



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:11 AM UTC

PDB ID : 4UPD / pdb_00004upd
Title : Open conformation of O. piceae sterol esterase mutant I544W
Authors : Gutierrez-Fernandez, J.; Vaquero, M.E.; Prieto, A.; Barriuso, J.; Gonzalez, M.J.; Hermoso, J.A.
Deposited on : 2014-06-16
Resolution : 2.40 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

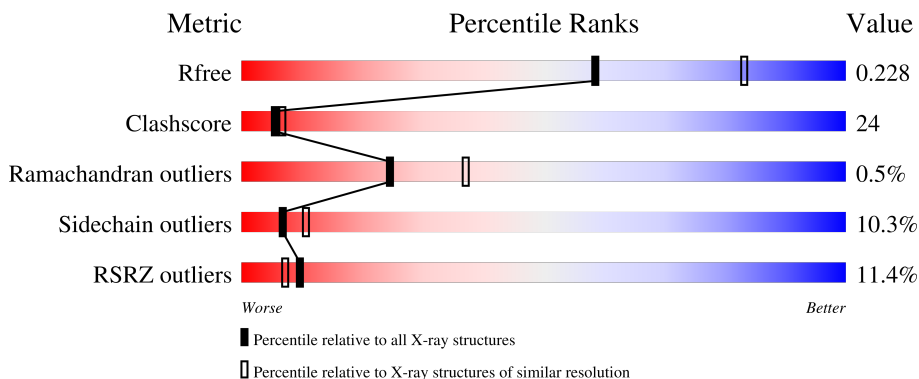
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. 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	545	 76% 18% ..
1	B	545	 22% 42% 45% 11% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8706 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.

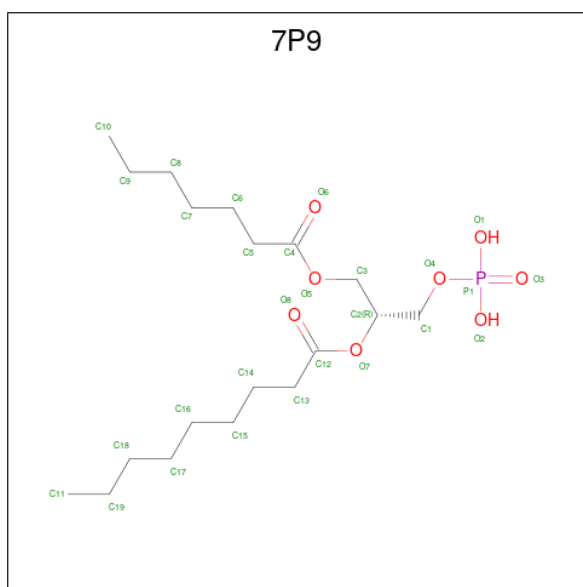
- Molecule 1 is a protein called STEROL ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	538	4137	2676	664	787	10	0	0	0
1	B	537	4126	2667	663	786	10	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

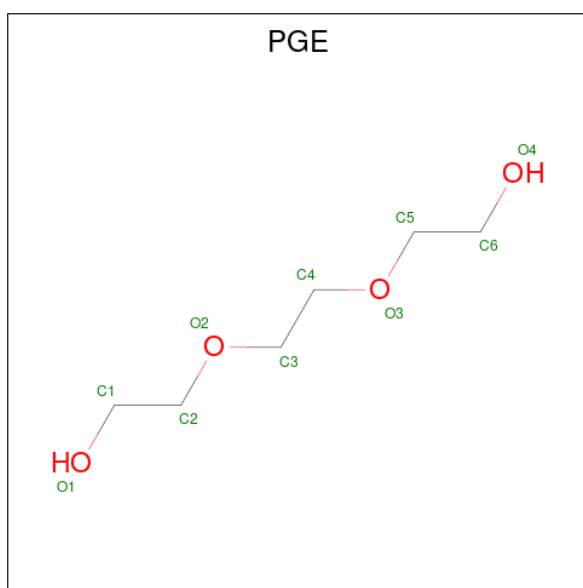
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLU	-	expression tag	UNP Q2TFW1
A	6	ALA	-	expression tag	UNP Q2TFW1
A	7	GLU	-	expression tag	UNP Q2TFW1
A	8	ALA	-	expression tag	UNP Q2TFW1
A	9	TYR	-	expression tag	UNP Q2TFW1
A	10	VAL	-	expression tag	UNP Q2TFW1
A	11	GLU	-	expression tag	UNP Q2TFW1
A	12	PHE	-	expression tag	UNP Q2TFW1
A	544	TRP	ILE	engineered mutation	UNP Q2TFW1
B	5	GLU	-	expression tag	UNP Q2TFW1
B	6	ALA	-	expression tag	UNP Q2TFW1
B	7	GLU	-	expression tag	UNP Q2TFW1
B	8	ALA	-	expression tag	UNP Q2TFW1
B	9	TYR	-	expression tag	UNP Q2TFW1
B	10	VAL	-	expression tag	UNP Q2TFW1
B	11	GLU	-	expression tag	UNP Q2TFW1
B	12	PHE	-	expression tag	UNP Q2TFW1
B	544	TRP	ILE	engineered mutation	UNP Q2TFW1

- Molecule 2 is [(2R)-2-heptanoyloxy-3-phosphonoxy-propyl] nonanoate (CCD ID: 7P9) (formula: C₁₉H₃₇O₈P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	O	P	0	0
			28	19	8	1		
2	B	1	Total	C	O	P	0	0
			28	19	8	1		

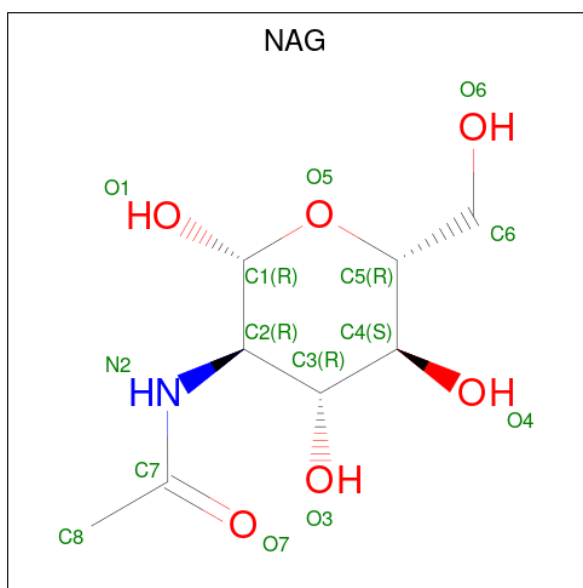
- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	O		0	0
			10	6	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

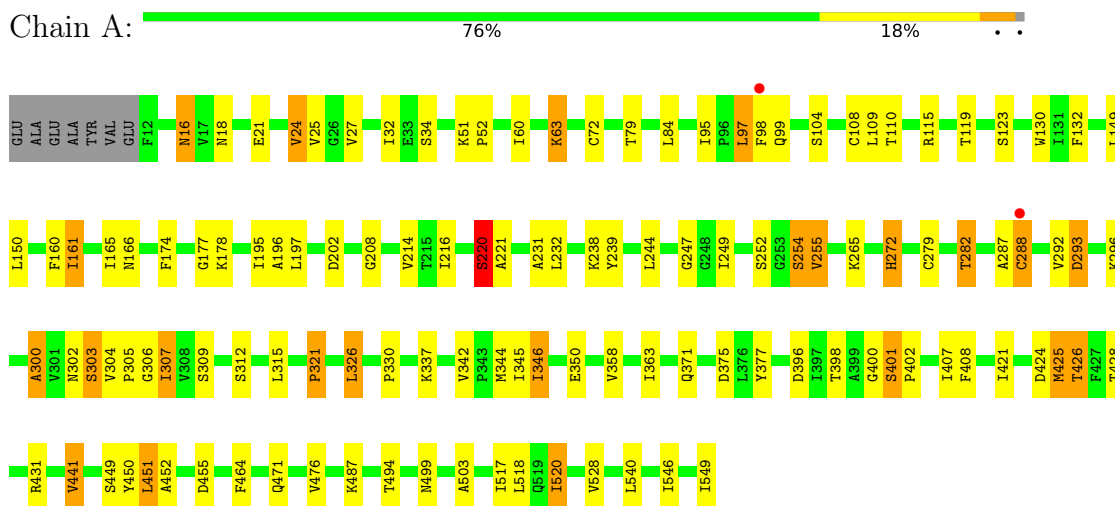
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	286	Total	O	0	0
			286	286		
5	B	49	Total	O	0	0
			49	49		

