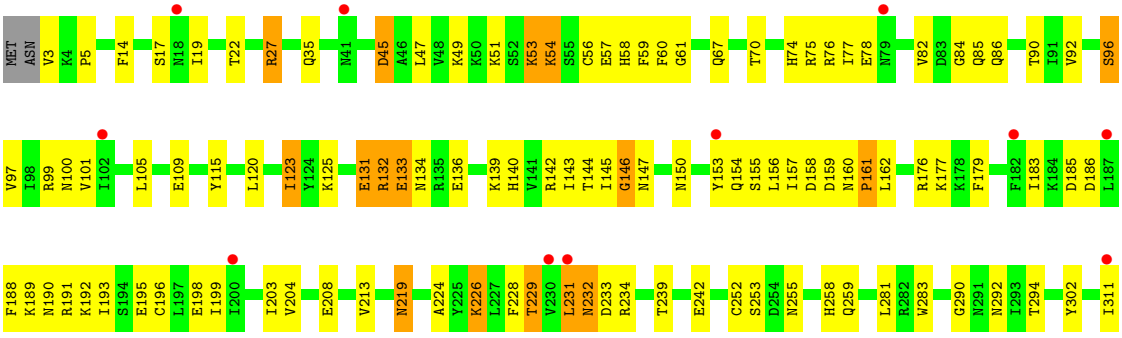
• Molecule 1: DUF262 domain-containing protein

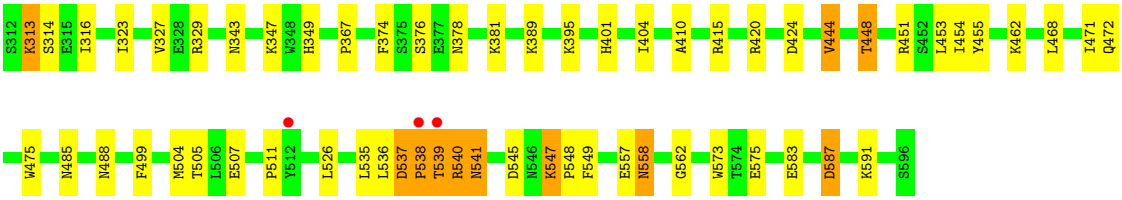
Chain B:



• Molecule 1: DUF262 domain-containing protein

Chain A:




S312
K313
S314
E315
I316
I323
V327
E328
R329
N343
K347
W348
H349
P367
F374
S375
S376
E377
N378
K381
K389
K395
H401
I404
A410
R415
R420
D424
V444
T448
R451
S452
L453
I454
Y455
K462
L468
I471
Q472
W475
N485
N488
F499
M504
T505
L506
E507
P511
Y512
L526
L535
L536
D537
P538
T539
R540
N541
D545
N546
K547
P548
F549
E557
N558
G562
W573
T574
E575
E583
D587
K591
S596

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	103.38Å 135.08Å 225.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 3.00 47.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.02-3.00) 99.5 (47.02-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.286 0.226 , 0.287	Depositor DCC
R_{free} test set	1610 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	85.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9861	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: EDO, PGE

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	0.45	2/5009 (0.0%)	0.66	2/6747 (0.0%)
1	B	0.43	0/4959	0.64	0/6677
All	All	0.44	2/9968 (0.0%)	0.65	2/13424 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	PRO	N-CD	5.42	1.55	1.47
1	A	538	PRO	N-CD	5.06	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	537	ASP	C-N-CD	5.85	140.68	128.40
1	A	160	ASN	C-N-CD	5.45	139.85	128.40

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	4909	0	4877	139	0
1	B	4860	0	4824	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	14	0	0
3	A	8	0	12	3	0
3	B	4	0	6	4	0
4	A	40	0	0	2	0
4	B	30	0	0	1	0
All	All	9861	0	9733	313	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 16.

