



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BIW
Title : CRYSTAL STRUCTURE OF APOCAROTENOID CLEAVAGE OXYGENASE FROM SYNECHOCYSTIS, NATIVE ENZYME
Authors : Kloer, D.P.; Ruch, S.; Al-Babili, S.; Beyer, P.; Schulz, G.E.
Deposited on : 2005-01-26
Resolution : 2.39 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

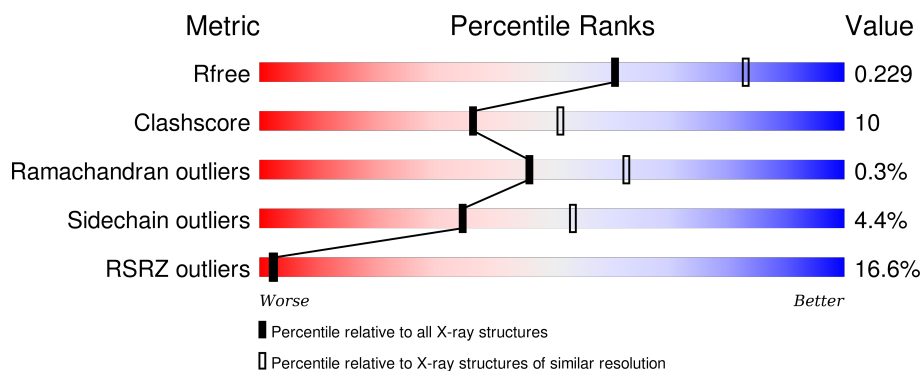
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	490	<div> <div>12%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	B	490	<div> <div>14%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	C	490	<div> <div>19%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	D	490	<div> <div>19%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3ON	A	1491	-	-	-	X
2	3ON	B	1491	-	-	-	X
2	3ON	C	1491	-	-	-	X
2	3ON	D	1491	-	-	-	X

2 Entry composition [i](#)

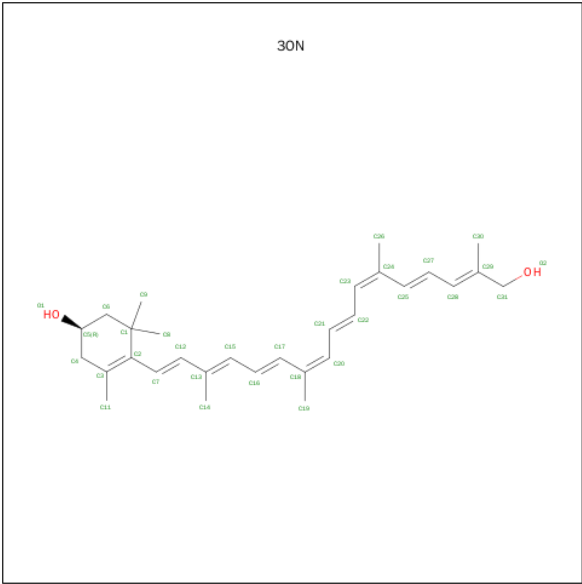
There are 4 unique types of molecules in this entry. The entry contains 15742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APOCAROTENOID-CLEAVING OXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			
1	B	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			
1	C	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			
1	D	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			

- Molecule 2 is (3R)-3-HYDROXY-8'-APOCAROTENOL (three-letter code: 3ON) (formula: C₃₀H₄₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			32	30	2		
2	B	1	Total	C	O	0	0
			32	30	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			32	30	2		
2	D	1	Total	C	O	0	0
			32	30	2		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

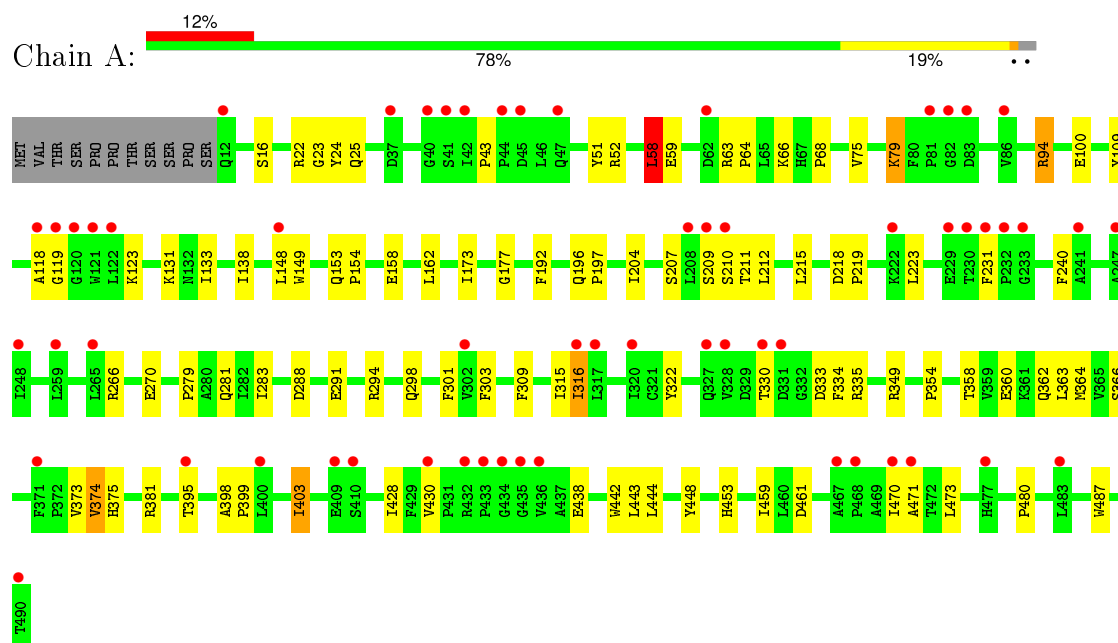
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	B	144	Total	O	0	0
			144	144		
4	C	121	Total	O	0	0
			121	121		
4	D	121	Total	O	0	0
			121	121		

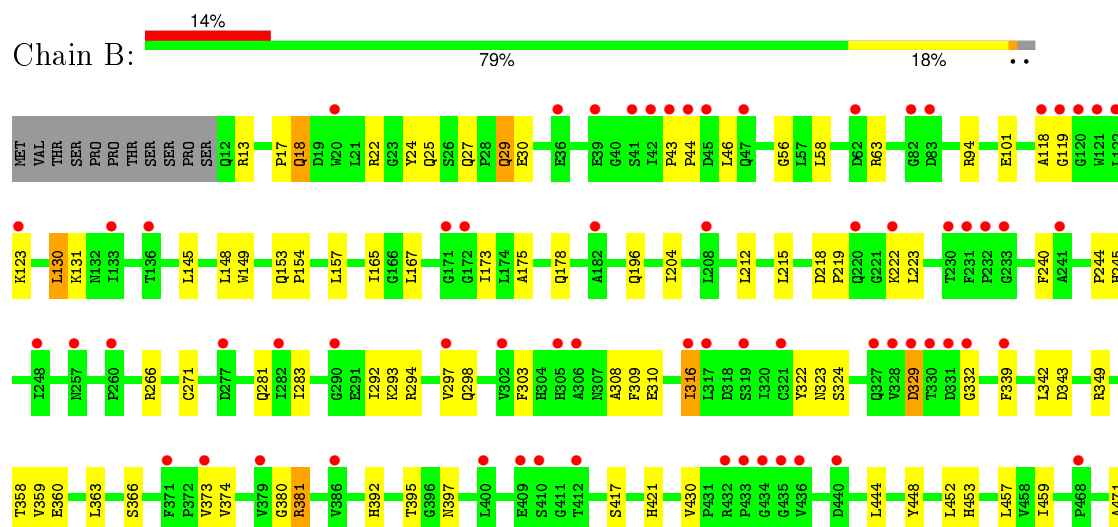
3 Residue-property plots

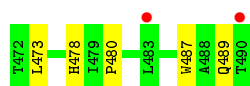
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: APOCAROTENOID-CLEAVING OXYGENASE