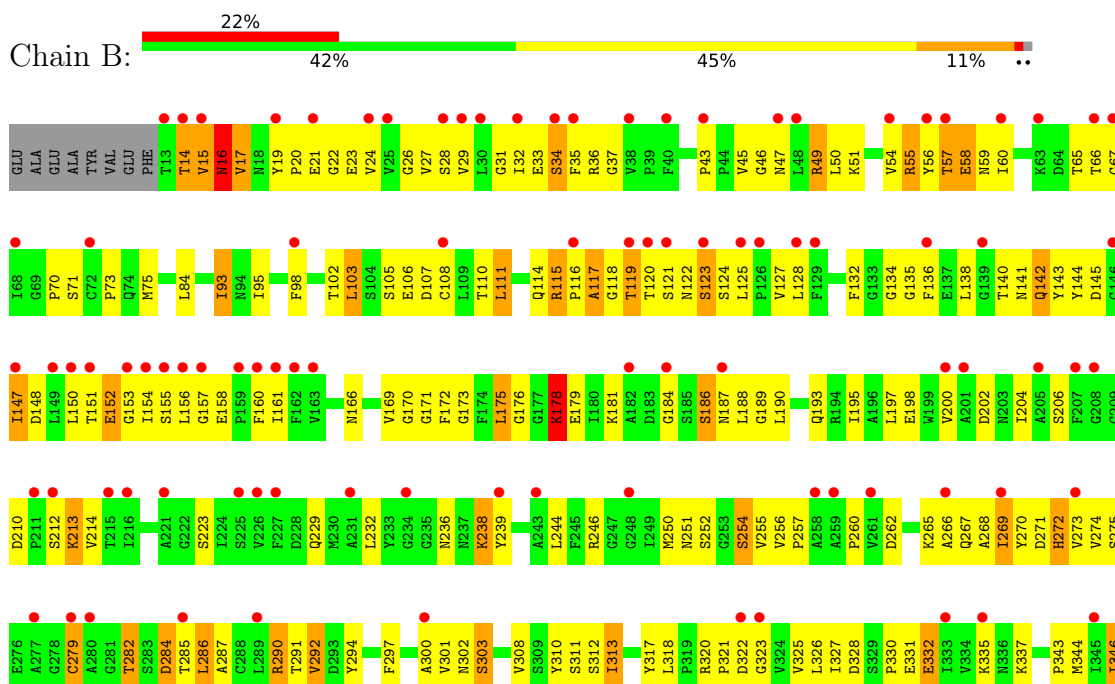
3 Residue-property plots

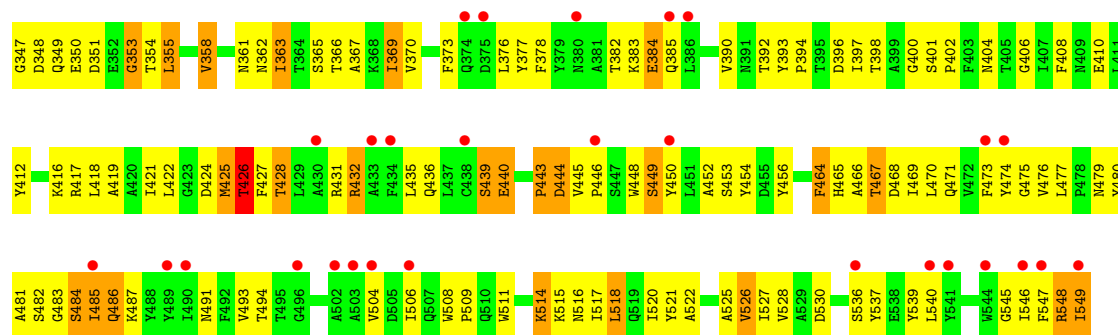
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: STEROL ESTERASE



• Molecule 1: STEROL ESTERASE





4 Data and refinement statistics i

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	164.86Å 164.86Å 94.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.29 – 2.40 58.29 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.29-2.40) 99.8 (58.29-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.40Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.196 , 0.248 0.205 , 0.228	Depositor DCC
R_{free} test set	2400 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, 0.333 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: NAG, PGE, 7P9

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	1.96	47/4243 (1.1%)	1.10	25/5787 (0.4%)
1	B	1.31	1/4231 (0.0%)	1.17	29/5771 (0.5%)
All	All	1.67	48/8474 (0.6%)	1.14	54/11558 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	ILE	C-O	-7.51	1.16	1.24
1	A	52	PRO	C-O	-7.35	1.18	1.25
1	A	312	SER	C-O	-7.34	1.17	1.24
1	A	220	SER	C-O	-6.99	1.18	1.24
1	A	24	VAL	C-O	-6.71	1.17	1.24
1	B	312	SER	C-O	-6.16	1.19	1.24
1	A	197	LEU	C-O	-6.10	1.17	1.24
1	A	520	ILE	C-O	-5.76	1.18	1.24
1	A	130	TRP	C-O	-5.71	1.17	1.24
1	A	342	VAL	C-O	-5.69	1.18	1.24
1	A	216	ILE	C-O	-5.69	1.17	1.24
1	A	239	TYR	C-O	-5.56	1.17	1.24
1	A	247	GLY	C-O	-5.53	1.18	1.24
1	A	342	VAL	CA-C	-5.50	1.48	1.52
1	A	99	GLN	C-O	-5.46	1.17	1.24
1	A	109	LEU	C-O	-5.46	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	VAL	C-O	-5.42	1.18	1.24
1	A	265	LYS	C-O	-5.42	1.17	1.24
1	A	452	ALA	C-O	-5.40	1.17	1.24
1	A	326	LEU	C-O	-5.39	1.17	1.24
1	A	195	ILE	C-O	-5.37	1.17	1.24
1	A	25	VAL	C-O	-5.35	1.18	1.24
1	A	110	THR	C-O	-5.34	1.17	1.23
1	A	321	PRO	C-O	-5.34	1.17	1.23
1	A	401	SER	C-O	-5.33	1.18	1.24
1	A	208	GLY	C-O	-5.33	1.17	1.24
1	A	161	ILE	C-O	-5.30	1.18	1.24
1	A	451	LEU	C-O	-5.30	1.18	1.24
1	A	249	ILE	C-O	-5.26	1.18	1.24
1	A	34	SER	C-O	-5.25	1.18	1.24
1	A	27	VAL	C-O	-5.25	1.18	1.24
1	A	177	GLY	C-O	-5.24	1.17	1.23
1	A	51	LYS	C-O	-5.23	1.18	1.24
1	A	244	LEU	C-O	-5.22	1.17	1.24
1	A	32	ILE	C-O	-5.22	1.18	1.24
1	A	214	VAL	C-O	-5.21	1.18	1.24
1	A	345	ILE	C-O	-5.21	1.18	1.24
1	A	292	VAL	C-O	-5.20	1.18	1.24
1	A	196	ALA	C-O	-5.17	1.18	1.24
1	A	344	MET	C-O	-5.14	1.17	1.23
1	A	231	ALA	C-O	-5.13	1.17	1.24
1	A	79	THR	C-O	-5.12	1.17	1.24
1	A	288	CYS	CA-CB	5.12	1.61	1.53
1	A	104	SER	C-O	-5.11	1.18	1.24
1	A	166	ASN	C-O	-5.08	1.17	1.24
1	A	518	LEU	C-O	-5.03	1.18	1.23
1	A	441	VAL	C-O	-5.03	1.19	1.24
1	A	377	TYR	CA-C	-5.01	1.49	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ILE	N-CA-C	11.09	121.06	110.30
1	B	17	VAL	N-CA-C	9.86	123.83	109.63
1	B	363	ILE	N-CA-C	8.26	115.05	106.21
1	A	123	SER	N-CA-C	7.78	119.76	111.28
1	B	202	ASP	N-CA-C	7.64	119.39	111.14
1	B	444	ASP	N-CA-CB	-7.38	106.72	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ASN	N-CA-C	7.33	120.31	109.24
1	A	494	THR	N-CA-C	7.32	119.04	111.14
1	B	173	GLY	N-CA-C	7.32	122.13	112.77
1	A	424	ASP	N-CA-C	7.30	119.03	111.14
1	B	443	PRO	CA-C-N	-7.08	115.74	126.86
1	B	443	PRO	C-N-CA	-7.08	115.74	126.86
1	B	353	GLY	N-CA-C	7.03	122.79	113.37
1	A	428	THR	N-CA-C	6.85	118.40	111.07
1	A	300	ALA	N-CA-C	6.70	118.38	111.14
1	B	358	VAL	N-CA-C	6.57	116.73	110.42
1	A	252	SER	N-CA-C	6.44	118.45	110.91
1	A	202	ASP	N-CA-C	6.25	118.17	111.36
1	B	282	THR	N-CA-C	-6.21	102.34	110.53
1	A	178	LYS	N-CA-C	6.10	118.00	111.36
1	A	358	VAL	N-CA-C	6.04	116.21	110.53
1	A	464	PHE	N-CA-C	6.01	118.28	110.53
1	B	426	THR	N-CA-C	5.94	117.84	111.36
1	B	428	THR	N-CA-C	5.93	117.41	111.07
1	A	375	ASP	N-CA-C	5.92	117.81	111.36
1	A	288	CYS	N-CA-C	-5.85	104.90	111.28
1	A	288	CYS	N-CA-CB	5.83	118.69	110.12
1	A	400	GLY	N-CA-C	5.82	121.57	112.31
1	B	440	GLU	N-CA-C	5.80	117.69	111.36
1	A	426	THR	N-CA-C	5.79	117.67	111.36
1	B	412	TYR	N-CA-C	-5.75	101.53	108.14
1	B	84	LEU	N-CA-C	5.72	117.52	111.28
1	A	408	PHE	N-CA-C	5.66	117.83	110.53
1	B	408	PHE	N-CA-C	5.50	117.97	110.55
1	A	287	ALA	N-CA-C	5.48	118.02	111.71
1	B	108	CYS	N-CA-C	5.47	120.83	113.72
1	B	445	VAL	N-CA-C	-5.44	102.16	107.55
1	A	302	ASN	CA-C-N	5.40	127.52	120.28
1	A	302	ASN	C-N-CA	5.40	127.52	120.28
1	B	71	SER	N-CA-C	-5.33	100.97	109.23
1	A	174	PHE	N-CA-C	5.29	119.50	112.30
1	B	49	ARG	N-CA-C	-5.28	103.17	110.35
1	B	464	PHE	N-CA-C	5.27	118.23	110.59
1	A	499	ASN	N-CA-C	5.26	119.70	113.28
1	A	231	ALA	N-CA-C	5.25	117.91	111.82
1	B	213	LYS	N-CA-C	-5.24	103.81	111.30
1	B	16	ASN	CA-C-N	5.22	127.50	120.50
1	B	16	ASN	C-N-CA	5.22	127.50	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	ASN	CA-C-N	5.22	127.28	120.28
1	B	361	ASN	C-N-CA	5.22	127.28	120.28
1	B	369	ILE	CB-CA-C	-5.22	105.09	112.14
1	A	21	GLU	N-CA-C	5.19	119.61	113.28
1	A	165	ILE	N-CA-C	5.16	117.11	109.17
1	B	344	MET	N-CA-C	5.09	116.98	108.99

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	VAL	Peptide
1	B	212	SER	Peptide

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	4137	0	4053	41	1
1	B	4126	0	4040	344	0
2	A	28	0	37	7	0
2	B	28	0	37	10	0
3	A	10	0	14	1	0
4	A	28	0	26	1	0
4	B	14	0	13	2	0
5	A	286	0	0	4	0
5	B	49	0	0	7	0
All	All	8706	0	8220	393	1

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 24.

