



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 AM UTC

PDB ID : 2WMZ / pdb_00002wmz
Title : Structure of a mutated TolC
Authors : Hinchliffe, P.; Pei, X.Y.; Symmons, M.F.; Koronakis, E.; Hughes, C.; Koronakis, V.
Deposited on : 2009-07-03
Resolution : 2.90 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)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

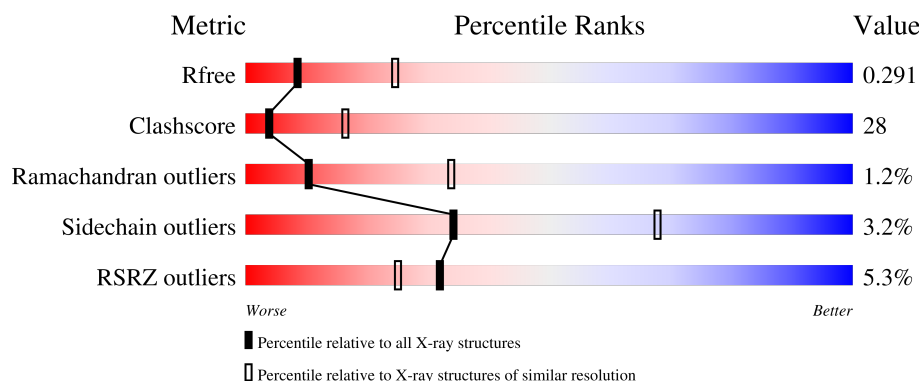
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	428	10% 51% 46% .
1	B	428	2% 53% 44% .
1	C	428	4% 51% 44% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9981 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 OUTER MEMBRANE PROTEIN TOLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3301	2035	583	678	5			
1	B	428	Total	C	N	O	S	0	0	0
			3301	2035	583	678	5			
1	C	428	Total	C	N	O	S	0	0	0
			3301	2035	583	678	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	LEU	VAL	SEE REMARK 999	UNP P02930
A	367	SER	ARG	engineered mutation	UNP P02930
B	169	LEU	VAL	SEE REMARK 999	UNP P02930
B	367	SER	ARG	engineered mutation	UNP P02930
C	169	LEU	VAL	SEE REMARK 999	UNP P02930
C	367	SER	ARG	engineered mutation	UNP P02930

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

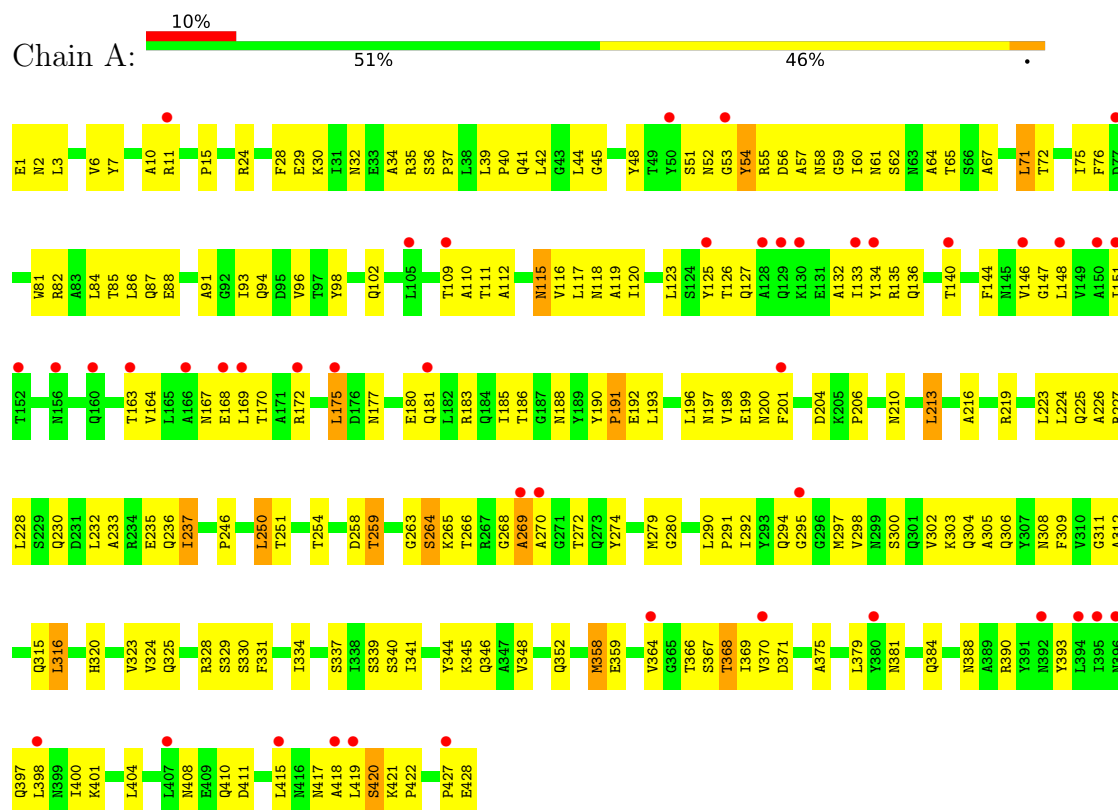
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	13	Total	O	0	0
			13	13		
5	C	2	Total	O	0	0
			2	2		