All (313) 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:105:LEU:HD13	1:A:193:ILE:HG21	1.29	1.10
1:B:309:GLU:HA	1:B:312:SER:HB3	1.13	1.09
1:B:545:ASP:CB	1:B:552:LYS:HE3	1.84	1.07
1:B:545:ASP:HB3	1:B:552:LYS:HE3	1.44	1.00
1:B:309:GLU:CA	1:B:312:SER:HB3	1.95	0.96
1:B:309:GLU:HA	1:B:312:SER:CB	1.99	0.93
1:A:57:GLU:HG2	1:A:59:PHE:CZ	2.05	0.92
1:A:226:LYS:O	1:A:229:THR:HG22	1.71	0.91
1:B:545:ASP:HB2	1:B:552:LYS:HE3	1.54	0.89
1:B:307:PHE:HD1	1:B:316:ILE:HG23	1.35	0.88
1:B:309:GLU:OE2	1:B:309:GLU:N	2.05	0.88
1:B:489:ARG:HG2	1:B:489:ARG:HH11	1.39	0.86
1:B:239:THR:HG22	1:B:240:GLU:N	1.91	0.84
1:A:232:ASN:HD22	1:A:233:ASP:N	1.77	0.83
1:A:35:GLN:HG3	1:A:234:ARG:HH21	1.44	0.82
1:A:105:LEU:CD1	1:A:193:ILE:HG21	2.10	0.82
1:B:307:PHE:HD1	1:B:316:ILE:CG2	1.93	0.81
1:B:307:PHE:CD1	1:B:316:ILE:HG23	2.15	0.81
1:A:233:ASP:O	1:A:234:ARG:HG3	1.80	0.80
1:B:307:PHE:CD1	1:B:316:ILE:CG2	2.66	0.78
1:B:125:LYS:O	1:B:142:ARG:CD	2.31	0.78
1:A:539:THR:OG1	1:A:540:ARG:HD2	1.84	0.77
1:B:312:SER:HA	1:B:316:ILE:HD11	1.67	0.77
1:A:60:PHE:CE1	1:A:84:GLY:HA2	2.20	0.76
1:B:536:LEU:HD13	1:B:543:LYS:HE3	1.65	0.76
1:B:549:PHE:CD2	1:B:573:TRP:HB2	2.21	0.75
1:A:57:GLU:HG2	1:A:59:PHE:CE2	2.22	0.74
1:B:308:ASN:O	1:B:311:ILE:HB	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ASN:HD22	1:A:541:ASN:H	1.33	0.74
1:A:59:PHE:O	1:A:213:VAL:HG12	1.89	0.73
1:B:308:ASN:O	1:B:312:SER:N	2.22	0.72
1:B:535:LEU:O	1:B:561:ILE:CD1	2.36	0.72
1:B:316:ILE:HD13	1:B:316:ILE:N	2.04	0.72
1:B:509:ILE:HD11	1:B:534:VAL:HG23	1.71	0.72
1:A:75:ARG:NH2	1:A:140:HIS:HB2	2.05	0.72
1:A:99:ARG:NH2	1:A:157:ILE:O	2.22	0.71
1:A:539:THR:CB	1:A:540:ARG:HD2	2.20	0.71
1:A:92:VAL:HG12	1:A:157:ILE:HD12	1.72	0.70
1:B:489:ARG:HG2	1:B:489:ARG:NH1	1.99	0.70
1:A:153:TYR:CE1	1:A:157:ILE:HD11	2.27	0.70
1:A:156:LEU:CD1	1:A:161:PRO:HB3	2.22	0.70
1:A:537:ASP:CG	1:A:540:ARG:HD3	2.11	0.70
1:A:538:PRO:HG2	1:A:539:THR:H	1.55	0.69
1:B:362:HIS:ND1	1:B:391:PHE:CD1	2.60	0.69
1:B:66:ALA:HA	1:B:218:THR:HG22	1.74	0.69
1:B:313:LYS:HG2	1:B:313:LYS:O	1.94	0.68
1:B:235:GLY:N	1:A:231:LEU:HD23	2.09	0.68
1:B:239:THR:HG23	1:B:278:THR:HG22	1.76	0.68
1:A:229:THR:HG21	4:A:737:HOH:O	1.94	0.67
1:A:154:GLN:OE1	1:A:154:GLN:HA	1.94	0.67
1:B:239:THR:HG22	1:B:240:GLU:H	1.57	0.67
1:B:539:THR:O	1:B:541:ASN:N	2.28	0.67
1:B:156:LEU:HD12	1:B:161:PRO:HB3	1.77	0.66
1:B:557:GLU:HG3	1:B:558:ASN:N	2.10	0.66
1:A:311:ILE:O	1:A:311:ILE:HG22	1.96	0.66
1:B:225:TYR:CE2	1:B:229:THR:HG21	2.31	0.66
1:B:561:ILE:HD11	1:B:564:HIS:CE1	2.30	0.65
1:B:536:LEU:CD1	1:B:543:LYS:HB3	2.26	0.65
1:B:125:LYS:O	1:B:142:ARG:HD2	1.95	0.65
1:B:547:LYS:N	1:B:552:LYS:HD2	2.11	0.65
1:A:22:THR:HG22	1:A:85:GLN:HG2	1.78	0.64
1:B:535:LEU:O	1:B:561:ILE:HD12	1.97	0.64