All (393) 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:366:THR:CA	1:B:369:ILE:HD13	1.45	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASP:OD2	1:B:213:LYS:HE2	1.24	1.34
1:B:158:GLU:OE1	1:B:494:THR:CB	1.77	1.31
1:B:482:SER:O	1:B:486:GLN:CG	1.82	1.26
1:B:269:ILE:O	1:B:273:VAL:HG23	1.30	1.25
1:B:158:GLU:OE1	1:B:494:THR:HB	1.27	1.24
1:B:366:THR:O	1:B:370:VAL:HG23	1.07	1.20
1:B:260:PRO:HB2	1:B:262:ASP:OD1	1.42	1.18
1:B:210:ASP:OD2	1:B:213:LYS:CE	1.92	1.16
1:B:443:PRO:O	1:B:444:ASP:HB3	1.44	1.16
1:B:350:GLU:OE1	1:B:453:SER:OG	1.62	1.15
1:B:480:TYR:O	1:B:484:SER:OG	1.65	1.12
1:B:300:ALA:O	1:B:303:SER:OG	1.66	1.12
1:B:366:THR:O	1:B:370:VAL:CG2	1.99	1.10
1:B:175:LEU:HD12	1:B:176:GLY:H	1.13	1.10
1:B:15:VAL:HG13	1:B:16:ASN:CG	1.76	1.09
1:B:116:PRO:HB3	1:B:154:ILE:HD11	1.08	1.07
1:B:366:THR:HA	1:B:369:ILE:CD1	1.83	1.07
1:B:482:SER:O	1:B:486:GLN:HG2	1.49	1.07
1:B:116:PRO:CB	1:B:154:ILE:HD11	1.85	1.06
1:B:15:VAL:O	1:B:26:GLY:N	1.89	1.06
1:A:72:CYS:SG	1:A:108:CYS:CB	2.44	1.05
1:B:393:TYR:OH	1:B:424:ASP:OD2	1.73	1.05
1:A:72:CYS:SG	1:A:108:CYS:SG	1.15	1.03
1:B:116:PRO:HB3	1:B:154:ILE:CD1	1.88	1.03
1:B:396:ASP:OD2	1:B:398:THR:OG1	1.77	1.03
1:B:349:GLN:OE1	1:B:452:ALA:HB3	1.56	1.02
1:B:385:GLN:HB3	1:B:539:TYR:OH	1.57	1.02
1:B:482:SER:O	1:B:486:GLN:HG3	1.58	1.01
1:B:366:THR:CA	1:B:369:ILE:CD1	2.32	1.00
1:B:158:GLU:OE1	1:B:494:THR:CG2	2.08	1.00
1:B:323:GLY:HA2	1:B:327:ILE:HA	1.41	0.99
1:B:286:LEU:HD11	1:B:290:ARG:NH2	1.75	0.99
1:B:141:ASN:CG	1:B:166:ASN:ND2	2.21	0.99
1:B:148:ASP:HA	1:B:151:THR:HB	1.42	0.98
1:B:514:LYS:HG3	1:B:516:ASN:ND2	1.78	0.97
1:B:143:TYR:O	1:B:474:TYR:OH	1.80	0.96
1:B:179:GLU:N	1:B:179:GLU:OE1	1.98	0.95
1:B:141:ASN:CG	1:B:166:ASN:HD21	1.77	0.92
1:B:178:LYS:HB3	1:B:179:GLU:OE1	1.70	0.92
1:B:19:TYR:HE1	1:B:21:GLU:HB2	1.33	0.91
1:B:279:CYS:O	1:B:282:THR:HG22	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASN:OD1	1:B:166:ASN:ND2	2.03	0.91
2:B:1550:7P9:H152	2:B:1550:7P9:H31C	1.52	0.90
1:B:369:ILE:HD12	1:B:369:ILE:H	1.35	0.90
1:B:382:THR:OG1	1:B:384:GLU:CG	2.20	0.89
1:A:293:ASP:OD1	5:A:2190:HOH:O	1.91	0.88
1:B:323:GLY:CA	1:B:327:ILE:HA	2.03	0.88
1:B:271:ASP:O	1:B:274:VAL:HG22	1.72	0.88
1:A:306:GLY:O	1:A:309:SER:OG	1.91	0.87
1:B:19:TYR:CE1	1:B:21:GLU:HB2	2.09	0.87
1:B:232:LEU:HD11	1:B:325:VAL:HG12	1.56	0.87
1:B:382:THR:OG1	1:B:384:GLU:HG3	1.74	0.87
1:B:331:GLU:OE2	1:B:548:ARG:NH2	2.08	0.85
1:B:439:SER:OG	1:B:511:TRP:HZ3	1.58	0.85
1:B:366:THR:HA	1:B:369:ILE:HD13	0.87	0.85
1:B:170:GLY:HA2	1:B:317:TYR:CD2	2.12	0.84
1:B:178:LYS:HB2	1:B:267:GLN:OE1	1.76	0.84
1:B:256:VAL:O	1:B:330:PRO:HG2	1.77	0.84
1:B:189:GLY:O	1:B:193:GLN:HG3	1.76	0.84
1:A:97:LEU:HD23	1:A:98:PHE:CE1	2.11	0.83
1:B:15:VAL:HG13	1:B:16:ASN:CB	2.08	0.83
1:B:93:ILE:HA	1:B:98:PHE:HD2	1.43	0.83
1:B:286:LEU:HD12	1:B:286:LEU:O	1.76	0.83
1:B:110:THR:OG1	5:B:2001:HOH:O	1.96	0.83
1:B:175:LEU:HD12	1:B:176:GLY:N	1.93	0.83
2:A:1550:7P9:H152	2:A:1550:7P9:H31C	1.59	0.83
1:B:346:ILE:HG12	1:B:431:ARG:HG3	1.61	0.82
1:B:349:GLN:OE1	1:B:452:ALA:CB	2.27	0.82
1:B:432:ARG:HG2	1:B:537:TYR:CE1	2.15	0.81
1:B:158:GLU:OE1	1:B:494:THR:HG21	1.79	0.81
1:B:141:ASN:ND2	1:B:166:ASN:HD22	1.79	0.80
1:B:141:ASN:ND2	1:B:166:ASN:ND2	2.30	0.80
1:B:246:ARG:NH2	1:B:493:VAL:O	2.12	0.79
1:A:300:ALA:O	1:A:303:SER:HB3	1.83	0.79
1:B:75:MET:HE3	1:B:302:ASN:HA	1.66	0.78
1:A:72:CYS:CB	1:A:108:CYS:SG	2.72	0.77
1:B:21:GLU:OE1	1:B:56:TYR:HB2	1.85	0.77
1:B:57:THR:C	1:B:58:GLU:OE2	2.20	0.77
1:B:15:VAL:HA	1:B:16:ASN:HB3	1.67	0.77
1:A:421:ILE:O	1:A:425:MET:HG2	1.85	0.77
1:B:200:VAL:O	1:B:204:ILE:HG22	1.85	0.76
1:B:443:PRO:O	1:B:444:ASP:CB	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:SER:OG	5:B:2013:HOH:O	2.04	0.76
1:A:396:ASP:OD2	1:A:398:THR:OG1	2.03	0.75
1:B:410:GLU:OE1	1:B:416:LYS:HG3	1.88	0.74
1:B:45:VAL:HG22	1:B:46:GLY:N	2.03	0.73
1:B:178:LYS:CB	1:B:179:GLU:OE1	2.37	0.73
1:B:382:THR:OG1	1:B:384:GLU:HG2	1.87	0.72
1:B:318:LEU:N	1:B:318:LEU:HD23	2.04	0.72
1:B:286:LEU:HD11	1:B:290:ARG:HH21	1.53	0.72
1:B:265:LYS:NZ	1:B:376:LEU:O	2.23	0.72
1:B:286:LEU:CD1	1:B:290:ARG:NH2	2.50	0.72
1:B:269:ILE:HA	1:B:272:HIS:NE2	2.04	0.71
1:B:373:PHE:CE2	1:B:425:MET:HE1	2.24	0.71
1:B:286:LEU:HD12	1:B:286:LEU:C	2.15	0.71
1:B:254:SER:OG	1:B:255:VAL:N	2.22	0.71
1:A:476:VAL:O	2:A:1550:7P9:H142	1.90	0.71
1:B:439:SER:HG	1:B:511:TRP:HZ3	0.76	0.70
1:B:279:CYS:O	1:B:282:THR:CG2	2.40	0.70
1:B:269:ILE:HA	1:B:272:HIS:CD2	2.25	0.70
1:B:400:GLY:HA3	1:B:416:LYS:HB3	1.74	0.69
2:A:1550:7P9:H31C	2:A:1550:7P9:C15	2.24	0.68
1:B:15:VAL:CG1	1:B:16:ASN:CG	2.63	0.68
1:A:254:SER:OG	1:A:255:VAL:N	2.28	0.67
1:B:266:ALA:O	1:B:269:ILE:HG13	1.95	0.67
1:B:14:THR:O	1:B:15:VAL:HG23	1.95	0.67
1:B:210:ASP:CG	1:B:213:LYS:HE2	2.17	0.67
1:B:15:VAL:HG13	1:B:16:ASN:HB3	1.74	0.67
1:B:418:LEU:HD12	1:B:422:LEU:HG	1.77	0.66
1:B:347:GLY:HA3	1:B:450:TYR:CE1	2.31	0.66
1:B:269:ILE:O	1:B:273:VAL:CG2	2.25	0.66
1:B:116:PRO:O	1:B:117:ALA:CB	2.44	0.66
1:B:15:VAL:CA	1:B:16:ASN:HB3	2.26	0.66
1:B:464:PHE:O	1:B:467:THR:OG1	2.13	0.65
1:B:115:ARG:HE	1:B:119:THR:HG23	1.61	0.65
1:B:210:ASP:OD2	1:B:213:LYS:HE3	1.94	0.65
1:B:223:SER:OG	1:B:250:MET:HB3	1.97	0.65
1:A:401:SER:HA	1:A:402:PRO:C	2.21	0.65
1:B:419:ALA:O	5:B:2026:HOH:O	2.15	0.64
1:B:93:ILE:HA	1:B:98:PHE:CD2	2.30	0.64
1:B:369:ILE:CD1	1:B:369:ILE:H	2.09	0.64
1:B:435:LEU:O	1:B:439:SER:OG	2.16	0.64
1:B:55:ARG:HH12	1:B:195:ILE:HG13	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:MET:HG3	1:B:302:ASN:CG	2.23	0.64
1:B:439:SER:OG	1:B:511:TRP:CZ3	2.39	0.64
1:B:16:ASN:OD1	1:B:17:VAL:N	2.31	0.63
1:B:514:LYS:NZ	1:B:516:ASN:HD22	1.95	0.63
1:B:171:GLY:O	5:B:2011:HOH:O	2.14	0.63
1:A:307:ILE:HD12	1:A:315:LEU:HD21	1.81	0.63