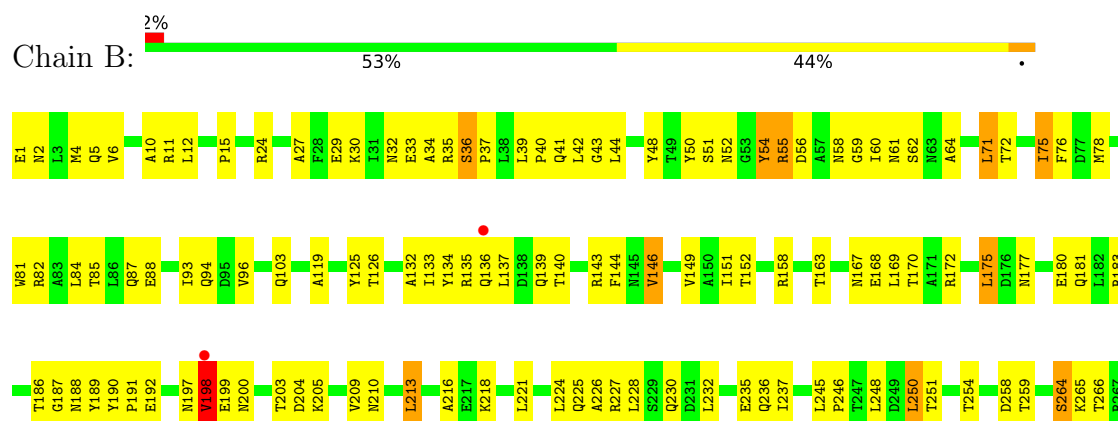
3 Residue-property plots [i](#)

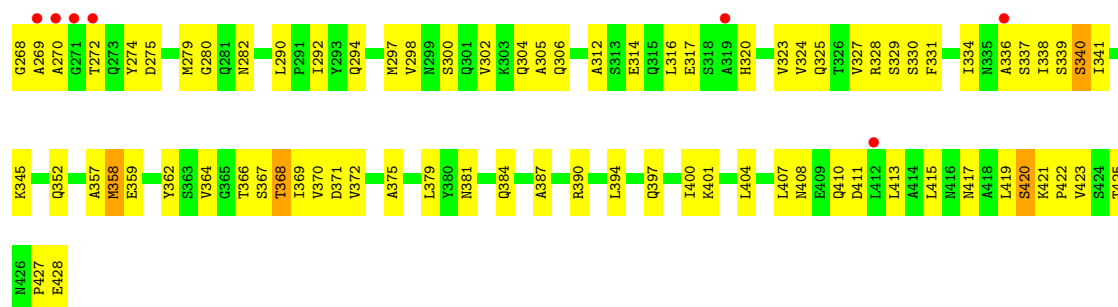
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