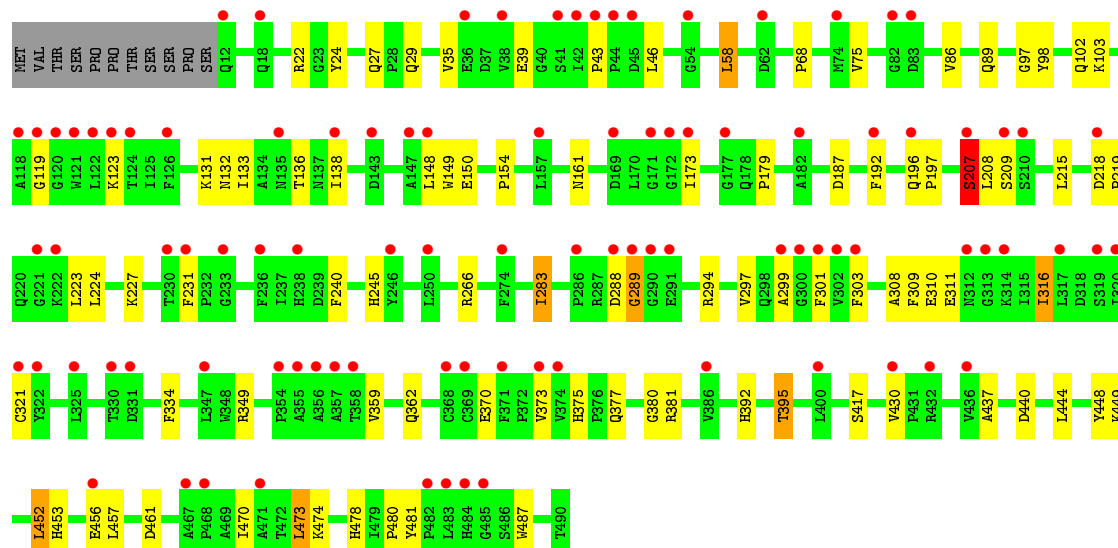
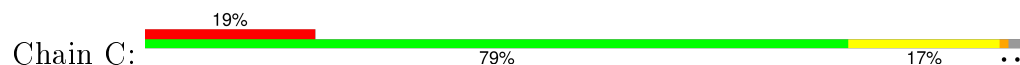


• Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE

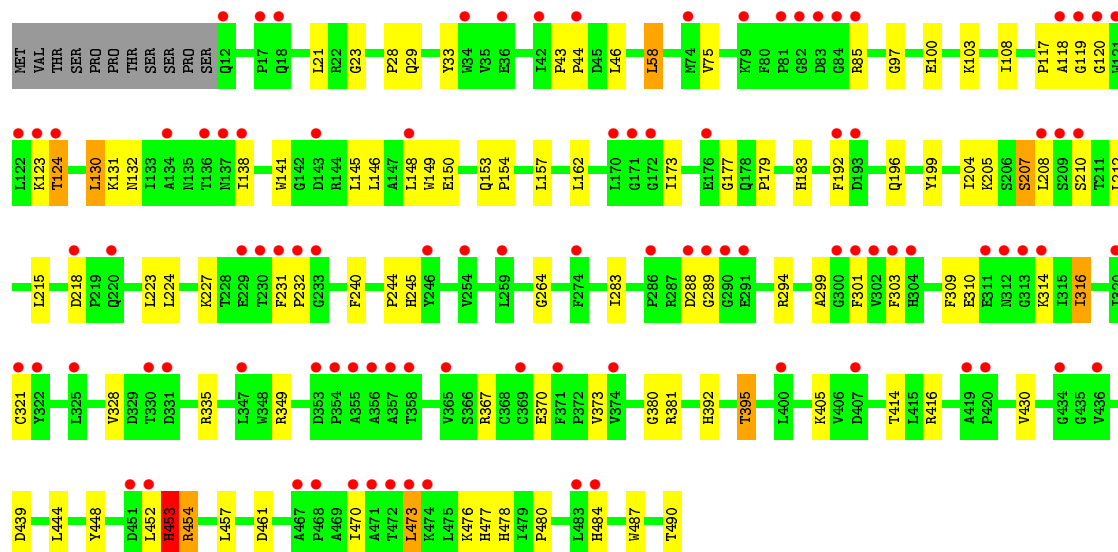
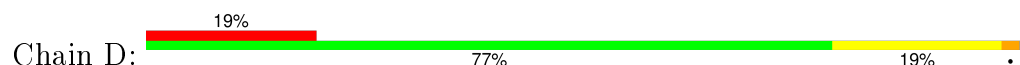




● Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE



● Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.05Å 125.28Å 203.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.41 – 2.39 43.76 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.41-2.39) 97.4 (43.76-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.224 0.187 , 0.229	Depositor DCC
R_{free} test set	5864 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.0	EDS
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 117337 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15742	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FE, 3ON

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	0.75	0/3880	0.78	4/5285 (0.1%)
1	B	0.73	0/3880	0.77	2/5284 (0.0%)
1	C	0.68	0/3880	0.74	4/5284 (0.1%)
1	D	0.68	1/3880 (0.0%)	0.75	5/5284 (0.1%)
All	All	0.71	1/15520 (0.0%)	0.76	15/21137 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	ARG	NE-CZ	5.53	1.40	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	LEU	CA-CB-CG	-7.67	97.67	115.30
1	D	299	ALA	C-N-CA	-6.76	108.10	122.30
1	C	283	ILE	CG1-CB-CG2	-6.73	96.60	111.40
1	A	58	LEU	CA-CB-CG	-6.52	100.29	115.30
1	A	374	VAL	CG1-CB-CG2	6.16	120.75	110.90
1	C	299	ALA	C-N-CA	-6.13	109.42	122.30
1	D	130	LEU	CA-CB-CG	5.84	128.72	115.30
1	B	381	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	381	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	395	THR	C-N-CA	-5.51	110.72	122.30
1	D	395	THR	C-N-CA	-5.49	110.77	122.30
1	B	130	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	C	58	LEU	CA-CB-CG	-5.28	103.15	115.30
1	D	453	HIS	N-CA-C	-5.20	96.97	111.00
1	A	395	THR	C-N-CA	-5.18	111.43	122.30

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	3767	0	3659	68	0
1	B	3767	0	3659	72	0
1	C	3767	0	3659	60	0
1	D	3767	0	3659	71	0
2	A	32	0	42	14	0
2	B	32	0	42	16	0
2	C	32	0	42	9	0
2	D	32	0	42	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	156	0	0	8	0
4	B	144	0	0	10	0
4	C	121	0	0	2	0
4	D	121	0	0	2	0
All	All	15742	0	14804	286	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 10.