1:B:236:ASN:OD1	1:B:238:LYS:HB2	1.99	0.63
1:A:487:LYS:HE3	1:A:503:ALA:O	1.99	0.62
2:B:1550:7P9:H31C	2:B:1550:7P9:C15	2.26	0.62
1:B:55:ARG:NH1	1:B:195:ILE:HG13	2.14	0.62
1:B:481:ALA:O	1:B:485:ILE:HG13	1.99	0.62
1:A:304:VAL:HB	1:A:305:PRO:CD	2.30	0.62
1:B:172:PHE:H	1:B:172:PHE:HD1	1.47	0.62
1:B:348:ASP:OD2	1:B:428:THR:HA	1.99	0.62
1:A:304:VAL:HB	1:A:305:PRO:HD2	1.81	0.62
1:B:382:THR:HG1	1:B:385:GLN:CD	2.05	0.62
1:B:111:LEU:C	1:B:111:LEU:HD12	2.25	0.62
1:B:410:GLU:OE1	1:B:410:GLU:HA	1.99	0.61
1:A:97:LEU:CD2	1:A:98:PHE:CE1	2.83	0.61
1:B:323:GLY:HA2	1:B:327:ILE:CA	2.25	0.61
1:B:527:ILE:HD12	1:B:527:ILE:H	1.64	0.61
1:B:19:TYR:HB2	1:B:20:PRO:HD2	1.83	0.61
1:B:156:LEU:HG	1:B:157:GLY:H	1.65	0.61
1:B:116:PRO:CG	1:B:154:ILE:HD11	2.31	0.61
1:B:198:GLU:HG2	1:B:239:TYR:CD1	2.35	0.61
1:B:292:VAL:HG12	1:B:297:PHE:HB2	1.82	0.60
1:B:527:ILE:HD12	1:B:527:ILE:N	2.16	0.60
1:B:476:VAL:O	2:B:1550:7P9:H132	2.01	0.60
1:B:282:THR:CG2	1:B:285:THR:HA	2.32	0.60
1:B:525:ALA:C	1:B:526:VAL:CG1	2.74	0.60
1:A:60:ILE:HD12	1:A:63:LYS:HD3	1.83	0.60
1:B:384:GLU:HG3	1:B:385:GLN:H	1.66	0.60
1:B:525:ALA:O	1:B:526:VAL:HG12	2.01	0.60
1:B:392:THR:HB	1:B:536:SER:OG	2.02	0.59
1:B:480:TYR:HB3	1:B:522:ALA:O	2.02	0.59
1:B:67:GLY:HA3	5:B:2002:HOH:O	2.01	0.59
1:B:425:MET:HG2	1:B:426:THR:H	1.67	0.59
1:A:450:TYR:CD2	1:A:520:ILE:HD12	2.39	0.58
1:B:355:LEU:HD13	1:B:464:PHE:CD2	2.38	0.58
1:B:363:ILE:CG2	1:B:369:ILE:HA	2.34	0.58
1:A:97:LEU:HD23	1:A:98:PHE:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:THR:N	1:B:385:GLN:OE1	2.35	0.58
1:B:37:GLY:HA2	5:B:2001:HOH:O	2.04	0.58
1:B:404:ASN:O	1:B:456:TYR:OH	2.20	0.58
1:B:178:LYS:HB3	1:B:179:GLU:CD	2.29	0.58
1:B:34:SER:HB3	1:B:114:GLN:HG2	1.86	0.57
1:B:49:ARG:HH21	1:B:106:GLU:CD	2.11	0.57
1:B:511:TRP:O	1:B:515:LYS:HA	2.04	0.57
1:B:160:PHE:HD2	1:B:161:ILE:O	1.87	0.57
1:B:401:SER:HA	1:B:402:PRO:C	2.29	0.57
1:B:148:ASP:CA	1:B:151:THR:HB	2.27	0.56
1:B:274:VAL:HG23	1:B:275:SER:N	2.18	0.56
1:B:483:GLY:HA2	1:B:486:GLN:HE21	1.69	0.56
1:B:509:PRO:HB2	1:B:514:LYS:HE3	1.86	0.56
1:B:178:LYS:HE3	1:B:267:GLN:OE1	2.04	0.56
1:B:45:VAL:CG2	1:B:46:GLY:N	2.67	0.56
1:B:525:ALA:C	1:B:526:VAL:HG13	2.29	0.56
1:B:172:PHE:CD1	1:B:172:PHE:N	2.73	0.56
1:B:331:GLU:HG2	1:B:332:GLU:N	2.21	0.56
1:B:252:SER:O	1:B:427:PHE:CD2	2.59	0.56
1:B:45:VAL:HG22	1:B:46:GLY:H	1.71	0.55
1:B:469:ILE:O	1:B:473:PHE:HB3	2.05	0.55
1:B:175:LEU:CD1	1:B:269:ILE:CD1	2.85	0.55
1:B:269:ILE:HD12	1:B:270:TYR:N	2.22	0.55
1:B:432:ARG:CG	1:B:537:TYR:CE1	2.87	0.55
1:B:32:ILE:HA	1:B:115:ARG:O	2.06	0.55
1:A:455:ASP:OD1	2:A:1550:7P9:HA	2.07	0.55
2:B:1550:7P9:H152	2:B:1550:7P9:C3	2.32	0.55
1:B:171:GLY:HA3	1:B:301:VAL:HG11	1.89	0.54
1:B:252:SER:O	1:B:427:PHE:CE2	2.60	0.54
1:B:385:GLN:CB	1:B:539:TYR:OH	2.43	0.54
1:B:132:PHE:CD1	1:B:132:PHE:C	2.85	0.54
1:B:232:LEU:HD11	1:B:325:VAL:CG1	2.32	0.54
1:B:269:ILE:C	1:B:273:VAL:HG23	2.23	0.54
1:B:549:ILE:HG13	1:B:549:ILE:O	2.06	0.54
1:B:116:PRO:O	1:B:117:ALA:HB3	2.07	0.54
1:B:377:TYR:O	1:B:549:ILE:HD12	2.08	0.54
1:B:55:ARG:NH1	1:B:195:ILE:CG1	2.71	0.54
1:B:327:ILE:HG13	1:B:328:ASP:N	2.23	0.54
1:B:425:MET:CG	1:B:426:THR:N	2.70	0.54
1:A:272:HIS:CE1	5:A:2077:HOH:O	2.61	0.54
1:B:446:PRO:HB2	1:B:448:TRP:CH2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ALA:O	1:B:526:VAL:CG1	2.56	0.53
1:B:514:LYS:HZ2	1:B:516:ASN:HD22	1.56	0.53
1:B:148:ASP:HA	1:B:151:THR:CB	2.29	0.53
1:B:418:LEU:HD12	1:B:418:LEU:O	2.09	0.53
1:B:373:PHE:HE2	1:B:425:MET:HE1	1.72	0.53
1:B:384:GLU:HG3	1:B:385:GLN:N	2.23	0.53
1:B:477:LEU:H	2:B:1550:7P9:H132	1.74	0.53
1:B:21:GLU:O	1:B:59:ASN:HA	2.09	0.52
1:B:321:PRO:HA	1:B:326:LEU:HB3	1.91	0.52
1:B:49:ARG:NE	1:B:106:GLU:OE2	2.20	0.52
1:A:255:VAL:HG13	1:A:330:PRO:HB2	1.92	0.52
1:B:232:LEU:CD1	1:B:325:VAL:HG12	2.33	0.52
1:B:514:LYS:HG3	1:B:516:ASN:HD22	1.66	0.52
1:B:318:LEU:N	1:B:318:LEU:CD2	2.73	0.52
1:B:353:GLY:HA3	1:B:419:ALA:O	2.10	0.51
1:B:471:GLN:HA	1:B:476:VAL:O	2.10	0.51
1:A:426:THR:HG21	3:A:1551:PGE:H6	1.92	0.51
1:B:366:THR:HG23	1:B:367:ALA:N	2.24	0.51
1:B:362:ASN:HB3	1:B:363:ILE:HD13	1.92	0.51
1:B:102:THR:C	1:B:103:LEU:HG	2.36	0.51
1:B:172:PHE:CE2	1:B:297:PHE:HE2	2.27	0.51
1:B:418:LEU:CD1	1:B:422:LEU:HG	2.40	0.51
1:A:346:ILE:HG12	1:A:431:ARG:HG3	1.92	0.50
1:B:73:PRO:HG2	1:B:172:PHE:CE2	2.46	0.50
1:B:17:VAL:O	1:B:23:GLU:HG3	2.11	0.50
1:B:134:GLY:HA3	1:B:138:LEU:O	2.11	0.50
1:B:540:LEU:HD12	1:B:547:PHE:CE2	2.46	0.50
1:B:43:PRO:O	1:B:45:VAL:HG12	2.12	0.50
1:B:310:TYR:CE2	4:B:1551:NAG:C1	2.94	0.50
1:B:351:ASP:OD1	1:B:402:PRO:HA	2.12	0.50
1:A:132:PHE:CD1	1:A:132:PHE:C	2.90	0.50
1:B:120:THR:H	1:B:123:SER:HB2	1.77	0.50
1:B:127:VAL:HB	1:B:214:VAL:HG22	1.93	0.50
1:B:369:ILE:HD12	1:B:369:ILE:N	2.15	0.50
1:B:473:PHE:C	1:B:473:PHE:CD1	2.89	0.50
1:A:337:LYS:HG3	1:A:441:VAL:HB	1.93	0.50
1:B:393:TYR:CD2	1:B:421:ILE:HG12	2.46	0.50
1:B:15:VAL:CG1	1:B:16:ASN:HB3	2.42	0.49
1:B:200:VAL:O	1:B:204:ILE:CG2	2.58	0.49
1:B:31:GLY:C	1:B:117:ALA:HB2	2.37	0.49
1:B:153:GLY:O	1:B:156:LEU:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:LEU:N	2:B:1550:7P9:H132	2.28	0.49
1:B:294:TYR:CD1	1:B:294:TYR:C	2.89	0.49
1:B:320:ARG:C	1:B:326:LEU:HD23	2.37	0.49
1:B:171:GLY:HA3	1:B:301:VAL:CG1	2.42	0.49
1:B:190:LEU:HD23	1:B:193:GLN:OE1	2.13	0.49
1:A:350:GLU:HA	1:A:451:LEU:HD11	1.95	0.49
1:B:15:VAL:CG1	1:B:16:ASN:CB	2.88	0.49
1:B:45:VAL:CG2	1:B:46:GLY:H	2.26	0.49
2:A:1550:7P9:H141	5:A:2257:HOH:O	2.12	0.49
1:B:274:VAL:CG2	1:B:275:SER:N	2.76	0.49
1:A:363:ILE:CD1	4:A:1552:NAG:H82	2.42	0.48
1:B:365:SER:O	1:B:369:ILE:N	2.40	0.48
1:B:393:TYR:O	1:B:417:ARG:NH2	2.44	0.48
1:B:471:GLN:NE2	2:B:1550:7P9:O8	2.46	0.48
1:B:509:PRO:CB	1:B:514:LYS:HE3	2.43	0.48
1:B:118:GLY:O	1:B:120:THR:HG23	2.14	0.48