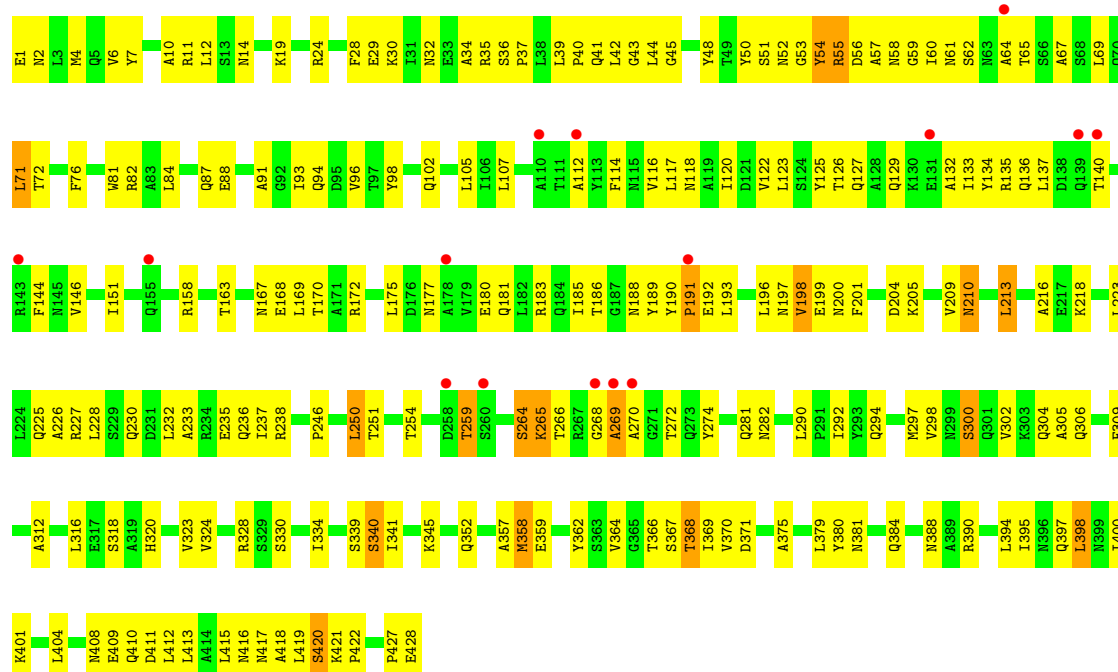


• Molecule 1: OUTER MEMBRANE PROTEIN TOLC





● Molecule 1: OUTER MEMBRANE PROTEIN TOLC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.69Å 135.22Å 136.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 2.90 29.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.93-2.90) 98.8 (29.93-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.301 0.244 , 0.291	Depositor DCC
R_{free} test set	2611 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	1.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9981	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.62% 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: PGE, NA, CL

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	0.46	0/3342	0.93	11/4539 (0.2%)
1	B	0.53	0/3342	0.95	11/4539 (0.2%)
1	C	0.50	0/3342	0.93	9/4539 (0.2%)
All	All	0.50	0/10026	0.94	31/13617 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ASN	N-CA-C	-6.96	102.60	112.13
1	B	381	ASN	N-CA-C	-6.95	102.61	112.13
1	C	381	ASN	N-CA-C	-6.84	102.76	112.13
1	A	345	LYS	N-CA-C	-6.52	104.17	111.28
1	A	56	ASP	N-CA-C	-6.09	105.11	112.54
1	B	56	ASP	N-CA-C	-5.98	105.24	112.54
1	C	345	LYS	N-CA-C	-5.73	105.03	111.28
1	C	56	ASP	N-CA-C	-5.73	105.39	112.38
1	C	375	ALA	N-CA-C	-5.70	105.15	111.36
1	B	175	LEU	N-CA-C	-5.63	105.24	111.71
1	B	345	LYS	N-CA-C	-5.62	105.15	111.28
1	B	375	ALA	N-CA-C	-5.53	105.40	111.82
1	A	54	TYR	N-CA-C	5.48	119.21	112.03
1	A	375	ALA	N-CA-C	-5.41	105.55	111.82
1	B	75	ILE	N-CA-C	-5.40	106.54	111.67
1	A	115	ASN	N-CA-C	-5.35	105.89	112.90
1	A	237	ILE	N-CA-C	-5.33	105.52	110.53
1	C	300	SER	N-CA-C	-5.31	105.60	111.71
1	C	54	TYR	N-CA-C	5.29	118.96	112.03
1	A	191	PRO	N-CA-C	-5.25	106.69	113.57
1	A	75	ILE	N-CA-C	-5.20	106.73	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	VAL	N-CA-C	-5.16	106.41	111.88
1	B	36	SER	CA-C-N	5.15	124.81	119.56
1	B	36	SER	C-N-CA	5.15	124.81	119.56
1	C	281	GLN	N-CA-C	5.15	117.07	108.99
1	A	316	LEU	N-CA-C	-5.13	105.77	111.36
1	B	54	TYR	N-CA-C	5.08	118.69	112.03
1	C	191	PRO	N-CA-C	-5.08	106.91	113.57
1	A	175	LEU	N-CA-C	-5.06	105.89	111.71
1	C	175	LEU	N-CA-C	-5.03	105.93	111.71
1	B	198	VAL	N-CA-C	5.01	119.11	111.89