All (286) 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)
2:B:1491:3ON:H25	4:B:2022:HOH:O	1.52	1.10
2:D:1491:3ON:H28	4:D:2005:HOH:O	1.50	1.09
2:A:1491:3ON:H25	4:A:2035:HOH:O	1.52	1.08
2:C:1491:3ON:H25	4:C:2042:HOH:O	1.66	0.96
2:A:1491:3ON:H28	4:A:2008:HOH:O	1.65	0.95
1:D:46:LEU:HD12	1:D:430:VAL:HG11	1.54	0.90
1:A:281:GLN:NE2	1:A:294:ARG:HD3	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:HH12	1:D:29:GLN:HE21	1.22	0.83
2:D:1491:3ON:H12	2:D:1491:3ON:H8C1	1.62	0.81
1:C:448:TYR:OH	1:C:453:HIS:HD2	1.64	0.80
1:C:449:LYS:HG2	1:C:456:GLU:OE1	1.83	0.79
1:D:454:ARG:CG	1:D:454:ARG:HH11	1.96	0.79
1:A:24:TYR:O	1:A:58:LEU:HD13	1.82	0.78
1:B:303:PHE:CD2	2:B:1491:3ON:H262	2.17	0.78
1:A:430:VAL:HG12	1:A:487:TRP:CG	2.17	0.78
1:B:130:LEU:HD21	2:B:1491:3ON:H113	1.66	0.77
1:D:303:PHE:CD2	2:D:1491:3ON:H263	2.20	0.77
1:D:370:GLU:HG3	2:D:1491:3ON:H302	1.67	0.77
1:D:454:ARG:HG3	1:D:454:ARG:HH11	1.51	0.75
1:B:430:VAL:HG21	1:B:444:LEU:HD11	1.69	0.74
1:A:281:GLN:HE22	1:A:294:ARG:HD3	1.49	0.74
1:A:211:THR:HG22	4:A:2081:HOH:O	1.87	0.74
1:B:448:TYR:OH	1:B:453:HIS:HD2	1.71	0.73
1:C:303:PHE:CD2	2:C:1491:3ON:H262	2.24	0.73
1:B:430:VAL:HG13	1:B:487:TRP:NE1	2.04	0.71
1:D:430:VAL:HG21	1:D:444:LEU:HD11	1.70	0.71
1:D:303:PHE:CD2	2:D:1491:3ON:C26	2.74	0.71
1:A:315:ILE:HD12	1:A:354:PRO:HG3	1.72	0.71
2:B:1491:3ON:H8C3	4:B:2075:HOH:O	1.91	0.70
1:C:309:PHE:CZ	1:C:316:ILE:HG12	2.27	0.69
1:A:333:ASP:OD2	1:A:335:ARG:NH1	2.25	0.69
1:A:430:VAL:HG11	1:A:444:LEU:HD11	1.74	0.69
1:B:204:ILE:HD12	1:B:212:LEU:HD12	1.72	0.69
1:A:153:GLN:NE2	1:A:177:GLY:H	1.91	0.69
1:B:245:HIS:HD2	1:B:310:GLU:OE1	1.76	0.67
1:A:430:VAL:HG12	1:A:487:TRP:CD2	2.29	0.67
1:A:283:ILE:HD13	1:A:294:ARG:HG2	1.76	0.67
1:B:149:TRP:CZ2	2:B:1491:3ON:H142	2.30	0.66
1:B:281:GLN:HG3	1:B:294:ARG:NH2	2.09	0.66
1:A:448:TYR:OH	1:A:453:HIS:HD2	1.77	0.66
1:B:24:TYR:O	1:B:58:LEU:HD22	1.95	0.66
1:D:46:LEU:CD1	1:D:430:VAL:HG11	2.25	0.66
1:C:24:TYR:O	1:C:58:LEU:HD13	1.95	0.66
1:A:430:VAL:CG2	1:A:442:TRP:HB2	2.24	0.66
1:A:173:ILE:CD1	1:A:223:LEU:HB2	2.24	0.66
1:C:370:GLU:HG3	2:C:1491:3ON:H302	1.75	0.66
1:D:448:TYR:OH	1:D:453:HIS:HD2	1.79	0.65
1:C:430:VAL:HG13	1:C:487:TRP:NE1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLU:OE2	4:B:2107:HOH:O	2.14	0.65
1:B:266:ARG:HH21	1:B:271:CYS:HA	1.61	0.65
1:B:324:SER:OG	1:B:343:ASP:OD2	2.14	0.65
1:C:316:ILE:HD13	1:C:349:ARG:NE	2.12	0.64
1:A:148:LEU:HD23	1:A:154:PRO:HB3	1.80	0.64
1:C:303:PHE:CG	2:C:1491:3ON:H262	2.34	0.63
1:D:204:ILE:HD12	1:D:212:LEU:HD12	1.81	0.63
1:D:309:PHE:CZ	1:D:316:ILE:HG12	2.33	0.62
1:A:210:SER:HB3	1:A:231:PHE:CZ	2.35	0.62
1:B:297:VAL:HB	1:B:359:VAL:HG11	1.82	0.62
1:A:281:GLN:OE1	1:A:283:ILE:HD11	1.99	0.61
1:A:298:GLN:HG3	1:B:30:GLU:O	1.99	0.61
1:B:392:HIS:HD2	1:B:417:SER:OG	1.83	0.61
1:C:392:HIS:HD2	1:C:417:SER:OG	1.84	0.61
2:B:1491:3ON:H12	2:B:1491:3ON:H9C1	1.82	0.61
1:D:405:LYS:NZ	1:D:439:ASP:OD2	2.30	0.60
1:B:46:LEU:HD12	1:B:430:VAL:HG11	1.83	0.60
1:B:145:LEU:HD23	1:B:157:LEU:HB2	1.83	0.60
1:C:303:PHE:CD2	2:C:1491:3ON:C26	2.85	0.60
1:A:43:PRO:HG3	1:A:470:ILE:HG21	1.84	0.59
1:D:430:VAL:CG2	1:D:444:LEU:HD11	2.33	0.59
1:A:316:ILE:HD13	1:A:349:ARG:NE	2.18	0.58
1:B:153:GLN:HB2	1:B:167:LEU:HD22	1.86	0.57
2:B:1491:3ON:H303	4:B:2042:HOH:O	2.03	0.57
1:A:430:VAL:HG12	1:A:487:TRP:CD1	2.38	0.57
1:D:153:GLN:NE2	1:D:177:GLY:H	2.01	0.57
1:B:119:GLY:HA3	1:B:123:LYS:HG3	1.85	0.57
1:C:227:LYS:NZ	1:C:289:GLY:HA2	2.20	0.57
1:C:136:THR:OG1	2:C:1491:3ON:H193	2.04	0.57
1:C:430:VAL:HG21	1:C:444:LEU:HD11	1.87	0.56
1:A:79:LYS:HB2	1:A:79:LYS:NZ	2.19	0.56
1:A:173:ILE:HD12	1:A:223:LEU:HB2	1.86	0.56
1:B:46:LEU:CD1	1:B:430:VAL:HG11	2.36	0.56
1:B:309:PHE:CZ	1:B:316:ILE:HG12	2.40	0.56
1:B:316:ILE:HD12	1:B:316:ILE:C	2.26	0.56
1:D:303:PHE:CG	2:D:1491:3ON:H262	2.40	0.56
1:B:173:ILE:HD12	1:B:223:LEU:HB2	1.88	0.56
1:A:309:PHE:CZ	1:A:316:ILE:HG12	2.40	0.55
1:C:448:TYR:OH	1:C:453:HIS:CD2	2.54	0.55
1:B:18:GLN:HE22	1:D:28:PRO:HB3	1.71	0.55
1:B:18:GLN:HE21	1:B:18:GLN:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TRP:CE2	2:A:1491:3ON:H142	2.41	0.55
1:A:303:PHE:CG	2:A:1491:3ON:H262	2.42	0.55
1:C:449:LYS:O	1:C:452:LEU:O	2.23	0.55
1:D:430:VAL:HG22	1:D:487:TRP:CG	2.42	0.55
1:A:196:GLN:HG3	1:A:197:PRO:HD2	1.88	0.55
1:C:187:ASP:OD1	1:C:381:ARG:NH2	2.40	0.55
1:C:89:GLN:HE22	1:C:161:ASN:HA	1.72	0.54
1:D:119:GLY:HA3	1:D:123:LYS:HG3	1.89	0.54
2:A:1491:3ON:H6C1	4:A:2084:HOH:O	2.07	0.54