1:B:477:TRP:CE2	1:B:489:ARG:HB2	2.32	0.64
1:B:239:THR:CG2	1:B:240:GLU:N	2.59	0.64
1:A:125:LYS:O	1:A:142:ARG:HD3	1.98	0.64
1:A:401:HIS:O	1:A:404:ILE:HG22	1.97	0.64
1:A:57:GLU:CG	1:A:59:PHE:CZ	2.79	0.63
1:A:132:ARG:HH21	1:A:132:ARG:HG3	1.63	0.63
1:A:123:ILE:HD11	1:A:204:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:OE2	1:A:133:GLU:HG2	1.99	0.63
1:A:58:HIS:CE1	1:A:61:GLY:HA3	2.34	0.62
1:B:561:ILE:HD11	1:B:564:HIS:NE2	2.14	0.62
1:A:14:PHE:O	1:A:142:ARG:NH2	2.33	0.62
1:B:308:ASN:CG	1:B:311:ILE:HG12	2.20	0.62
1:A:233:ASP:O	1:A:234:ARG:CG	2.48	0.62
1:A:507:GLU:HB2	1:A:536:LEU:HD11	1.82	0.61
1:A:539:THR:OG1	1:A:540:ARG:NH1	2.33	0.61
1:A:541:ASN:HD22	1:A:541:ASN:N	1.98	0.61
1:B:308:ASN:ND2	1:B:311:ILE:HG12	2.14	0.61
1:B:499:PHE:HB3	1:B:504:MET:HE1	1.83	0.60
1:A:53:LYS:HG3	1:A:54:LYS:H	1.67	0.60
1:A:468:LEU:HD22	3:A:601:EDO:H11	1.84	0.60
1:A:229:THR:CG2	4:A:737:HOH:O	2.50	0.60
1:B:60:PHE:CZ	1:B:84:GLY:HA2	2.37	0.59
1:A:75:ARG:HH21	1:A:140:HIS:HB2	1.67	0.59
1:A:538:PRO:HG2	1:A:539:THR:N	2.17	0.59
1:B:18:ASN:O	1:B:142:ARG:NH2	2.35	0.59
1:A:75:ARG:CZ	1:A:140:HIS:HB2	2.33	0.59
1:B:266:TRP:O	1:B:270:LEU:HG	2.02	0.59
1:B:524:GLU:OE1	1:B:527:LYS:NZ	2.34	0.59
1:B:58:HIS:NE2	1:B:61:GLY:HA3	2.18	0.59
1:B:499:PHE:HB3	1:B:504:MET:CE	2.33	0.59
1:B:344:ASN:HB3	1:B:346:ASN:ND2	2.18	0.59
1:B:66:ALA:O	1:B:67:GLN:HG3	2.02	0.59
1:B:75:ARG:HG3	1:B:140:HIS:CB	2.33	0.59
1:B:239:THR:CG2	1:B:240:GLU:H	2.16	0.59
1:B:545:ASP:HB2	1:B:552:LYS:CE	2.30	0.58
1:A:58:HIS:NE2	1:A:61:GLY:HA3	2.19	0.58
1:B:58:HIS:CE1	1:B:61:GLY:HA3	2.38	0.58
1:B:451:ARG:NH1	1:B:583:GLU:OE1	2.37	0.58
1:B:296:SER:HB3	1:A:234:ARG:HH11	1.68	0.57
1:A:96:SER:HB3	1:A:157:ILE:HG23	1.85	0.57
1:B:22:THR:HG22	1:B:85:GLN:HG2	1.86	0.57
1:A:47:LEU:O	1:A:51:LYS:HE2	2.05	0.57
1:B:239:THR:HG21	1:B:277:VAL:CG1	2.35	0.57
1:B:537:ASP:O	1:B:543:LYS:HD3	2.05	0.57
1:B:547:LYS:HB3	1:B:548:PRO:HD2	1.86	0.57
1:B:60:PHE:CE2	1:B:84:GLY:HA2	2.40	0.56
1:B:218:THR:HG21	1:B:224:ALA:HB2	1.87	0.56
1:B:309:GLU:C	1:B:312:SER:H	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ARG:HH11	1:B:489:ARG:CG	2.14	0.56
1:B:316:ILE:HD13	1:B:316:ILE:H	1.69	0.56
1:A:27:ARG:NE	1:A:242:GLU:OE2	2.32	0.56
1:A:451:ARG:NH1	1:A:583:GLU:OE2	2.38	0.55
1:B:308:ASN:OD1	1:B:311:ILE:HG12	2.06	0.55
1:B:452:SER:O	1:B:454:ILE:HD12	2.06	0.55
1:B:102:ILE:HD11	1:B:200:ILE:HD12	1.89	0.55
1:B:308:ASN:ND2	1:B:311:ILE:CG1	2.69	0.55
1:B:507:GLU:HB2	1:B:536:LEU:HG	1.89	0.55
1:B:537:ASP:OD1	1:B:539:THR:HB	2.06	0.54
1:A:156:LEU:HD13	1:A:161:PRO:HB3	1.90	0.54
1:B:14:PHE:O	1:B:142:ARG:NH1	2.41	0.54
1:B:51:LYS:N	1:B:51:LYS:HD2	2.22	0.54
1:B:534:VAL:HG21	1:B:567:ILE:HD13	1.90	0.53
1:A:156:LEU:HD12	1:A:161:PRO:HB3	1.90	0.53
1:B:60:PHE:CE1	3:B:602:EDO:H21	2.42	0.53