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	3301	0	3248	204	0
1	B	3301	0	3248	208	0
1	C	3301	0	3248	197	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	10	0	14	0	0
3	B	20	0	28	1	0
3	C	20	0	28	1	0
4	B	1	0	0	0	0
5	A	9	0	0	1	0
5	B	13	0	0	3	0
5	C	2	0	0	0	0
All	All	9981	0	9814	560	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 28.

All (560) 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:364:VAL:HG23	1:A:366:THR:HG23	1.38	1.04
1:C:172:ARG:HD3	1:C:427:PRO:HB2	1.44	0.97
1:C:364:VAL:HG23	1:C:366:THR:HG23	1.47	0.94
1:B:136:GLN:HE21	1:B:359:GLU:HG2	1.32	0.91
1:A:172:ARG:HD3	1:A:427:PRO:HB2	1.56	0.88
1:B:172:ARG:HD3	1:B:427:PRO:HB2	1.56	0.87
1:C:125:TYR:HD2	1:C:384:GLN:HG2	1.40	0.86
1:A:6:VAL:HG22	1:A:190:TYR:CE2	2.12	0.84
1:A:268:GLY:O	1:A:270:ALA:N	2.15	0.80
1:A:292:ILE:HG21	1:C:42:LEU:HD23	1.64	0.79
1:B:136:GLN:NE2	1:B:359:GLU:HG2	1.98	0.79
1:C:172:ARG:CD	1:C:427:PRO:HB2	2.12	0.78
1:B:41:GLN:HE22	1:C:294:GLN:HB3	1.47	0.78
1:B:96:VAL:CG1	1:B:225:GLN:HG3	2.14	0.77
1:B:216:ALA:HB2	1:B:404:LEU:HD23	1.65	0.77
1:A:294:GLN:HB3	1:C:41:GLN:HE22	1.50	0.76
1:C:96:VAL:CG1	1:C:225:GLN:HG3	2.16	0.76
1:B:183:ARG:HA	1:B:188:ASN:O	1.86	0.75
1:C:64:ALA:HB2	1:C:259:THR:HG23	1.68	0.75
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.53	0.74
1:B:96:VAL:HG11	1:B:225:GLN:HG3	1.67	0.74
1:A:330:SER:HB3	1:A:400:ILE:HG12	1.70	0.74
1:A:197:ASN:HA	1:A:421:LYS:HZ1	1.53	0.73
1:A:41:GLN:HE22	1:B:294:GLN:HB3	1.53	0.73
1:B:401:LYS:HE3	1:B:411:ASP:OD1	1.88	0.73
1:A:64:ALA:HB2	1:A:259:THR:HG23	1.71	0.72
1:B:197:ASN:HA	1:B:421:LYS:HZ1	1.55	0.72
1:B:183:ARG:HG2	1:B:189:TYR:CZ	2.25	0.71
1:B:36:SER:HB3	1:B:37:PRO:HD3	1.72	0.71
1:A:250:LEU:C	1:A:250:LEU:HD23	2.15	0.71
1:A:197:ASN:HA	1:A:421:LYS:NZ	2.06	0.71
1:B:268:GLY:O	1:B:270:ALA:N	2.24	0.71
1:B:172:ARG:CD	1:B:427:PRO:HB2	2.21	0.70
1:B:364:VAL:HG23	1:B:366:THR:HG23	1.74	0.70
1:C:183:ARG:HG3	1:C:183:ARG:HH11	1.57	0.70
1:A:180:GLU:OE2	1:A:180:GLU:HA	1.91	0.70
1:A:401:LYS:HE3	1:A:411:ASP:OD1	1.92	0.70
1:B:144:PHE:CZ	1:B:151:ILE:HD13	2.27	0.70
1:B:146:VAL:HG12	1:B:146:VAL:O	1.92	0.70
1:A:297:MET:HB2	1:C:36:SER:OG	1.93	0.69
1:C:268:GLY:O	1:C:270:ALA:N	2.24	0.69
1:C:114:PHE:HD2	1:C:395:ILE:HD11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:HD23	1:B:250:LEU:C	2.18	0.69