1:D:454:ARG:CG	1:D:454:ARG:NH1	2.63	0.54
1:A:153:GLN:HE21	1:A:177:GLY:H	1.54	0.54
1:B:308:ALA:HA	1:B:316:ILE:O	2.07	0.54
1:B:303:PHE:CD2	2:B:1491:3ON:C26	2.87	0.54
1:C:375:HIS:CE1	1:C:377:GLN:HG2	2.43	0.54
1:D:245:HIS:HD2	1:D:310:GLU:OE1	1.90	0.54
1:B:322:TYR:OH	2:B:1491:3ON:H302	2.08	0.54
1:A:303:PHE:CD1	2:A:1491:3ON:H23	2.43	0.54
1:A:210:SER:HB3	1:A:231:PHE:CE2	2.43	0.54
1:D:316:ILE:HD13	1:D:349:ARG:CD	2.38	0.54
1:C:283:ILE:HG23	1:C:294:ARG:HG2	1.90	0.54
1:D:119:GLY:HA3	1:D:123:LYS:CG	2.38	0.54
1:C:46:LEU:CD1	1:C:430:VAL:HG11	2.37	0.53
2:A:1491:3ON:H8C1	2:A:1491:3ON:H12	1.89	0.53
1:A:430:VAL:HG23	1:A:442:TRP:HE3	1.73	0.53
1:D:448:TYR:OH	1:D:453:HIS:CD2	2.60	0.53
1:B:149:TRP:CE2	2:B:1491:3ON:H142	2.43	0.53
1:B:25:GLN:O	1:B:478:HIS:HE1	1.92	0.53
1:A:149:TRP:CZ2	2:A:1491:3ON:H142	2.44	0.52
1:C:375:HIS:HE1	1:C:377:GLN:HG2	1.74	0.52
1:B:298:GLN:NE2	4:B:2090:HOH:O	2.42	0.52
1:C:218:ASP:HB2	1:C:219:PRO:CD	2.39	0.52
1:A:66:LYS:NZ	1:A:270:GLU:OE2	2.40	0.52
1:A:303:PHE:CD2	2:A:1491:3ON:H262	2.45	0.52
1:A:281:GLN:NE2	1:A:294:ARG:CD	2.68	0.52
1:B:22:ARG:HG2	1:B:453:HIS:CD2	2.45	0.52
2:A:1491:3ON:C12	2:A:1491:3ON:H8C1	2.40	0.52
1:D:430:VAL:HG22	1:D:487:TRP:CD2	2.44	0.52
1:A:461:ASP:HB2	1:A:470:ILE:HD11	1.90	0.52
1:D:303:PHE:CG	2:D:1491:3ON:C26	2.92	0.51
1:D:283:ILE:CD1	1:D:294:ARG:HE	2.23	0.51
1:C:457:LEU:HD23	1:C:473:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1491:3ON:H8C3	4:A:2084:HOH:O	2.09	0.51
1:D:218:ASP:HB3	1:D:224:LEU:HD21	1.92	0.51
1:B:56:GLY:HA2	1:B:480:PRO:HG2	1.92	0.51
1:D:316:ILE:HD13	1:D:349:ARG:NE	2.26	0.50
1:B:218:ASP:HB2	1:B:219:PRO:CD	2.41	0.50
1:C:192:PHE:CE1	1:C:288:ASP:HB3	2.45	0.50
1:C:218:ASP:HB2	1:C:219:PRO:HD2	1.93	0.50
1:D:75:VAL:HG12	1:D:162:LEU:HD13	1.94	0.50
1:D:303:PHE:CD2	2:D:1491:3ON:H262	2.46	0.50
1:D:118:ALA:O	1:D:123:LYS:HG3	2.12	0.49
1:D:210:SER:HB3	1:D:231:PHE:CZ	2.47	0.49
1:A:291:GLU:OE1	1:A:291:GLU:HA	2.11	0.49
1:C:119:GLY:HA3	1:C:123:LYS:HG3	1.94	0.49
1:D:192:PHE:CE1	1:D:288:ASP:HB3	2.48	0.49
1:B:489:GLN:NE2	4:B:2144:HOH:O	2.46	0.49
1:D:245:HIS:CD2	1:D:310:GLU:OE1	2.65	0.49
1:B:27:GLN:HE21	1:B:29:GLN:H	1.60	0.49
1:D:179:PRO:HD3	1:D:205:LYS:HE3	1.95	0.49
1:C:97:GLY:HA3	1:C:131:LYS:HG3	1.94	0.49
1:A:204:ILE:HD12	1:A:212:LEU:HD12	1.96	0.48
1:A:316:ILE:C	1:A:316:ILE:HD12	2.33	0.48
1:C:245:HIS:HD2	1:C:310:GLU:OE1	1.96	0.48
1:B:13:ARG:HH12	1:D:29:GLN:NE2	2.02	0.48
1:C:39:GLU:OE1	1:C:474:LYS:HD2	2.13	0.48
1:B:17:PRO:HD2	1:D:28:PRO:HB2	1.96	0.48
1:C:196:GLN:HG3	1:C:197:PRO:HD2	1.94	0.48
1:D:148:LEU:HD23	1:D:154:PRO:HB3	1.95	0.48
1:B:149:TRP:CE2	2:B:1491:3ON:C14	2.96	0.47
1:B:430:VAL:CG1	4:B:2144:HOH:O	2.62	0.47
1:B:63:ARG:HH11	1:B:118:ALA:HB2	1.79	0.47
1:D:150:GLU:O	1:D:179:PRO:HB3	2.14	0.47
1:A:100:GLU:OE1	1:A:109:TYR:OH	2.26	0.47
1:D:303:PHE:CE2	2:D:1491:3ON:H263	2.48	0.47
1:B:25:GLN:O	1:B:478:HIS:CE1	2.68	0.47
1:A:204:ILE:HA	1:A:211:THR:O	2.15	0.47
1:A:22:ARG:HG2	1:A:453:HIS:CD2	2.50	0.47
1:B:430:VAL:HG22	1:B:487:TRP:CG	2.50	0.47
1:A:68:PRO:HD3	1:A:334:PHE:CD2	2.50	0.47
1:B:316:ILE:HD13	1:B:349:ARG:HG3	1.96	0.47
1:B:342:LEU:HB2	1:B:397:ASN:ND2	2.30	0.46
1:A:375:HIS:HD2	1:A:438:GLU:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:HD21	1:D:335:ARG:HA	1.97	0.46
1:C:119:GLY:HA3	1:C:123:LYS:CG	2.45	0.46
1:A:75:VAL:HG12	1:A:162:LEU:HD13	1.98	0.46
1:D:227:LYS:NZ	1:D:289:GLY:HA2	2.31	0.46
1:C:27:GLN:HE21	1:C:29:GLN:H	1.62	0.46
2:C:1491:3ON:H22	4:C:2042:HOH:O	2.15	0.46
1:D:430:VAL:HG13	1:D:487:TRP:NE1	2.31	0.46
1:B:459:ILE:HD12	1:B:471:ALA:HB3	1.98	0.46
1:B:457:LEU:HD23	1:B:473:LEU:HD22	1.98	0.46
1:C:207:SER:OG	1:C:208:LEU:N	2.48	0.46
1:C:227:LYS:HZ3	1:C:289:GLY:HA2	1.80	0.46
1:B:430:VAL:HG21	1:B:444:LEU:CD1	2.43	0.45
2:C:1491:3ON:H261	2:C:1491:3ON:H27	1.43	0.45
1:A:430:VAL:HG23	1:A:430:VAL:O	2.16	0.45
1:A:22:ARG:HG3	1:A:25:GLN:NE2	2.32	0.45
1:B:218:ASP:OD2	1:B:222:LYS:HB2	2.16	0.45
1:D:210:SER:HB2	1:D:231:PHE:CE1	2.52	0.45
1:B:43:PRO:HA	1:B:44:PRO:HD3	1.89	0.45
1:D:132:ASN:HA	1:D:149:TRP:CZ3	2.51	0.45
1:D:303:PHE:CB	2:D:1491:3ON:H262	2.47	0.45
1:C:309:PHE:CZ	1:C:316:ILE:CG1	2.99	0.45
1:B:244:PRO:HD3	1:B:380:GLY:O	2.17	0.45
1:B:303:PHE:CG	2:B:1491:3ON:H262	2.51	0.45
1:C:43:PRO:HG3	1:C:470:ILE:HG21	1.98	0.45
1:B:175:ALA:O	1:B:178:GLN:HB3	2.16	0.45
1:B:303:PHE:CD1	2:B:1491:3ON:H23	2.51	0.45
2:B:1491:3ON:H6C1	4:B:2075:HOH:O	2.16	0.44
1:C:173:ILE:HD12	1:C:223:LEU:HB2	1.99	0.44
1:C:132:ASN:HA	1:C:149:TRP:CZ3	2.53	0.44