1:B:75:ARG:HG3	1:B:140:HIS:HB3	1.89	0.53
1:B:188:PHE:CD1	1:B:199:ILE:HD11	2.43	0.53
1:B:58:HIS:CE1	1:B:61:GLY:CA	2.91	0.53
1:B:557:GLU:HB2	4:B:704:HOH:O	2.09	0.53
1:A:232:ASN:HD22	1:A:232:ASN:C	2.08	0.53
1:A:537:ASP:OD1	1:A:538:PRO:HD2	2.09	0.53
1:B:7:TYR:CZ	1:A:219:ASN:HB2	2.44	0.52
1:A:76:ARG:NH1	1:A:77:ILE:HD11	2.25	0.52
1:B:102:ILE:O	1:B:116:ARG:NH2	2.42	0.52
1:B:296:SER:HB3	1:A:234:ARG:NH1	2.24	0.52
1:B:511:PRO:HG3	1:B:547:LYS:O	2.09	0.52
1:A:226:LYS:O	1:A:229:THR:CG2	2.53	0.52
1:A:471:ILE:HG13	3:A:601:EDO:H22	1.90	0.52
1:B:239:THR:HG23	1:B:278:THR:CG2	2.38	0.52
1:A:349:HIS:CG	1:A:381:LYS:HG2	2.45	0.52
1:B:244:LEU:O	1:B:248:THR:HB	2.09	0.52
1:B:545:ASP:N	1:B:545:ASP:OD1	2.42	0.52
1:B:248:THR:CG2	1:B:262:ILE:HG21	2.40	0.52
1:B:536:LEU:HD12	1:B:543:LYS:HB3	1.91	0.52
1:B:31:TRP:CZ3	1:B:90:THR:HG21	2.45	0.51
1:A:53:LYS:CG	1:A:54:LYS:H	2.22	0.51
1:B:110:ASP:OD1	1:B:110:ASP:O	2.29	0.51
1:B:536:LEU:HD13	1:B:543:LYS:HB3	1.91	0.51
1:A:444:VAL:O	1:A:448:THR:HG22	2.10	0.51
1:A:199:ILE:O	1:A:203:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASP:O	1:A:159:ASP:HB3	2.11	0.51
1:B:307:PHE:CE1	1:B:316:ILE:HG22	2.46	0.51
1:B:475:TRP:CE2	1:B:562:GLY:HA3	2.46	0.51
1:B:188:PHE:HD1	1:B:199:ILE:HD11	1.75	0.51
1:A:192:LYS:O	1:A:195:GLU:N	2.43	0.51
1:B:468:LEU:O	1:B:469:MET:C	2.49	0.50
1:A:58:HIS:CE1	1:A:61:GLY:CA	2.94	0.50
1:B:109:GLU:O	1:B:111:LYS:HG2	2.12	0.50
1:B:225:TYR:O	1:B:229:THR:HG23	2.10	0.50
1:B:500:ASP:OD1	1:B:502:ASN:N	2.44	0.50
1:B:59:PHE:O	1:B:60:PHE:C	2.48	0.50
1:B:534:VAL:HG21	1:B:567:ILE:CD1	2.42	0.50
1:B:42:ASP:CB	1:B:59:PHE:HZ	2.25	0.49
1:B:308:ASN:H	1:B:311:ILE:HB	1.77	0.49
1:B:125:LYS:O	1:B:142:ARG:NE	2.45	0.49
1:A:133:GLU:CD	1:A:134:ASN:H	2.15	0.49
1:A:541:ASN:N	1:A:541:ASN:ND2	2.60	0.49
1:B:478:LEU:HD21	1:B:592:VAL:HG23	1.93	0.49
1:A:75:ARG:NE	1:A:140:HIS:HB2	2.26	0.49
1:A:224:ALA:O	1:A:228:PHE:CE2	2.65	0.49
1:A:349:HIS:CE1	1:A:381:LYS:HB3	2.48	0.49
1:B:42:ASP:HB3	1:B:59:PHE:HZ	1.76	0.49
1:A:311:ILE:O	1:A:311:ILE:CG2	2.60	0.49
1:A:541:ASN:H	1:A:541:ASN:ND2	2.08	0.49
1:A:105:LEU:CD1	1:A:193:ILE:CG2	2.86	0.49
1:B:102:ILE:HD11	1:B:200:ILE:CD1	2.43	0.48
1:B:258:HIS:CD2	1:B:314:SER:HB2	2.48	0.48
1:A:190:ASN:O	1:A:190:ASN:ND2	2.46	0.48
1:B:312:SER:O	1:B:312:SER:OG	2.28	0.48
1:B:42:ASP:HB3	1:B:59:PHE:CZ	2.48	0.48
1:B:60:PHE:HB2	1:B:87:ARG:HH11	1.79	0.48
1:B:73:GLY:HA2	1:B:78:GLU:HB3	1.94	0.48
1:B:287:MET:SD	1:B:371:ALA:HB2	2.53	0.48
1:B:337:GLU:OE1	1:A:462:LYS:HE2	2.12	0.48
1:B:85:GLN:O	1:B:89:SER:HB2	2.13	0.48
1:B:509:ILE:HD11	1:B:534:VAL:CG2	2.43	0.48
1:A:19:ILE:HG13	1:A:75:ARG:HB2	1.96	0.48
1:B:362:HIS:CD2	1:B:365:ALA:HB2	2.48	0.48
1:B:239:THR:HG21	1:B:277:VAL:HG12	1.94	0.48
1:B:60:PHE:O	1:B:61:GLY:C	2.52	0.48