1:A:308:ASN:HB2	5:A:2009:HOH:O	1.91	0.68
1:B:183:ARG:HG3	1:B:183:ARG:HH11	1.57	0.68
1:C:250:LEU:C	1:C:250:LEU:HD23	2.17	0.68
1:C:96:VAL:HG11	1:C:225:GLN:HG3	1.74	0.68
1:A:292:ILE:CG2	1:C:42:LEU:HD23	2.24	0.68
1:B:330:SER:HB3	1:B:400:ILE:HG12	1.76	0.68
1:B:6:VAL:HG22	1:B:190:TYR:CE2	2.29	0.67
1:A:144:PHE:CZ	1:A:151:ILE:HD13	2.29	0.67
1:C:320:HIS:O	1:C:323:VAL:HG12	1.94	0.66
1:B:125:TYR:HD2	1:B:384:GLN:HG2	1.61	0.66
1:A:125:TYR:HD2	1:A:384:GLN:HG2	1.61	0.66
1:A:339:SER:C	1:C:169:LEU:HD11	2.21	0.65
1:C:6:VAL:HG22	1:C:190:TYR:CE2	2.31	0.65
1:B:136:GLN:NE2	1:B:372:VAL:HG11	2.11	0.65
1:C:401:LYS:HE3	1:C:411:ASP:OD1	1.97	0.65
1:B:60:ILE:C	1:B:61:ASN:HD22	2.05	0.65
1:B:197:ASN:HA	1:B:421:LYS:NZ	2.12	0.65
1:C:180:GLU:OE2	1:C:180:GLU:HA	1.97	0.65
1:C:266:THR:HA	1:C:274:TYR:HD2	1.62	0.65
1:A:36:SER:OG	1:B:297:MET:HB2	1.96	0.65
1:B:137:LEU:HD21	1:B:158:ARG:HD2	1.79	0.64
1:A:72:THR:HG22	1:A:251:THR:HG22	1.78	0.64
1:C:330:SER:HB3	1:C:400:ILE:HG12	1.80	0.64
1:C:341:ILE:HD11	1:C:390:ARG:HA	1.80	0.64
1:C:146:VAL:HG12	1:C:146:VAL:O	1.97	0.64
1:A:266:THR:HA	1:A:274:TYR:HD2	1.63	0.63
1:B:266:THR:HA	1:B:274:TYR:HD2	1.64	0.63
1:C:60:ILE:C	1:C:61:ASN:HD22	2.06	0.63
1:A:60:ILE:C	1:A:61:ASN:HD22	2.06	0.63
1:A:232:LEU:O	1:A:236:GLN:HG3	1.99	0.63
5:B:2004:HOH:O	1:C:297:MET:HE3	1.98	0.63
1:C:36:SER:HB3	1:C:37:PRO:HD3	1.81	0.63
1:C:334:ILE:HD11	1:C:397:GLN:HG2	1.81	0.63
1:A:136:GLN:NE2	1:A:359:GLU:HG2	2.14	0.62
1:C:51:SER:HB2	1:C:62:SER:OG	1.98	0.62
1:B:352:GLN:HA	1:B:379:LEU:HD13	1.82	0.62
1:B:136:GLN:CD	1:B:372:VAL:HG11	2.24	0.62
1:C:368:THR:HG23	1:C:371:ASP:CG	2.24	0.62
1:B:64:ALA:HB2	1:B:259:THR:HG23	1.82	0.62
1:A:358:MET:HG3	1:A:371:ASP:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:VAL:O	1:B:327:VAL:HG23	1.98	0.61
1:A:36:SER:HB3	1:A:37:PRO:HD3	1.80	0.61
1:A:146:VAL:HG12	1:A:146:VAL:O	2.00	0.61
1:B:298:VAL:O	1:B:302:VAL:HG23	2.00	0.61
1:B:51:SER:HB2	1:B:62:SER:OG	2.00	0.61
1:B:394:LEU:HD22	1:B:415:LEU:HD22	1.83	0.61
1:B:169:LEU:HD11	1:C:339:SER:C	2.26	0.61
1:B:341:ILE:HD11	1:B:390:ARG:HA	1.82	0.61
1:C:226:ALA:HB1	1:C:316:LEU:HA	1.81	0.60
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.67	0.60