1:A:52:ARG:NH2	1:A:428:ILE:HG12	2.32	0.44
1:C:136:THR:OG1	2:C:1491:3ON:C19	2.66	0.44
1:B:119:GLY:HA3	1:B:123:LYS:CG	2.48	0.44
1:C:461:ASP:HB2	1:C:470:ILE:HD11	1.98	0.44
1:C:35:VAL:HB	1:C:86:VAL:HG13	2.00	0.44
1:A:430:VAL:HG23	1:A:442:TRP:HB2	1.99	0.44
1:B:18:GLN:HE21	1:B:18:GLN:N	2.14	0.44
1:C:297:VAL:HB	1:C:359:VAL:HG11	1.99	0.44
1:C:218:ASP:HB3	1:C:224:LEU:HD21	1.98	0.44
1:A:398:ALA:HB1	1:A:399:PRO:HD2	2.00	0.43
1:D:461:ASP:HB2	1:D:470:ILE:HD11	2.00	0.43
1:B:316:ILE:HD13	1:B:349:ARG:NE	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:HA	1:D:146:LEU:O	2.17	0.43
1:D:141:TRP:CE2	1:D:199:TYR:HB2	2.53	0.43
1:A:119:GLY:HA3	1:A:123:LYS:HG3	1.99	0.43
1:A:298:GLN:CG	1:B:30:GLU:O	2.64	0.43
1:A:192:PHE:CE1	1:A:288:ASP:HB3	2.53	0.43
1:D:173:ILE:HD12	1:D:223:LEU:HD22	2.00	0.43
1:C:301:PHE:O	1:C:321:CYS:HA	2.18	0.43
1:B:283:ILE:HG23	1:B:292:ILE:CG2	2.49	0.43
1:A:131:LYS:HE3	1:A:133:ILE:CG2	2.48	0.43
2:D:1491:3ON:H12	2:D:1491:3ON:C8	2.43	0.43
1:B:309:PHE:CZ	1:B:316:ILE:CG1	3.02	0.43
1:B:18:GLN:HE22	1:D:28:PRO:CB	2.32	0.43
1:D:43:PRO:HA	1:D:44:PRO:HD3	1.95	0.43
1:D:23:GLY:O	1:D:480:PRO:HA	2.17	0.43
1:D:124:THR:OG1	1:D:264:GLY:CA	2.67	0.43
1:A:63:ARG:HD2	1:A:118:ALA:HB2	2.01	0.43
2:A:1491:3ON:C28	4:A:2008:HOH:O	2.42	0.43
1:D:244:PRO:HD3	1:D:380:GLY:O	2.19	0.43
1:B:309:PHE:CE2	1:B:316:ILE:HG13	2.54	0.42
2:D:1491:3ON:H25	4:D:2005:HOH:O	2.18	0.42
1:A:59:GLU:CB	1:A:64:PRO:HA	2.49	0.42
1:C:308:ALA:O	1:C:380:GLY:HA2	2.19	0.42
1:A:430:VAL:CG1	1:A:444:LEU:HD11	2.45	0.42
1:C:480:PRO:O	1:C:481:TYR:C	2.58	0.42
1:C:75:VAL:HG11	1:C:138:ILE:CD1	2.50	0.42
1:A:363:LEU:HD21	1:A:366:SER:HB3	2.01	0.42
1:A:459:ILE:HD12	1:A:471:ALA:HB3	2.00	0.42
1:B:165:ILE:HD13	1:B:165:ILE:N	2.35	0.42
1:C:148:LEU:HD23	1:C:154:PRO:HB3	2.00	0.42
1:C:437:ALA:HB3	1:C:440:ASP:HB2	2.02	0.42
1:C:98:TYR:O	1:C:102:GLN:HG2	2.20	0.42
2:B:1491:3ON:H261	2:B:1491:3ON:H27	1.27	0.42
1:D:231:PHE:HA	1:D:232:PRO:HD3	1.95	0.42
1:C:430:VAL:HG21	1:C:444:LEU:CD1	2.50	0.41
1:A:403:ILE:HD11	1:A:443:LEU:CD1	2.50	0.41
1:D:108:ILE:O	1:D:117:PRO:HG3	2.20	0.41
1:D:367:ARG:NH1	1:D:392:HIS:O	2.48	0.41
2:A:1491:3ON:H141	2:A:1491:3ON:H16	1.92	0.41
1:C:430:VAL:HG22	1:C:487:TRP:CG	2.56	0.41
1:C:392:HIS:CD2	1:C:417:SER:OG	2.69	0.41
1:A:218:ASP:HB2	1:A:219:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:N	1:A:322:TYR:O	2.50	0.41
1:D:33:TYR:CE1	1:D:476:LYS:HD2	2.55	0.41
1:C:22:ARG:HG2	1:C:453:HIS:CD2	2.55	0.41
1:C:309:PHE:CE2	1:C:316:ILE:CG1	3.04	0.41
1:B:363:LEU:HD21	1:B:366:SER:HB3	2.01	0.41
1:A:51:TYR:HB3	1:A:138:ILE:HD13	2.02	0.41
1:D:301:PHE:O	1:D:321:CYS:HA	2.20	0.41
1:D:207:SER:HB3	1:D:208:LEU:H	1.69	0.41
1:D:97:GLY:HA3	1:D:131:LYS:HG3	2.03	0.41
1:C:131:LYS:HE3	1:C:133:ILE:CG2	2.50	0.41
1:B:101:GLU:OE1	1:B:131:LYS:NZ	2.42	0.41
1:B:329:ASP:OD2	1:B:332:GLY:HA3	2.20	0.41
1:A:430:VAL:CG1	1:A:487:TRP:CD2	3.02	0.41
1:D:309:PHE:CZ	1:D:316:ILE:CG1	3.02	0.41
1:C:123:LYS:HD3	1:C:123:LYS:HA	1.90	0.41
1:B:323:ASN:ND2	4:B:2098:HOH:O	2.34	0.41
1:D:477:HIS:HD2	1:D:478:HIS:O	2.04	0.41
1:B:148:LEU:HD23	1:B:154:PRO:HB3	2.02	0.41
2:A:1491:3ON:H261	2:A:1491:3ON:H27	1.36	0.41
1:B:421:HIS:CE1	4:B:2123:HOH:O	2.74	0.41
1:C:150:GLU:O	1:C:179:PRO:HB3	2.21	0.41
1:B:149:TRP:NE1	2:B:1491:3ON:H141	2.35	0.40
1:A:298:GLN:HA	4:A:2102:HOH:O	2.21	0.40
1:D:173:ILE:HD12	1:D:223:LEU:HB2	2.03	0.40
1:D:120:GLY:O	1:D:124:THR:HG23	2.21	0.40
1:A:23:GLY:O	1:A:480:PRO:HA	2.20	0.40
1:A:94:ARG:NH2	4:A:2037:HOH:O	2.53	0.40
1:D:145:LEU:HD23	1:D:157:LEU:HB2	2.03	0.40
1:D:457:LEU:HB3	1:D:473:LEU:HD22	2.03	0.40
1:C:68:PRO:HD3	1:C:334:PHE:CD2	2.57	0.40
1:D:183:HIS:HE1	1:D:484:HIS:CE1	2.39	0.40
1:D:210:SER:CB	1:D:231:PHE:CZ	3.04	0.40
1:A:403:ILE:HD11	1:A:443:LEU:HD13	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	477/490 (97%)	461 (97%)	15 (3%)	1 (0%)	52	69
1	B	477/490 (97%)	459 (96%)	17 (4%)	1 (0%)	52	69
1	C	477/490 (97%)	461 (97%)	14 (3%)	2 (0%)	39	56
1	D	477/490 (97%)	458 (96%)	17 (4%)	2 (0%)	39	56
All	All	1908/1960 (97%)	1839 (96%)	63 (3%)	6 (0%)	46	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	PHE
1	C	207	SER
1	D	452	LEU
1	D	453	HIS
1	A	330	THR
1	C	289	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	399/410 (97%)	379 (95%)	20 (5%)	30	48
1	B	399/410 (97%)	384 (96%)	15 (4%)	40	60
1	C	399/410 (97%)	384 (96%)	15 (4%)	40	60
1	D	399/410 (97%)	379 (95%)	20 (5%)	30	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1596/1640 (97%)	1526 (96%)	70 (4%)	35 53