1:B:135:ARG:H	1:B:135:ARG:HD3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLY:HA2	1:B:169:HIS:HD2	1.77	0.48
1:B:366:MET:HE2	1:B:369:LEU:HD12	1.97	0.47
1:A:185:ASP:O	1:A:189:LYS:HB2	2.13	0.47
1:A:323:ILE:O	1:A:327:VAL:HG23	2.14	0.47
1:B:33:ASP:OD1	1:B:174:ARG:NH2	2.47	0.47
1:A:86:GLN:O	1:A:90:THR:HG23	2.14	0.47
1:A:132:ARG:HH21	1:A:132:ARG:CG	2.27	0.47
1:B:185:ASP:O	1:B:189:LYS:HD3	2.15	0.47
1:B:135:ARG:HD3	1:B:135:ARG:N	2.28	0.47
1:B:579:LYS:O	1:B:583:GLU:HG2	2.15	0.47
1:A:150:ASN:O	1:A:154:GLN:HG2	2.15	0.47
1:A:191:ARG:HB2	1:A:196:CYS:SG	2.55	0.47
1:A:537:ASP:OD1	1:A:540:ARG:HD3	2.14	0.47
1:A:539:THR:C	1:A:540:ARG:HD2	2.35	0.47
1:B:7:TYR:OH	1:A:219:ASN:HB2	2.15	0.47
1:A:92:VAL:HB	1:A:153:TYR:OH	2.14	0.47
1:A:82:VAL:HG12	1:A:82:VAL:O	2.15	0.47
1:B:145:ILE:HD11	1:B:153:TYR:HB2	1.97	0.46
1:B:165:THR:HG22	1:B:165:THR:O	2.15	0.46
1:B:547:LYS:H	1:B:552:LYS:HD2	1.78	0.46
1:B:547:LYS:HB2	1:B:552:LYS:HG3	1.97	0.46
1:B:549:PHE:HD2	1:B:573:TRP:HB2	1.78	0.46
1:A:70:THR:HA	1:A:76:ARG:O	2.15	0.46
1:A:60:PHE:O	1:A:61:GLY:C	2.50	0.46
1:A:22:THR:CG2	1:A:145:ILE:HA	2.46	0.46
1:A:22:THR:HG23	1:A:145:ILE:HA	1.97	0.46
1:A:504:MET:HG2	1:A:535:LEU:CD1	2.46	0.46
1:A:311:ILE:HA	1:A:313:LYS:HD2	1.97	0.45
1:B:307:PHE:CE1	1:B:316:ILE:CG2	2.99	0.45
1:B:219:ASN:HA	1:A:5:PRO:HG3	1.97	0.45
1:B:311:ILE:HG22	1:B:316:ILE:CD1	2.47	0.45
1:B:235:GLY:N	1:A:231:LEU:CD2	2.79	0.45
1:B:239:THR:HG21	1:B:277:VAL:HG11	1.98	0.45
1:A:96:SER:CB	1:A:157:ILE:HG23	2.46	0.45
1:A:538:PRO:CG	1:A:539:THR:H	2.23	0.45
1:B:132:ARG:HG2	1:B:137:ILE:HG22	1.99	0.45
1:B:309:GLU:C	1:B:312:SER:HB3	2.35	0.45
1:A:101:VAL:CG1	1:A:188:PHE:HE2	2.30	0.45
1:B:534:VAL:HG12	1:B:535:LEU:O	2.17	0.45
1:A:329:ARG:CZ	1:A:374:PHE:CE1	3.00	0.45
1:A:444:VAL:O	1:A:448:THR:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:O	1:B:50:LYS:HB2	2.17	0.45
1:B:69:LYS:HB2	1:B:78:GLU:OE2	2.17	0.44
1:A:549:PHE:CD2	1:A:573:TRP:HB2	2.52	0.44
1:A:539:THR:C	1:A:540:ARG:CD	2.86	0.44
1:B:348:TRP:NE1	1:B:473:GLU:OE2	2.42	0.44
1:B:527:LYS:O	1:B:528:ASN:HB2	2.18	0.44
1:B:84:GLY:HA2	3:B:602:EDO:H12	1.99	0.44
1:B:135:ARG:HH21	1:B:135:ARG:HG3	1.81	0.44
1:A:193:ILE:HG22	1:A:193:ILE:O	2.17	0.44
1:A:290:GLY:HA2	1:A:410:ALA:O	2.18	0.44
1:B:132:ARG:NH2	1:B:134:ASN:O	2.49	0.43
1:B:135:ARG:HH21	1:B:135:ARG:CG	2.31	0.43
1:A:253:SER:HA	1:A:259:GLN:OE1	2.17	0.43
1:A:526:LEU:HD21	1:A:575:GLU:HG3	2.00	0.43
1:B:521:MET:HB3	1:B:521:MET:HE2	1.88	0.43
1:B:293:ILE:HD13	1:B:301:GLU:HG3	2.00	0.43
1:A:125:LYS:NZ	1:A:208:GLU:OE2	2.51	0.43
1:B:60:PHE:O	1:B:60:PHE:CG	2.70	0.43
1:A:258:HIS:NE2	1:A:314:SER:HB2	2.34	0.43
1:B:550:ILE:HG13	1:B:551:ASP:OD1	2.18	0.43
1:A:499:PHE:HB3	1:A:504:MET:CE	2.48	0.43
1:B:102:ILE:HD12	1:B:197:LEU:CD2	2.49	0.43