1:A:330:SER:HB3	1:A:400:ILE:CG1	2.30	0.60
1:B:180:GLU:OE2	1:B:180:GLU:HA	1.99	0.60
1:C:136:GLN:O	1:C:140:THR:HG23	2.02	0.60
1:A:250:LEU:HD23	1:A:251:THR:N	2.16	0.60
1:B:246:PRO:HB3	1:B:290:LEU:HD13	1.83	0.60
1:C:43:GLY:HA3	3:C:1431:PGE:H32	1.83	0.60
1:B:36:SER:OG	1:C:297:MET:HB2	2.02	0.60
1:A:368:THR:HG23	1:A:371:ASP:CG	2.27	0.59
1:C:4:MET:HE1	1:C:409:GLU:O	2.02	0.59
1:C:216:ALA:HB2	1:C:404:LEU:HD23	1.83	0.59
1:C:250:LEU:HD23	1:C:251:THR:N	2.17	0.59
1:A:51:SER:HB2	1:A:62:SER:OG	2.02	0.59
1:A:96:VAL:CG1	1:A:225:GLN:HG3	2.32	0.59
1:C:144:PHE:CZ	1:C:151:ILE:HD13	2.38	0.59
1:C:213:LEU:HD21	1:C:324:VAL:HG22	1.85	0.59
1:C:4:MET:HE3	1:C:413:LEU:HB2	1.84	0.58
1:B:137:LEU:HD11	1:B:158:ARG:HG2	1.85	0.58
1:A:10:ALA:HB2	1:A:186:THR:HA	1.85	0.58
1:B:237:ILE:HA	1:B:305:ALA:HB1	1.85	0.58
1:B:250:LEU:HD23	1:B:251:THR:N	2.18	0.58
1:C:246:PRO:HB3	1:C:290:LEU:HD13	1.86	0.58
1:C:362:TYR:HD1	1:C:367:SER:O	1.87	0.58
1:A:132:ALA:HA	1:A:135:ARG:HE	1.69	0.58
1:B:44:LEU:HB2	1:C:292:ILE:HD11	1.85	0.58
1:C:394:LEU:HD22	1:C:415:LEU:HD22	1.86	0.58
1:A:246:PRO:HB3	1:A:290:LEU:HD13	1.85	0.57
1:B:169:LEU:HD23	1:B:170:THR:N	2.19	0.57
1:C:1:GLU:O	1:C:193:LEU:HA	2.04	0.57
1:A:42:LEU:HD23	1:B:292:ILE:HG21	1.85	0.57
1:C:72:THR:HG22	1:C:251:THR:HG22	1.86	0.57
1:C:125:TYR:HD2	1:C:384:GLN:CG	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:MET:HG3	1:C:371:ASP:HB3	1.86	0.57
1:B:203:THR:HG21	1:B:338:ILE:HG23	1.86	0.57
1:B:358:MET:HE3	1:B:367:SER:HB3	1.87	0.57
1:C:254:THR:HG23	1:C:254:THR:O	2.03	0.57
1:A:320:HIS:O	1:A:323:VAL:HG12	2.05	0.57
1:B:232:LEU:O	1:B:236:GLN:HG3	2.05	0.57
1:C:132:ALA:HA	1:C:135:ARG:HE	1.69	0.57
1:B:169:LEU:HD23	1:B:169:LEU:C	2.29	0.56
1:C:169:LEU:C	1:C:169:LEU:HD23	2.30	0.56
1:A:216:ALA:HB2	1:A:404:LEU:HD23	1.86	0.56
1:C:136:GLN:HE21	1:C:359:GLU:HG2	1.69	0.56
1:C:169:LEU:HD23	1:C:170:THR:N	2.20	0.56
1:C:197:ASN:HA	1:C:421:LYS:HZ1	1.71	0.56
1:B:213:LEU:HD21	1:B:324:VAL:HG22	1.87	0.56
1:C:352:GLN:HA	1:C:379:LEU:HD13	1.88	0.56
1:A:96:VAL:HG11	1:A:225:GLN:HG3	1.87	0.56
1:B:71:LEU:C	1:B:71:LEU:HD23	2.31	0.56
1:B:227:ARG:HG2	1:B:227:ARG:HH11	1.71	0.56
1:B:139:GLN:HE21	1:B:362:TYR:HD2	1.55	0.55
1:B:272:THR:HG22	1:B:272:THR:O	2.06	0.55
1:B:72:THR:HG22	1:B:251:THR:HG22	1.88	0.55