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	58	LEU
1	A	79	LYS
1	A	94	ARG
1	A	158	GLU
1	A	207	SER
1	A	209	SER
1	A	215	LEU
1	A	240	PHE
1	A	266	ARG
1	A	279	PRO
1	A	316	ILE
1	A	358	THR
1	A	360	GLU
1	A	362	GLN
1	A	364	MET
1	A	373	VAL
1	A	374	VAL
1	A	403	ILE
1	A	473	LEU
1	B	18	GLN
1	B	29	GLN
1	B	94	ARG
1	B	196	GLN
1	B	215	LEU
1	B	240	PHE
1	B	293	LYS
1	B	316	ILE
1	B	329	ASP
1	B	358	THR
1	B	373	VAL
1	B	374	VAL
1	B	381	ARG
1	B	395	THR
1	B	452	LEU
1	C	103	LYS
1	C	207	SER

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Mol	Chain	Res	Type
1	C	209	SER
1	C	215	LEU
1	C	231	PHE
1	C	240	PHE
1	C	266	ARG
1	C	311	GLU
1	C	316	ILE
1	C	362	GLN
1	C	373	VAL
1	C	395	THR
1	C	452	LEU
1	C	473	LEU
1	C	478	HIS
1	D	58	LEU
1	D	100	GLU
1	D	103	LYS
1	D	124	THR
1	D	130	LEU
1	D	196	GLN
1	D	207	SER
1	D	215	LEU
1	D	240	PHE
1	D	314	LYS
1	D	316	ILE
1	D	328	VAL
1	D	373	VAL
1	D	381	ARG
1	D	395	THR
1	D	414	THR
1	D	416	ARG
1	D	454	ARG
1	D	473	LEU
1	D	490	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	29	GLN
1	A	153	GLN
1	A	245	HIS
1	A	453	HIS