1:B:308:VAL:HG12	1:B:308:VAL:O	2.12	0.48
1:B:270:TYR:O	1:B:274:VAL:HG13	2.13	0.48
1:B:393:TYR:OH	1:B:424:ASP:CG	2.54	0.48
1:B:476:VAL:HG12	1:B:477:LEU:HD23	1.96	0.48
1:B:15:VAL:HG13	1:B:16:ASN:OD1	2.12	0.48
1:B:144:TYR:HE1	1:B:469:ILE:HD12	1.79	0.47
1:B:300:ALA:C	1:B:303:SER:OG	2.51	0.47
1:B:323:GLY:C	1:B:327:ILE:HA	2.39	0.47
1:A:455:ASP:OD1	2:A:1550:7P9:H131	2.13	0.47
1:B:140:THR:HG23	1:B:142:GLN:H	1.79	0.47
1:B:251:ASN:N	1:B:251:ASN:HD22	2.12	0.47
1:B:14:THR:C	1:B:15:VAL:HG23	2.39	0.47
1:B:58:GLU:N	1:B:58:GLU:CD	2.73	0.47
1:B:246:ARG:O	1:B:343:PRO:HD2	2.14	0.47
1:B:482:SER:O	1:B:486:GLN:CD	2.53	0.47
1:B:509:PRO:CB	1:B:514:LYS:CE	2.92	0.47
1:B:158:GLU:CD	1:B:494:THR:HG21	2.40	0.47
1:B:178:LYS:O	1:B:181:LYS:HB3	2.15	0.47
1:B:257:PRO:HB2	1:B:548:ARG:HA	1.97	0.47
1:B:271:ASP:O	1:B:274:VAL:CG2	2.54	0.47
1:B:321:PRO:N	1:B:326:LEU:HD23	2.28	0.47
1:B:425:MET:HG2	1:B:426:THR:N	2.30	0.47
1:B:514:LYS:HG3	1:B:516:ASN:CG	2.38	0.47
1:B:197:LEU:O	1:B:200:VAL:HB	2.15	0.47
1:B:125:LEU:O	1:B:210:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLY:HA2	5:B:2013:HOH:O	2.14	0.46
1:B:313:ILE:HD11	1:B:422:LEU:HB3	1.98	0.46
1:B:426:THR:HB	1:B:427:PHE:CD1	2.51	0.46
1:B:318:LEU:HD23	1:B:318:LEU:H	1.75	0.46
1:B:378:PHE:CD1	1:B:547:PHE:HA	2.51	0.46
1:B:49:ARG:NH2	1:B:106:GLU:OE1	2.23	0.46
1:B:58:GLU:OE2	1:B:58:GLU:N	2.47	0.46
1:B:145:ASP:N	1:B:474:TYR:OH	2.37	0.46
1:B:73:PRO:CG	1:B:172:PHE:CE2	2.99	0.46
1:B:479:ASN:O	1:B:482:SER:OG	2.27	0.46
1:B:349:GLN:OE1	1:B:349:GLN:HA	2.16	0.46
1:B:128:LEU:HD23	1:B:160:PHE:CE2	2.50	0.46
1:B:393:TYR:HA	1:B:394:PRO:HD3	1.82	0.46
1:B:70:PRO:C	1:B:142:GLN:NE2	2.74	0.46
1:A:279:CYS:O	1:A:282:THR:OG1	2.30	0.45
1:B:19:TYR:N	1:B:22:GLY:O	2.43	0.45
1:B:509:PRO:HB3	1:B:514:LYS:HE2	1.98	0.45
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.75	0.45
1:B:390:VAL:O	1:B:417:ARG:NH2	2.49	0.45
1:B:468:ASP:OD1	1:B:468:ASP:N	2.41	0.45
1:B:73:PRO:HG2	1:B:172:PHE:CD2	2.52	0.45
1:B:31:GLY:O	1:B:117:ALA:HB2	2.17	0.45
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.67	0.45
1:B:175:LEU:CD1	1:B:269:ILE:HD12	2.46	0.45
1:A:115:ARG:HD2	1:A:119:THR:HB	1.99	0.45
1:A:425:MET:O	5:A:2248:HOH:O	2.21	0.45
1:A:449:SER:HB3	1:A:517:ILE:HG22	1.98	0.45
1:B:105:SER:C	1:B:107:ASP:N	2.75	0.45
1:B:158:GLU:OE1	1:B:494:THR:OG1	2.31	0.45
1:B:366:THR:HB	1:B:417:ARG:HH12	1.81	0.45
1:A:16:ASN:HB2	1:A:24:VAL:O	2.15	0.45
1:B:50:LEU:HA	1:B:50:LEU:HD23	1.78	0.45
1:B:158:GLU:CG	1:B:494:THR:HG21	2.46	0.45
1:B:354:THR:O	1:B:358:VAL:HG23	2.16	0.45
1:B:465:HIS:O	1:B:466:ALA:HB3	2.17	0.45
1:B:310:TYR:CZ	4:B:1551:NAG:H5	2.52	0.45
1:B:363:ILE:HG22	1:B:369:ILE:HG13	1.99	0.45
1:B:156:LEU:HG	1:B:157:GLY:N	2.32	0.44
1:B:508:TRP:CD2	1:B:518:LEU:HD12	2.52	0.44
1:A:150:LEU:HD11	1:A:160:PHE:O	2.17	0.44
1:B:373:PHE:HA	1:B:377:TYR:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:VAL:CG1	1:B:16:ASN:OD1	2.66	0.44
1:B:476:VAL:C	2:B:1550:7P9:H132	2.42	0.44
1:B:432:ARG:HA	1:B:435:LEU:HD12	2.00	0.44
1:B:480:TYR:CD1	1:B:480:TYR:C	2.96	0.44
1:B:140:THR:HG21	1:B:142:GLN:OE1	2.17	0.44
1:B:151:THR:O	1:B:155:SER:N	2.47	0.44
1:B:36:ARG:O	1:B:65:THR:HB	2.18	0.43
1:B:321:PRO:CA	1:B:326:LEU:HD23	2.48	0.43
2:B:1550:7P9:H31C	2:B:1550:7P9:C14	2.48	0.43
2:B:1550:7P9:C16	2:B:1550:7P9:H72C	2.48	0.43
1:B:398:THR:HG22	1:B:406:GLY:HA2	2.00	0.43
1:B:213:LYS:HA	1:B:246:ARG:HD3	2.01	0.43
1:B:158:GLU:OE2	1:B:491:ASN:OD1	2.36	0.43
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.72	0.43
1:B:57:THR:C	1:B:58:GLU:CD	2.87	0.43
1:B:517:ILE:HG23	1:B:530:ASP:HB2	2.00	0.43
1:A:321:PRO:HA	1:A:326:LEU:HB3	2.00	0.43
1:B:21:GLU:O	1:B:59:ASN:CG	2.62	0.43
1:B:349:GLN:NE2	1:B:468:ASP:HB3	2.34	0.43
1:A:346:ILE:O	1:A:449:SER:HA	2.19	0.43
1:B:473:PHE:CD1	1:B:473:PHE:O	2.72	0.43
1:A:471:GLN:OE1	2:A:1550:7P9:O8	2.36	0.42
1:B:111:LEU:C	1:B:111:LEU:CD1	2.92	0.42
1:B:135:GLY:O	1:B:136:PHE:HB2	2.18	0.42
1:B:432:ARG:HG2	1:B:537:TYR:CD1	2.52	0.42
1:B:152:GLU:HA	1:B:155:SER:HB3	2.01	0.42
1:B:35:PHE:CD1	1:B:35:PHE:N	2.88	0.42
1:B:520:ILE:HG22	1:B:521:TYR:O	2.19	0.42
1:B:172:PHE:CE2	1:B:297:PHE:CE2	3.07	0.42
1:B:75:MET:HG3	1:B:302:ASN:OD1	2.19	0.42
1:B:27:VAL:HG13	1:B:27:VAL:O	2.19	0.42
1:B:115:ARG:HB2	1:B:119:THR:HG21	2.02	0.42
1:B:449:SER:C	1:B:508:TRP:HZ2	2.28	0.42
1:B:176:GLY:O	1:B:270:TYR:HB2	2.20	0.41
1:B:321:PRO:HA	1:B:326:LEU:HD23	2.01	0.41
1:A:220:SER:HB3	1:A:221:ALA:H	1.63	0.41
1:B:150:LEU:HD21	1:B:160:PHE:O	2.20	0.41
1:B:284:ASP:CG	1:B:287:ALA:H	2.22	0.41
1:B:287:ALA:HA	1:B:290:ARG:NH1	2.35	0.41
1:B:431:ARG:HD2	1:B:449:SER:OG	2.21	0.41
1:B:448:TRP:CE3	1:B:448:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASN:OD1	1:B:17:VAL:CG2	2.69	0.41
1:B:450:TYR:HB3	1:B:508:TRP:CZ2	2.55	0.41
1:B:28:SER:HB2	1:B:33:GLU:HG2	2.01	0.41
1:B:75:MET:HE3	1:B:302:ASN:CA	2.45	0.41
1:B:346:ILE:O	1:B:449:SER:HA	2.20	0.41
1:B:436:GLN:NE2	1:B:440:GLU:OE2	2.45	0.41
1:B:150:LEU:HA	1:B:150:LEU:HD23	1.80	0.41
1:B:17:VAL:O	1:B:24:VAL:N	2.41	0.41
1:B:431:ARG:HE	1:B:431:ARG:HB3	1.73	0.41
1:B:545:GLY:O	1:B:548:ARG:HG2	2.21	0.41
1:B:115:ARG:NE	1:B:119:THR:HG23	2.31	0.41
1:B:179:GLU:N	1:B:179:GLU:CD	2.73	0.41
1:B:527:ILE:N	1:B:527:ILE:CD1	2.82	0.41
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.88	0.41
1:B:232:LEU:HD12	1:B:232:LEU:HA	1.96	0.40
1:B:268:ALA:O	1:B:272:HIS:CD2	2.74	0.40
1:B:454:TYR:CD1	1:B:471:GLN:HG2	2.57	0.40
1:B:16:ASN:OD1	1:B:17:VAL:HG23	2.21	0.40
1:B:51:LYS:C	1:B:188:LEU:HD22	2.46	0.40
1:B:322:ASP:OD1	1:B:322:ASP:N	2.54	0.40
1:B:471:GLN:O	1:B:475:GLY:HA2	2.22	0.40
1:B:509:PRO:HB2	1:B:514:LYS:CE	2.52	0.40
1:B:187:ASN:O	1:B:190:LEU:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:OD1	1:A:296:LYS:NZ[7_554]	1.87	0.33