1:B:308:ASN:HB2	1:B:309:GLU:OE2	2.17	0.43
1:A:252:CYS:O	1:A:259:GLN:HG3	2.18	0.43
1:B:539:THR:O	1:B:540:ARG:C	2.56	0.43
1:A:504:MET:CG	1:A:535:LEU:CD1	2.96	0.43
1:B:595:PHE:O	1:B:596:SER:HB3	2.18	0.43
1:A:100:ASN:HD21	1:A:159:ASP:HB2	1.84	0.43
1:A:499:PHE:HB3	1:A:504:MET:HE2	2.01	0.43
1:A:45:ASP:O	1:A:49:LYS:HG2	2.19	0.42
1:B:102:ILE:CG2	1:B:116:ARG:HG2	2.49	0.42
1:B:311:ILE:HG22	1:B:316:ILE:HD12	2.01	0.42
1:B:11:GLY:O	1:B:15:LYS:N	2.49	0.42
1:B:462:LYS:N	1:B:463:PRO:CD	2.82	0.42
1:A:57:GLU:CG	1:A:59:PHE:CE2	2.99	0.42
1:A:557:GLU:CG	1:A:558:ASN:N	2.83	0.42
1:B:14:PHE:HD2	1:B:142:ARG:HD3	1.83	0.42
1:B:543:LYS:N	1:B:543:LYS:HD2	2.34	0.42
1:A:485:ASN:O	1:A:488:ASN:HB3	2.19	0.42
1:A:504:MET:HG3	1:A:535:LEU:HD11	2.02	0.42
1:B:69:LYS:HG3	1:A:3:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:CE1	1:B:245:LYS:HE2	2.55	0.42
1:A:54:LYS:HE3	1:A:56:CYS:HB2	2.01	0.42
1:A:475:TRP:NE1	1:A:562:GLY:HA3	2.34	0.42
1:B:537:ASP:OD1	1:B:539:THR:N	2.52	0.42
1:B:563:ILE:O	1:B:563:ILE:HG13	2.20	0.42
1:A:97:VAL:HG11	1:A:179:PHE:HB3	2.01	0.42
1:A:125:LYS:O	1:A:142:ARG:CD	2.65	0.42
1:A:472:GLN:HB2	3:A:601:EDO:O2	2.20	0.42
1:B:461:ASN:C	1:B:463:PRO:HD2	2.40	0.42
1:B:365:ALA:O	1:B:368:LEU:HB3	2.19	0.41
1:A:74:HIS:O	1:A:75:ARG:NH1	2.45	0.41
1:B:239:THR:CG2	1:B:278:THR:HG22	2.48	0.41
1:A:511:PRO:HG3	1:A:548:PRO:HA	2.01	0.41
1:A:537:ASP:CG	1:A:540:ARG:CD	2.86	0.41
1:B:129:LEU:HD23	1:B:129:LEU:O	2.20	0.41
1:B:239:THR:HG22	1:B:241:GLY:H	1.85	0.41
1:A:17:SER:CB	1:A:76:ARG:HD3	2.51	0.41
1:B:349:HIS:CE1	1:B:381:LYS:HB3	2.55	0.41
1:B:510:TYR:HB3	1:B:532:ASN:OD1	2.20	0.41
1:A:19:ILE:HD13	1:A:19:ILE:HA	1.95	0.41
1:A:232:ASN:C	1:A:232:ASN:ND2	2.73	0.41
1:B:83:ASP:OD1	3:B:602:EDO:H22	2.20	0.41
1:A:232:ASN:HD22	1:A:233:ASP:H	1.59	0.41
1:B:86:GLN:HB2	3:B:602:EDO:H11	2.03	0.41
1:A:454:ILE:HG22	1:A:455:TYR:O	2.21	0.41
1:A:587:ASP:OD2	1:A:591:LYS:NZ	2.53	0.41
1:B:285:LEU:HD22	1:B:302:TYR:CD2	2.56	0.41
1:A:547:LYS:HB2	1:A:548:PRO:HD2	2.02	0.41
1:B:44:GLN:O	1:B:45:ASP:C	2.58	0.40
1:B:59:PHE:O	1:B:61:GLY:N	2.54	0.40
1:B:66:ALA:O	1:B:67:GLN:CG	2.68	0.40
1:A:475:TRP:CD1	1:A:562:GLY:HA3	2.56	0.40
1:A:539:THR:CB	1:A:540:ARG:HH11	2.33	0.40
1:B:504:MET:O	1:A:347:LYS:NZ	2.55	0.40
1:A:145:ILE:O	1:A:146:GLY:O	2.39	0.40
1:B:142:ARG:HH21	1:B:142:ARG:HG2	1.86	0.40
1:B:356:LEU:HD13	1:B:388:SER:HA	2.04	0.40
1:A:283:TRP:CD1	1:A:367:PRO:HD3	2.57	0.40
1:B:454:ILE:HG22	1:B:455:TYR:O	2.21	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	592/596 (99%)	522 (88%)	68 (12%)	2 (0%)	37 70
1	B	584/596 (98%)	519 (89%)	64 (11%)	1 (0%)	44 77
All	All	1176/1192 (99%)	1041 (88%)	132 (11%)	3 (0%)	37 70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ILE
1	B	441	PRO
1	A	146	GLY