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Mol	Chain	Res	Type
1	B	18	GLN
1	B	27	GLN
1	B	29	GLN
1	B	153	GLN
1	B	196	GLN
1	B	226	GLN
1	B	245	HIS
1	B	362	GLN
1	B	392	HIS
1	B	453	HIS
1	B	477	HIS
1	B	478	HIS
1	C	25	GLN
1	C	27	GLN
1	C	89	GLN
1	C	153	GLN
1	C	245	HIS
1	C	362	GLN
1	C	392	HIS
1	C	421	HIS
1	C	453	HIS
1	C	477	HIS
1	C	478	HIS
1	D	25	GLN
1	D	29	GLN
1	D	96	GLN
1	D	116	GLN
1	D	153	GLN
1	D	245	HIS
1	D	312	ASN
1	D	421	HIS
1	D	453	HIS
1	D	477	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	3ON	A	1491	-	31,32,32	1.16	3 (9%)	40,42,42	2.64	19 (47%)
2	3ON	B	1491	-	31,32,32	1.20	1 (3%)	40,42,42	2.78	17 (42%)
2	3ON	C	1491	-	31,32,32	1.26	3 (9%)	40,42,42	2.29	11 (27%)
2	3ON	D	1491	-	31,32,32	1.39	6 (19%)	40,42,42	2.41	11 (27%)