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	536/545 (98%)	523 (98%)	12 (2%)	1 (0%)	43	58
1	B	535/545 (98%)	512 (96%)	19 (4%)	4 (1%)	18	28
All	All	1071/1090 (98%)	1035 (97%)	31 (3%)	5 (0%)	24	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	117	ALA
1	B	178	LYS
1	B	254	SER
1	B	16	ASN
1	A	254	SER

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	443/448 (99%)	421 (95%)	22 (5%)	22	38
1	B	442/448 (99%)	373 (84%)	69 (16%)	2	3
All	All	885/896 (99%)	794 (90%)	91 (10%)	7	11

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	84	LEU
1	A	95	ILE
1	A	97	LEU
1	A	149	LEU
1	A	161	ILE
1	A	220	SER
1	A	232	LEU
1	A	238	LYS
1	A	272	HIS
1	A	282	THR

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Mol	Chain	Res	Type
1	A	288	CYS
1	A	293	ASP
1	A	303	SER
1	A	307	ILE
1	A	371	GLN
1	A	407	ILE
1	A	425	MET
1	A	528	VAL
1	A	540	LEU
1	A	546	ILE
1	A	549	ILE
1	B	14	THR
1	B	29	VAL
1	B	34	SER
1	B	47	ASN
1	B	54	VAL
1	B	55	ARG
1	B	57	THR
1	B	58	GLU
1	B	60	ILE
1	B	66	THR
1	B	93	ILE
1	B	95	ILE
1	B	103	LEU
1	B	111	LEU
1	B	115	ARG
1	B	119	THR
1	B	121	SER
1	B	122	ASN
1	B	123	SER
1	B	124	SER
1	B	142	GLN
1	B	147	ILE
1	B	152	GLU
1	B	169	VAL
1	B	175	LEU
1	B	178	LYS
1	B	186	SER
1	B	206	SER
1	B	229	GLN
1	B	238	LYS
1	B	269	ILE

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Mol	Chain	Res	Type
1	B	272	HIS
1	B	279	CYS
1	B	284	ASP
1	B	286	LEU
1	B	290	ARG
1	B	291	THR
1	B	292	VAL
1	B	303	SER
1	B	311	SER
1	B	313	ILE
1	B	332	GLU
1	B	335	LYS
1	B	337	LYS
1	B	346	ILE
1	B	355	LEU
1	B	383	LYS
1	B	384	GLU
1	B	397	ILE
1	B	425	MET
1	B	426	THR
1	B	432	ARG
1	B	439	SER
1	B	449	SER
1	B	467	THR
1	B	470	LEU
1	B	484	SER
1	B	485	ILE
1	B	486	GLN
1	B	487	LYS
1	B	504	VAL
1	B	506	ILE
1	B	514	LYS
1	B	518	LEU
1	B	526	VAL
1	B	528	VAL
1	B	546	ILE
1	B	548	ARG
1	B	549	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	409	ASN
1	A	507	GLN
1	A	519	GLN
1	B	18	ASN
1	B	166	ASN
1	B	203	ASN
1	B	251	ASN
1	B	272	HIS
1	B	336	ASN
1	B	404	ASN
1	B	471	GLN
1	B	486	GLN
1	B	507	GLN
1	B	516	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](#)

6 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
4	NAG	A	1552	1	14,14,15	0.29	0	17,19,21	0.56	0
2	7P9	B	1550	-	27,27,27	1.86	5 (18%)	30,32,32	1.98	5 (16%)
3	PGE	A	1551	-	9,9,9	1.13	0	8,8,8	0.65	0
4	NAG	A	1553	1	14,14,15	0.46	0	17,19,21	0.85	0
4	NAG	B	1551	1	14,14,15	0.84	0	17,19,21	2.18	5 (29%)
2	7P9	A	1550	-	27,27,27	1.76	5 (18%)	30,32,32	2.18	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1552	1	-	2/6/23/26	0/1/1/1
2	7P9	B	1550	-	-	18/29/29/29	-
3	PGE	A	1551	-	-	2/7/7/7	-
4	NAG	A	1553	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1551	1	-	1/6/23/26	0/1/1/1
2	7P9	A	1550	-	-	15/29/29/29	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1550	7P9	O8-C12	5.93	1.40	1.22
2	A	1550	7P9	O8-C12	5.78	1.39	1.22
2	B	1550	7P9	O6-C4	5.25	1.38	1.22
2	A	1550	7P9	O6-C4	4.76	1.36	1.22
2	B	1550	7P9	O5-C4	3.01	1.42	1.33
2	B	1550	7P9	O7-C12	2.86	1.42	1.34
2	A	1550	7P9	O7-C12	2.74	1.42	1.34
2	A	1550	7P9	O5-C4	2.68	1.41	1.33
2	B	1550	7P9	O7-C2	-2.45	1.40	1.46
2	A	1550	7P9	O7-C2	-2.27	1.41	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1550	7P9	O7-C12-O8	-7.19	106.91	123.70
2	B	1550	7P9	O7-C12-O8	-5.74	110.28	123.70
2	B	1550	7P9	O5-C4-O6	-5.49	109.88	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1550	7P9	O5-C4-O6	-5.44	110.02	123.63
4	B	1551	NAG	C1-O5-C5	-5.31	105.07	112.19
4	B	1551	NAG	C4-C3-C2	5.06	118.44	111.02
2	A	1550	7P9	O8-C12-C13	-4.60	105.81	123.78
2	B	1550	7P9	O6-C4-C5	-4.35	106.76	123.78
2	B	1550	7P9	O8-C12-C13	-4.21	107.30	123.78
2	A	1550	7P9	O6-C4-C5	-3.46	110.25	123.78
2	A	1550	7P9	C3-C2-C1	-2.63	105.64	111.78
4	B	1551	NAG	C1-C2-N2	-2.58	106.37	110.43
2	B	1550	7P9	O7-C12-C13	-2.31	106.49	111.48
4	B	1551	NAG	O4-C4-C3	-2.30	104.95	110.38
2	A	1550	7P9	C3-O5-C4	-2.13	109.35	117.12
4	B	1551	NAG	O3-C3-C2	-2.04	105.16	109.40

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1550	7P9	O6-C4-O5-C3
2	A	1550	7P9	O8-C12-O7-C2
2	A	1550	7P9	C13-C12-O7-C2
2	B	1550	7P9	C1-O4-P1-O3
2	B	1550	7P9	C2-C3-O5-C4
2	B	1550	7P9	O8-C12-O7-C2
2	B	1550	7P9	O6-C4-O5-C3
2	A	1550	7P9	C2-C3-O5-C4
2	A	1550	7P9	C5-C4-O5-C3
2	B	1550	7P9	C5-C4-O5-C3
3	A	1551	PGE	O2-C3-C4-O3
2	B	1550	7P9	C4-C5-C6-C7
2	A	1550	7P9	C4-C5-C6-C7
2	A	1550	7P9	C12-C13-C14-C15
2	A	1550	7P9	C16-C17-C18-C19
2	B	1550	7P9	C6-C7-C8-C9
2	B	1550	7P9	C5-C6-C7-C8
2	B	1550	7P9	C13-C12-O7-C2
2	A	1550	7P9	C5-C6-C7-C8
2	A	1550	7P9	C6-C7-C8-C9
2	A	1550	7P9	O4-C1-C2-O7
4	B	1551	NAG	O5-C5-C6-O6
4	A	1552	NAG	C4-C5-C6-O6
2	B	1550	7P9	C1-C2-C3-O5