1:C:133:ILE:HG22	1:C:133:ILE:O	2.05	0.55
1:A:172:ARG:CD	1:A:427:PRO:HB2	2.31	0.55
1:A:272:THR:HG22	1:A:272:THR:O	2.07	0.55
1:C:328:ARG:HH11	1:C:328:ARG:HG2	1.71	0.55
1:A:1:GLU:O	1:A:193:LEU:HA	2.07	0.55
1:B:264:SER:C	1:B:266:THR:H	2.15	0.55
1:C:125:TYR:CD2	1:C:384:GLN:HG2	2.32	0.55
1:C:192:GLU:OE1	1:C:422:PRO:HB3	2.07	0.55
1:A:280:GLY:HA3	1:C:54:TYR:CD1	2.42	0.54
1:C:197:ASN:HA	1:C:421:LYS:NZ	2.22	0.54
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.23	0.54
1:B:27:ALA:HA	5:B:2002:HOH:O	2.06	0.54
1:B:334:ILE:HD11	1:B:397:GLN:HG2	1.89	0.54
1:B:84:LEU:O	1:B:88:GLU:HG3	2.07	0.54
1:B:126:THR:HG21	1:B:168:GLU:HA	1.90	0.54
1:A:71:LEU:HD23	1:A:71:LEU:C	2.33	0.54
1:A:337:SER:O	1:A:341:ILE:HG13	2.08	0.54
1:B:320:HIS:O	1:B:323:VAL:HG12	2.07	0.54
1:B:358:MET:HG3	1:B:371:ASP:HB3	1.90	0.54
1:C:237:ILE:HA	1:C:305:ALA:HB1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ALA:HB2	1:A:185:ILE:HD12	1.88	0.54
1:A:226:ALA:HB1	1:A:316:LEU:HA	1.88	0.54
1:B:4:MET:HE3	1:B:413:LEU:HB2	1.90	0.54
1:C:136:GLN:NE2	1:C:359:GLU:HG2	2.23	0.54
1:C:272:THR:HG22	1:C:272:THR:O	2.07	0.54
1:A:264:SER:C	1:A:266:THR:H	2.16	0.53
1:A:294:GLN:HA	1:C:41:GLN:NE2	2.22	0.53
1:B:200:ASN:HD22	1:B:200:ASN:N	2.07	0.53
1:A:41:GLN:HB2	1:A:72:THR:OG1	2.08	0.53
1:A:298:VAL:O	1:A:302:VAL:HG23	2.09	0.53
1:B:358:MET:HE3	1:B:367:SER:CB	2.39	0.53
1:C:417:ASN:N	1:C:417:ASN:HD22	2.04	0.53
1:A:136:GLN:HE21	1:A:359:GLU:HG2	1.74	0.53
1:A:398:LEU:HD11	1:A:415:LEU:HD11	1.90	0.53
1:B:36:SER:CB	1:B:37:PRO:HD3	2.39	0.53
1:C:71:LEU:C	1:C:71:LEU:HD23	2.34	0.53
1:A:169:LEU:C	1:A:169:LEU:HD23	2.34	0.53
1:A:330:SER:CB	1:A:400:ILE:HG12	2.38	0.53
1:A:340:SER:N	1:C:169:LEU:HD11	2.24	0.53
1:B:226:ALA:HB1	1:B:316:LEU:HA	1.90	0.53
1:B:203:THR:CB	1:B:338:ILE:HG23	2.38	0.53
1:B:203:THR:OG1	1:B:338:ILE:HG23	2.07	0.53
1:C:118:ASN:HD21	1:C:388:ASN:ND2	2.07	0.53
1:C:417:ASN:C	1:C:419:LEU:H	2.16	0.53
1:A:169:LEU:HD23	1:A:170:THR:N	2.23	0.52
1:B:41:GLN:HB2	1:B:72:THR:OG1	2.09	0.52
1:C:6:VAL:CG1	1:C:186:THR:HG21	2.40	0.52
1:A:132:ALA:CB	1:A:135:ARG:HH21	2.22	0.52
1:A:177:ASN:O	1:A:181:GLN:HG2	2.10	0.52
1:A:219:ARG:HB2	1:A:404:LEU:O	2.10	0.52
1:C:30:LYS:HB3	1:C:87:GLN:OE1	2.10	0.52
1:B:133:ILE:HG22	1:B:133:ILE:O	2.10	0.52
1:C:137:LEU:HD21	1:C:158:