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	3ON	A	1491	-	-	0/26/45/45	0/1/1/1
2	3ON	B	1491	-	-	0/26/45/45	0/1/1/1
2	3ON	C	1491	-	-	0/26/45/45	0/1/1/1
2	3ON	D	1491	-	-	0/26/45/45	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1491	3ON	C28-C29	2.05	1.36	1.34
2	D	1491	3ON	C23-C24	2.06	1.38	1.35
2	A	1491	3ON	C1-C2	2.16	1.56	1.53
2	D	1491	3ON	C4-C3	2.19	1.54	1.51
2	D	1491	3ON	C7-C2	2.20	1.53	1.45
2	D	1491	3ON	C28-C29	2.22	1.36	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1491	3ON	C3-C2	2.25	1.37	1.34
2	C	1491	3ON	C28-C29	2.34	1.36	1.34
2	A	1491	3ON	C6-C5	2.41	1.56	1.52
2	B	1491	3ON	C20-C18	2.59	1.39	1.35
2	D	1491	3ON	C1-C2	2.64	1.57	1.53
2	C	1491	3ON	C6-C5	2.72	1.56	1.52
2	C	1491	3ON	C1-C2	3.19	1.58	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1491	3ON	C26-C24-C25	-5.98	108.14	118.10
2	B	1491	3ON	C1-C2-C3	-5.90	113.99	122.66
2	B	1491	3ON	C26-C24-C25	-5.65	108.69	118.10
2	A	1491	3ON	C22-C21-C20	-4.93	112.48	123.39
2	C	1491	3ON	C1-C2-C3	-4.80	115.61	122.66
2	C	1491	3ON	C26-C24-C25	-4.80	110.11	118.10
2	B	1491	3ON	C11-C3-C2	-4.68	120.01	124.61
2	A	1491	3ON	C26-C24-C25	-4.66	110.35	118.10
2	A	1491	3ON	C1-C2-C3	-4.43	116.16	122.66
2	D	1491	3ON	C11-C3-C2	-4.42	120.27	124.61
2	B	1491	3ON	C22-C21-C20	-4.22	114.06	123.39
2	C	1491	3ON	C19-C18-C20	-4.19	116.71	122.90
2	A	1491	3ON	C11-C3-C2	-3.94	120.74	124.61
2	D	1491	3ON	C19-C18-C20	-3.80	117.29	122.90
2	B	1491	3ON	C19-C18-C17	-3.46	112.33	118.10
2	B	1491	3ON	C27-C25-C24	-3.30	116.61	126.32
2	D	1491	3ON	C1-C2-C3	-3.26	117.87	122.66
2	B	1491	3ON	C14-C13-C15	-3.22	118.15	122.90
2	A	1491	3ON	C27-C25-C24	-2.99	117.53	126.32
2	B	1491	3ON	C21-C20-C18	-2.97	122.91	127.20
2	A	1491	3ON	C19-C18-C20	-2.93	118.58	122.90
2	D	1491	3ON	C28-C27-C25	-2.55	115.35	123.13
2	D	1491	3ON	C19-C18-C17	-2.46	114.00	118.10
2	A	1491	3ON	C26-C24-C23	-2.28	119.54	122.90
2	B	1491	3ON	C22-C23-C24	-2.27	123.92	127.20
2	A	1491	3ON	C19-C18-C17	-2.26	114.33	118.10
2	B	1491	3ON	C16-C15-C13	-2.23	123.98	127.20
2	C	1491	3ON	C22-C23-C24	-2.23	123.98	127.20
2	A	1491	3ON	C14-C13-C15	-2.21	119.63	122.90
2	C	1491	3ON	C27-C25-C24	-2.08	120.18	126.32
2	A	1491	3ON	C21-C20-C18	-2.07	124.21	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1491	3ON	C15-C16-C17	-2.03	116.96	123.13
2	A	1491	3ON	C12-C13-C15	2.10	122.37	118.98
2	A	1491	3ON	C6-C5-C4	2.11	114.06	110.32
2	A	1491	3ON	C6-C1-C2	2.16	113.94	110.49
2	D	1491	3ON	C21-C22-C23	2.22	128.30	123.39
2	C	1491	3ON	C11-C3-C4	2.47	118.75	114.24
2	B	1491	3ON	C12-C13-C15	2.66	123.28	118.98
2	B	1491	3ON	C1-C6-C5	3.07	120.62	113.41
2	A	1491	3ON	C11-C3-C4	3.19	120.06	114.24
2	B	1491	3ON	C1-C2-C7	3.22	124.83	115.82
2	D	1491	3ON	C1-C2-C7	3.22	124.83	115.82
2	A	1491	3ON	C1-C2-C7	3.30	125.06	115.82
2	B	1491	3ON	C11-C3-C4	3.46	120.55	114.24
2	A	1491	3ON	C1-C6-C5	3.58	121.81	113.41
2	D	1491	3ON	C9-C1-C2	3.81	116.27	110.30
2	C	1491	3ON	C9-C1-C2	3.90	116.42	110.30
2	C	1491	3ON	C1-C2-C7	4.09	127.28	115.82
2	A	1491	3ON	C21-C22-C23	4.25	132.80	123.39
2	B	1491	3ON	C17-C18-C20	4.64	126.46	118.98
2	B	1491	3ON	C21-C22-C23	5.01	134.46	123.39
2	A	1491	3ON	C17-C18-C20	5.03	127.09	118.98
2	C	1491	3ON	C25-C24-C23	5.13	127.25	118.98
2	C	1491	3ON	C17-C18-C20	5.92	128.51	118.98
2	D	1491	3ON	C17-C18-C20	6.03	128.70	118.98
2	B	1491	3ON	C25-C24-C23	6.20	128.98	118.98
2	D	1491	3ON	C25-C24-C23	6.45	129.37	118.98
2	A	1491	3ON	C25-C24-C23	6.47	129.41	118.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1491	3ON	14	0
2	B	1491	3ON	16	0
2	C	1491	3ON	9	0
2	D	1491	3ON	12	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	479/490 (97%)	1.02	59 (12%) 5 5	55, 63, 74, 86	0
1	B	479/490 (97%)	1.07	69 (14%) 3 3	54, 63, 74, 86	0
1	C	479/490 (97%)	1.28	95 (19%) 1 1	56, 63, 74, 86	0
1	D	479/490 (97%)	1.29	95 (19%) 1 1	55, 63, 74, 87	0
All	All	1916/1960 (97%)	1.16	318 (16%) 2 2	54, 63, 74, 87	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	THR	8.7
1	A	331	ASP	8.2
1	B	330	THR	8.1
1	D	121	TRP	6.7
1	A	232	PRO	6.6
1	C	436	VAL	6.6
1	A	208	LEU	6.5
1	B	121	TRP	6.4
1	C	119	GLY	6.4
1	D	233	GLY	6.3
1	C	230	THR	6.2
1	C	121	TRP	6.2
1	C	356	ALA	6.2
1	A	433	PRO	5.7
1	B	329	ASP	5.6
1	D	231	PHE	5.6
1	C	355	ALA	5.6
1	D	313	GLY	5.5
1	B	122	LEU	5.3
1	D	289	GLY	5.2
1	B	331	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	312	ASN	5.1
1	B	436	VAL	5.0
1	D	331	ASP	5.0
1	C	289	GLY	5.0
1	B	412	THR	4.9
1	D	467	ALA	4.8
1	C	118	ALA	4.8
1	D	312	ASN	4.8
1	A	328	VAL	4.8
1	B	328	VAL	4.8
1	D	355	ALA	4.7
1	B	208	LEU	4.6
1	D	232	PRO	4.6
1	C	171	GLY	4.6
1	D	357	ALA	4.6
1	D	83	ASP	4.6
1	A	120	GLY	4.6
1	B	62	ASP	4.5
1	D	356	ALA	4.5
1	D	171	GLY	4.5
1	A	121	TRP	4.5
1	B	327	GLN	4.5
1	B	232	PRO	4.5
1	D	288	ASP	4.4
1	C	120	GLY	4.4
1	D	436	VAL	4.4
1	D	122	LEU	4.3
1	D	483	LEU	4.3
1	D	434	GLY	4.3
1	A	122	LEU	4.2
1	C	371	PHE	4.2
1	D	44	PRO	4.2
1	A	231	PHE	4.1
1	D	176	GLU	4.1
1	D	12	GLN	4.1
1	C	290	GLY	4.1
1	D	192	PHE	4.0
1	A	42	ILE	4.0
1	D	118	ALA	4.0
1	C	483	LEU	4.0
1	D	18	GLN	3.9
1	D	82	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	330	THR	3.9
1	A	434	GLY	3.9
1	D	230	THR	3.9
1	D	371	PHE	3.8
1	C	218	ASP	3.8
1	C	45	ASP	3.8
1	D	314	LYS	3.7
1	C	291	GLU	3.7
1	C	357	ALA	3.7
1	C	320	ILE	3.7
1	D	302	VAL	3.7
1	C	172	GLY	3.7
1	B	43	PRO	3.6
1	C	233	GLY	3.6
1	C	288	ASP	3.6
1	C	358	THR	3.6
1	D	290	GLY	3.6
1	C	44	PRO	3.6
1	B	233	GLY	3.5
1	C	467	ALA	3.5
1	D	321	CYS	3.5
1	D	123	LYS	3.5
1	D	452	LEU	3.5
1	D	193	ASP	3.5
1	D	301	PHE	3.5
1	A	327	GLN	3.4
1	D	358	THR	3.4
1	A	490	THR	3.4
1	D	320	ILE	3.4
1	C	354	PRO	3.4
1	B	483	LEU	3.4
1	C	330	THR	3.4
1	C	173	ILE	3.4
1	D	347	LEU	3.3
1	C	303	PHE	3.3
1	D	209	SER	3.3
1	B	230	THR	3.3
1	D	124	THR	3.3
1	A	44	PRO	3.3
1	A	47	GLN	3.3
1	A	45	ASP	3.3
1	A	119	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	42	ILE	3.2
1	B	44	PRO	3.2
1	A	41	SER	3.2
1	C	209	SER	3.2
1	C	210	SER	3.2
1	B	120	GLY	3.2
1	C	83	ASP	3.2
1	C	148	LEU	3.2
1	C	322	TYR	3.2
1	A	483	LEU	3.2
1	B	82	GLY	3.1
1	B	435	GLY	3.1
1	C	456	GLU	3.1
1	C	236	PHE	3.1
1	C	124	THR	3.1
1	A	468	PRO	3.1
1	C	62	ASP	3.1
1	A	230	THR	3.1
1	D	120	GLY	3.1
1	D	300	GLY	3.1
1	C	471	ALA	3.1
1	B	231	PHE	3.1
1	B	490	THR	3.0
1	C	286	PRO	3.0
1	C	143	ASP	3.0
1	C	126	PHE	3.0
1	D	134	ALA	3.0
1	B	171	GLY	3.0
1	B	306	ALA	3.0
1	C	321	CYS	3.0
1	C	331	ASP	3.0
1	D	84	GLY	3.0
1	A	229	GLU	2.9
1	A	210	SER	2.9
1	D	119	GLY	2.9
1	C	182	ALA	2.9
1	D	143	ASP	2.9
1	D	451	ASP	2.9
1	C	432	ARG	2.9
1	A	470	ILE	2.9
1	C	250	LEU	2.9
1	D	208	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	430	VAL	2.8
1	C	123	LYS	2.8
1	C	314	LYS	2.8
1	C	18	GLN	2.8
1	C	301	PHE	2.8
1	D	303	PHE	2.8
1	D	229	GLU	2.8
1	A	395	THR	2.8
1	B	386	VAL	2.8
1	C	246	TYR	2.8
1	B	118	ALA	2.8
1	D	81	PRO	2.8
1	C	484	HIS	2.7
1	D	353	ASP	2.7
1	C	231	PHE	2.7
1	A	118	ALA	2.7
1	D	291	GLU	2.7
1	C	347	LEU	2.7
1	D	471	ALA	2.7
1	B	290	GLY	2.7
1	D	470	ILE	2.7
1	A	432	ARG	2.7
1	A	259	LEU	2.7
1	D	210	SER	2.7
1	B	302	VAL	2.7
1	D	254	VAL	2.7
1	B	257	ASN	2.6
1	A	371	PHE	2.6
1	D	274	PHE	2.6
1	A	400	LEU	2.6
1	B	119	GLY	2.6
1	B	248	ILE	2.6
1	D	218	ASP	2.6
1	B	41	SER	2.6
1	C	373	VAL	2.6
1	A	12	GLN	2.6
1	D	472	THR	2.6
1	B	371	PHE	2.6
1	C	468	PRO	2.6
1	D	286	PRO	2.6
1	B	172	GLY	2.6
1	B	434	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	400	LEU	2.6
1	C	207	SER	2.5
1	C	74	MET	2.5
1	D	420	PRO	2.5
1	A	467	ALA	2.5
1	B	317	LEU	2.5
1	B	45	ASP	2.5
1	C	12	GLN	2.5
1	A	81	PRO	2.5
1	C	369	CYS	2.5
1	D	136	THR	2.5
1	C	313	GLY	2.5
1	C	386	VAL	2.5
1	D	220	GLN	2.5
1	A	209	SER	2.5
1	C	169	ASP	2.5
1	B	136	THR	2.4
1	C	36	GLU	2.4
1	C	325	LEU	2.4
1	C	302	VAL	2.4
1	C	82	GLY	2.4
1	A	248	ILE	2.4
1	D	172	GLY	2.4
1	B	260	PRO	2.4
1	B	433	PRO	2.4
1	A	265	LEU	2.4
1	C	122	LEU	2.4
1	D	400	LEU	2.4
1	A	247	ALA	2.4
1	B	468	PRO	2.4
1	B	400	LEU	2.4
1	C	274	PHE	2.4
1	A	233	GLY	2.4
1	B	123	LYS	2.4
1	B	36	GLU	2.3
1	C	138	ILE	2.3
1	C	430	VAL	2.3
1	B	83	ASP	2.3
1	B	305	HIS	2.3
1	D	42	ILE	2.3
1	A	471	ALA	2.3
1	C	192	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	436	VAL	2.3
1	A	241	ALA	2.3
1	A	40	GLY	2.3
1	A	435	GLY	2.3
1	C	177	GLY	2.3
1	D	36	GLU	2.3
1	D	484	HIS	2.3
1	D	311	GLU	2.3
1	B	42	ILE	2.3
1	B	39	GLU	2.3
1	D	325	LEU	2.3
1	D	354	PRO	2.2
1	C	300	GLY	2.2
1	D	369	CYS	2.2
1	B	410	SER	2.2
1	D	170	LEU	2.2
1	C	222	LYS	2.2
1	D	79	LYS	2.2
1	A	86	VAL	2.2
1	A	477	HIS	2.2
1	B	321	CYS	2.2
1	D	322	TYR	2.2
1	A	222	LYS	2.2
1	C	157	LEU	2.2
1	C	54	GLY	2.2
1	A	37	ASP	2.2
1	A	409	GLU	2.2
1	D	34	TRP	2.2
1	B	133	ILE	2.2
1	B	432	ARG	2.2
1	B	47	GLN	2.2
1	D	137	ASN	2.2
1	D	474	LYS	2.2
1	B	332	GLY	2.2
1	B	277	ASP	2.2
1	C	317	LEU	2.2
1	C	299	ALA	2.2
1	A	302	VAL	2.2
1	A	82	GLY	2.2
1	C	221	GLY	2.2
1	D	17	PRO	2.2
1	B	220	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	196	GLN	2.2
1	C	319	SER	2.2
1	B	241	ALA	2.2
1	D	419	ALA	2.2
1	A	320	ILE	2.2
1	B	282	ILE	2.2
1	B	222	LYS	2.1
1	B	440	ASP	2.1
1	D	407	ASP	2.1
1	D	85	ARG	2.1
1	D	374	VAL	2.1
1	C	43	PRO	2.1
1	D	246	TYR	2.1
1	C	368	CYS	2.1
1	B	20	TRP	2.1
1	B	339	PHE	2.1
1	D	304	HIS	2.1
1	D	148	LEU	2.1
1	B	316	ILE	2.1
1	C	374	VAL	2.1
1	D	473	LEU	2.1
1	A	83	ASP	2.1
1	C	38	VAL	2.1
1	C	41	SER	2.1
1	A	148	LEU	2.1
1	A	410	SER	2.1
1	D	468	PRO	2.1
1	B	373	VAL	2.1
1	D	74	MET	2.0
1	C	147	ALA	2.0
1	A	62	ASP	2.0
1	C	135	ASN	2.0
1	D	365	VAL	2.0
1	B	182	ALA	2.0
1	B	319	SER	2.0
1	B	409	GLU	2.0
1	C	482	PRO	2.0
1	A	316	ILE	2.0
1	C	485	GLY	2.0
1	D	138	ILE	2.0
1	B	297	VAL	2.0
1	B	379	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	317	LEU	2.0
1	D	259	LEU	2.0
1	C	238	HIS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	3ON	B	1491	32/32	0.45	0.56	8.42	62,84,99,100	0
2	3ON	D	1491	32/32	0.47	0.54	5.31	78,88,98,98	0
2	3ON	C	1491	32/32	0.49	0.53	5.01	75,89,103,104	0
2	3ON	A	1491	32/32	0.61	0.41	4.41	61,80,89,90	0
3	FE	A	1492	1/1	1.00	0.02	-	43,43,43,43	0
3	FE	B	1492	1/1	0.99	0.04	-	45,45,45,45	0
3	FE	C	1492	1/1	0.99	0.03	-	51,51,51,51	0
3	FE	D	1492	1/1	0.98	0.04	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.