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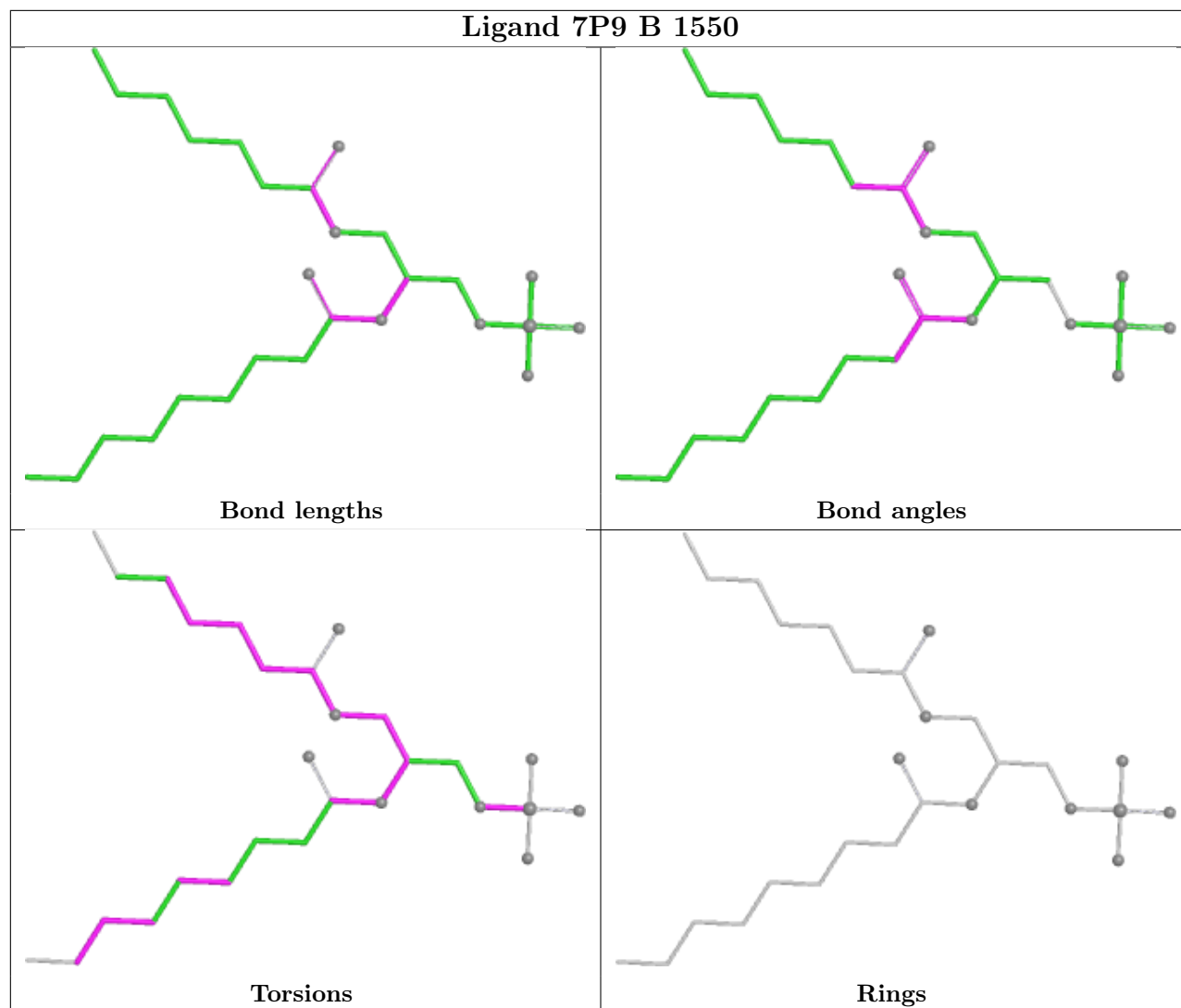
Mol	Chain	Res	Type	Atoms
2	A	1550	7P9	C3-C2-O7-C12
2	B	1550	7P9	C14-C15-C16-C17
2	A	1550	7P9	O4-C1-C2-C3
2	B	1550	7P9	O5-C4-C5-C6
2	B	1550	7P9	C17-C18-C19-C11
3	A	1551	PGE	O1-C1-C2-O2
4	A	1552	NAG	O5-C5-C6-O6
2	B	1550	7P9	O7-C2-C3-O5
2	B	1550	7P9	C3-C2-O7-C12
2	B	1550	7P9	C16-C17-C18-C19
2	A	1550	7P9	O5-C4-C5-C6
2	B	1550	7P9	C1-O4-P1-O2
2	A	1550	7P9	C14-C15-C16-C17
2	B	1550	7P9	C1-C2-O7-C12

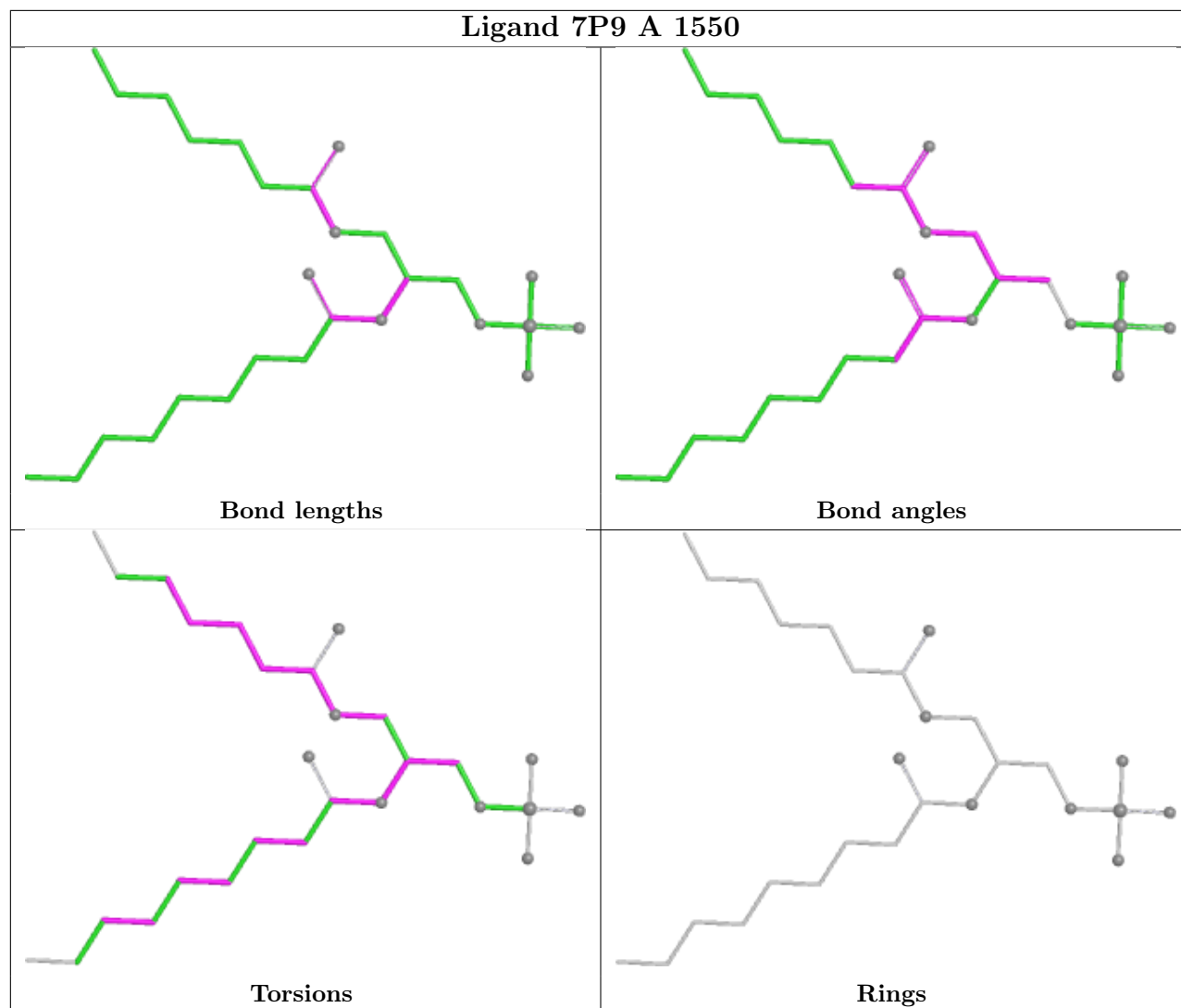
There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1552	NAG	1	0
2	B	1550	7P9	10	0
3	A	1551	PGE	1	0
4	B	1551	NAG	2	0
2	A	1550	7P9	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 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	538/545 (98%)	-0.35	2 (0%) 88 86	22, 35, 46, 62	0
1	B	537/545 (98%)	1.32	121 (22%) 2 2	42, 72, 103, 116	0
All	All	1075/1090 (98%)	0.49	123 (11%) 10 7	22, 46, 96, 116	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	SER	4.9
1	B	430	ALA	4.4
1	B	227	PHE	4.0
1	B	30	LEU	3.9
1	B	182	ALA	3.7
1	B	547	PHE	3.7
1	B	156	LEU	3.6
1	B	67	GLY	3.5
1	A	288	CYS	3.5
1	B	154	ILE	3.5
1	B	434	PHE	3.4
1	B	200	VAL	3.3
1	B	147	ILE	3.3
1	B	438	CYS	3.3
1	B	150	LEU	3.2
1	B	504	VAL	3.2
1	B	125	LEU	3.2
1	B	433	ALA	3.1
1	B	157	GLY	3.0
1	B	386	LEU	3.0
1	B	60	ILE	2.9
1	B	40	PHE	2.9
1	B	29	VAL	2.9
1	B	129	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	21	GLU	2.9
1	B	160	PHE	2.9
1	B	38	VAL	2.8
1	B	248	GLY	2.8
1	B	345	ILE	2.8
1	B	24	VAL	2.8
1	B	208	GLY	2.8
1	B	285	THR	2.8
1	B	216	ILE	2.7
1	B	155	SER	2.7
1	B	212	SER	2.7
1	B	226	VAL	2.7
1	B	162	PHE	2.7
1	B	25	VAL	2.7
1	B	56	TYR	2.7
1	B	541	TYR	2.7
1	B	116	PRO	2.6
1	B	32	ILE	2.6
1	B	269	ILE	2.6
1	B	289	LEU	2.6
1	B	259	ALA	2.6
1	B	277	ALA	2.6
1	B	14	THR	2.6
1	B	335	LYS	2.6
1	B	490	ILE	2.6
1	A	98	PHE	2.5
1	B	108	CYS	2.5
1	B	231	ALA	2.5
1	B	57	THR	2.5
1	B	66	THR	2.5
1	B	234	GLY	2.5
1	B	205	ALA	2.5
1	B	13	THR	2.5
1	B	149	LEU	2.5
1	B	215	THR	2.5
1	B	323	GLY	2.5
1	B	35	PHE	2.5
1	B	119	THR	2.5
1	B	446	PRO	2.4
1	B	19	TYR	2.4
1	B	489	TYR	2.4
1	B	540	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	207	PHE	2.4
1	B	126	PRO	2.4
1	B	151	THR	2.4
1	B	68	ILE	2.4
1	B	549	ILE	2.4
1	B	136	PHE	2.4
1	B	163	VAL	2.4
1	B	201	ALA	2.4
1	B	266	ALA	2.4
1	B	161	ILE	2.4
1	B	279	CYS	2.4
1	B	54	VAL	2.4
1	B	128	LEU	2.3
1	B	322	ASP	2.3
1	B	72	CYS	2.3
1	B	243	ALA	2.3
1	B	123	SER	2.3
1	B	485	ILE	2.3
1	B	502	ALA	2.3
1	B	544	TRP	2.3
1	B	187	ASN	2.3
1	B	375	ASP	2.3
1	B	211	PRO	2.3
1	B	450	TYR	2.3
1	B	48	LEU	2.2
1	B	280	ALA	2.2
1	B	120	THR	2.2
1	B	139	GLY	2.2
1	B	273	VAL	2.2
1	B	239	TYR	2.2
1	B	146	GLY	2.2
1	B	121	SER	2.2
1	B	159	PRO	2.2
1	B	261	VAL	2.2
1	B	258	ALA	2.2
1	B	473	PHE	2.2
1	B	374	GLN	2.1
1	B	385	GLN	2.1
1	B	496	GLY	2.1
1	B	474	TYR	2.1
1	B	536	SER	2.1
1	B	43	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	63	LYS	2.1
1	B	221	ALA	2.1
1	B	503	ALA	2.1
1	B	506	ILE	2.1
1	B	546	ILE	2.1
1	B	28	SER	2.1
1	B	333	ILE	2.1
1	B	98	PHE	2.1
1	B	380	ASN	2.1
1	B	184	GLY	2.1
1	B	15	VAL	2.0
1	B	153	GLY	2.0
1	B	300	ALA	2.0
1	B	47	ASN	2.0
1	B	34	SER	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 oligosaccharides in this entry.