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	554/556 (100%)	497 (90%)	57 (10%)	6 24
1	B	548/556 (99%)	493 (90%)	55 (10%)	6 25
All	All	1102/1112 (99%)	990 (90%)	112 (10%)	6 24

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	GLU
1	B	50	LYS
1	B	51	LYS

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Mol	Chain	Res	Type
1	B	52	SER
1	B	56	CYS
1	B	69	LYS
1	B	85	GLN
1	B	110	ASP
1	B	115	TYR
1	B	121	LYS
1	B	129	LEU
1	B	133	GLU
1	B	135	ARG
1	B	144	THR
1	B	155	SER
1	B	168	SER
1	B	169	HIS
1	B	177	LYS
1	B	184	LYS
1	B	198	GLU
1	B	218	THR
1	B	219	ASN
1	B	226	LYS
1	B	228	PHE
1	B	248	THR
1	B	255	ASN
1	B	276	LYS
1	B	294	THR
1	B	304	LYS
1	B	309	GLU
1	B	312	SER
1	B	315	GLU
1	B	316	ILE
1	B	357	ILE
1	B	378	ASN
1	B	388	SER
1	B	401	HIS
1	B	407	LYS
1	B	424	ASP
1	B	425	ILE
1	B	471	ILE
1	B	487	LEU
1	B	519	LYS
1	B	522	ASP
1	B	527	LYS

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Mol	Chain	Res	Type
1	B	540	ARG
1	B	542	ASN
1	B	543	LYS
1	B	545	ASP
1	B	546	ASN
1	B	553	LYS
1	B	556	PHE
1	B	558	ASN
1	B	577	SER
1	B	587	ASP
1	A	27	ARG
1	A	45	ASP
1	A	53	LYS
1	A	54	LYS
1	A	67	GLN
1	A	78	GLU
1	A	96	SER
1	A	109	GLU
1	A	115	TYR
1	A	120	LEU
1	A	123	ILE
1	A	131	GLU
1	A	132	ARG
1	A	133	GLU
1	A	136	GLU
1	A	139	LYS
1	A	143	ILE
1	A	144	THR
1	A	147	ASN
1	A	155	SER
1	A	162	LEU
1	A	176	ARG
1	A	177	LYS
1	A	183	ILE
1	A	186	ASP
1	A	198	GLU
1	A	219	ASN
1	A	226	LYS
1	A	229	THR
1	A	231	LEU
1	A	232	ASN
1	A	239	THR

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	281	LEU
1	A	292	ASN
1	A	294	THR
1	A	302	TYR
1	A	313	LYS
1	A	343	ASN
1	A	376	SER
1	A	378	ASN
1	A	389	LYS
1	A	395	LYS
1	A	415	ARG
1	A	420	ARG
1	A	424	ASP
1	A	444	VAL
1	A	448	THR
1	A	453	LEU
1	A	505	THR
1	A	539	THR
1	A	540	ARG
1	A	541	ASN
1	A	545	ASP
1	A	547	LYS
1	A	558	ASN
1	A	587	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	169	HIS
1	B	542	ASN
1	B	546	ASN
1	A	18	ASN
1	A	38	GLN
1	A	67	GLN
1	A	86	GLN
1	A	100	ASN
1	A	106	ASN
1	A	232	ASN
1	A	343	ASN
1	A	456	GLN
1	A	541	ASN

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Mol	Chain	Res	Type
1	A	544	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	601	-	3,3,3	0.91	0	2,2,2	0.57	0
3	EDO	B	602	-	3,3,3	0.38	0	2,2,2	0.80	0
2	PGE	B	601	-	9,9,9	0.53	0	8,8,8	0.18	0
3	EDO	A	602	-	3,3,3	0.67	0	2,2,2	0.29	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
3	EDO	A	601	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	602	-	-	0/1/1/1	-
2	PGE	B	601	-	-	4/7/7/7	-
3	EDO	A	602	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	PGE	O1-C1-C2-O2
3	A	601	EDO	O1-C1-C2-O2
3	A	602	EDO	O1-C1-C2-O2
2	B	601	PGE	C4-C3-O2-C2
2	B	601	PGE	C6-C5-O3-C4
2	B	601	PGE	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	EDO	3	0
3	B	602	EDO	4	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	594/596 (99%)	0.02	14 (2%)	59	37	48, 89, 142, 177	0
1	B	588/596 (98%)	0.01	18 (3%)	51	30	48, 87, 137, 229	0
All	All	1182/1192 (99%)	0.01	32 (2%)	56	34	48, 88, 139, 229	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	VAL	3.7
1	B	73	GLY	3.6
1	A	187	LEU	3.4
1	A	153	TYR	3.3
1	B	314	SER	3.3
1	B	219	ASN	3.2
1	B	78	GLU	3.1
1	B	562	GLY	3.1
1	A	200	ILE	3.0
1	A	231	LEU	2.9
1	B	455	TYR	2.8
1	A	311	ILE	2.8
1	B	66	ALA	2.8
1	B	74	HIS	2.6
1	A	512	TYR	2.6
1	B	199	ILE	2.6
1	A	41	ASN	2.6
1	B	75	ARG	2.5
1	B	201	ASP	2.5
1	A	182	PHE	2.4
1	B	113	SER	2.4
1	B	490	LEU	2.4
1	A	18	ASN	2.3
1	B	69	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	239	THR	2.2
1	A	102	ILE	2.2
1	A	538	PRO	2.1
1	A	539	THR	2.1
1	B	179	PHE	2.1
1	B	538	PRO	2.1
1	B	397	ILE	2.0
1	A	79	ASN	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	EDO	A	602	4/4	0.73	0.21	63,69,70,77	0
3	EDO	A	601	4/4	0.79	0.17	46,56,56,60	0
3	EDO	B	602	4/4	0.88	0.15	47,58,61,69	0
2	PGE	B	601	10/10	0.89	0.12	74,103,116,120	0

6.5 Other polymers (i)

There are no such residues in this entry.