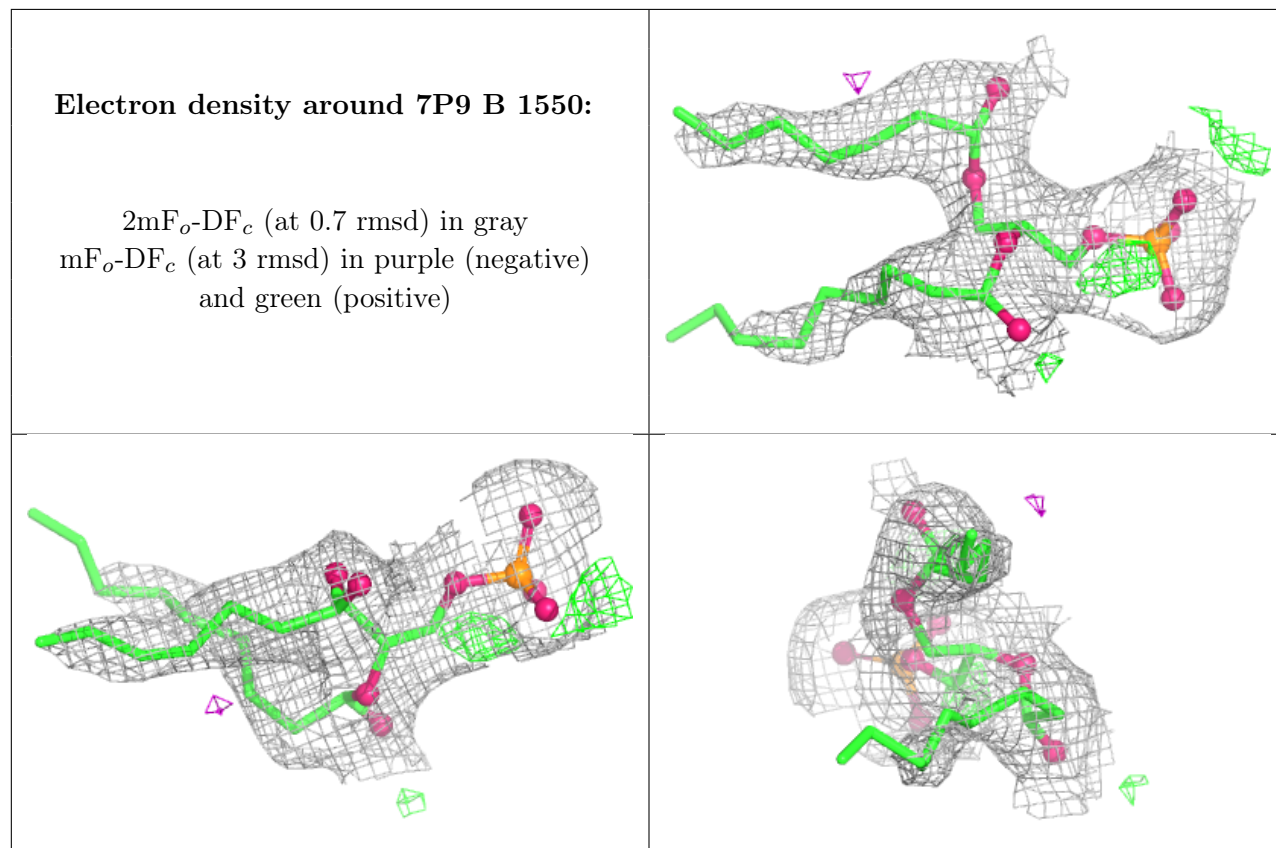
6.4 Ligands [i](#)

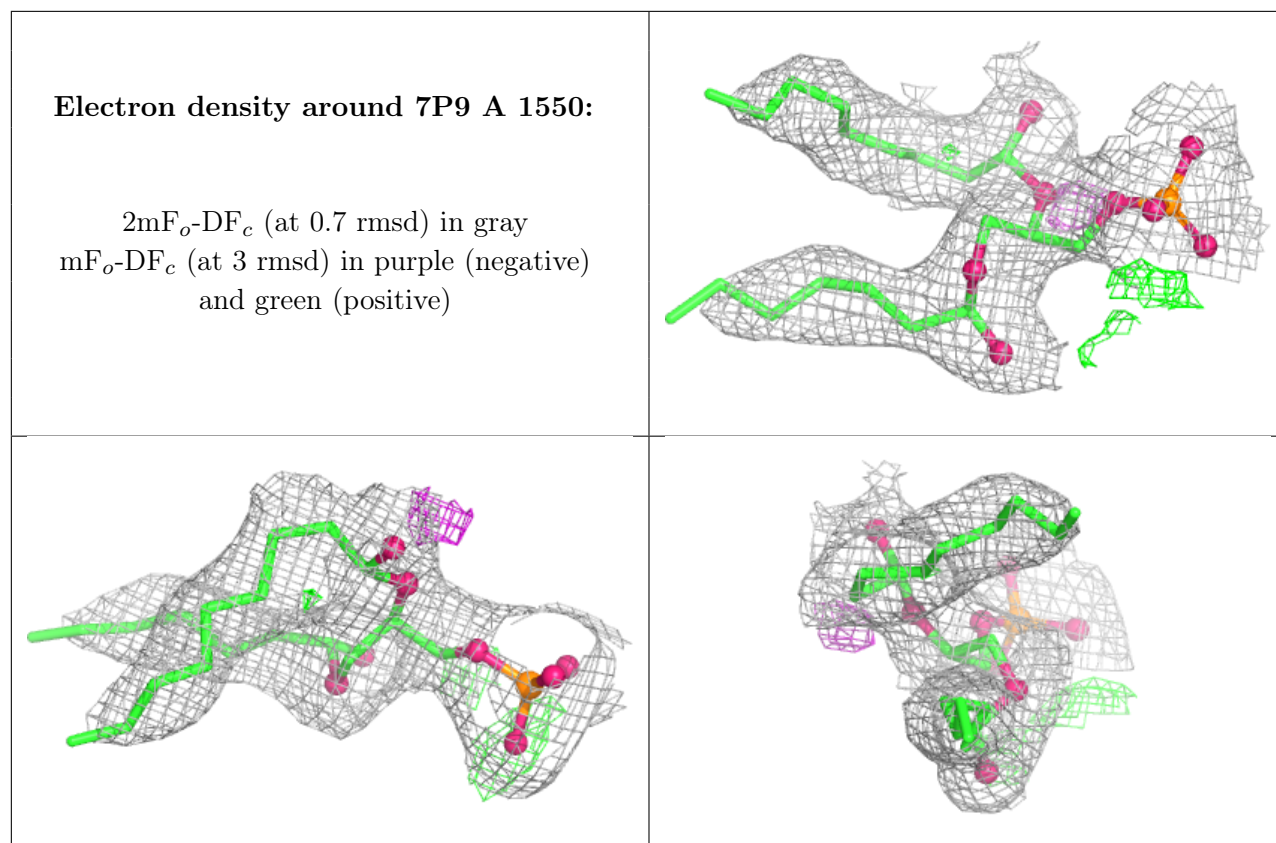
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	1551	14/15	0.70	0.14	75,81,85,85	0
4	NAG	A	1552	14/15	0.81	0.13	42,48,51,59	0
4	NAG	A	1553	14/15	0.87	0.11	44,56,60,62	0
3	PGE	A	1551	10/10	0.88	0.14	47,52,55,56	0
2	7P9	B	1550	28/28	0.89	0.14	52,63,76,84	0
2	7P9	A	1550	28/28	0.92	0.12	39,51,62,66	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.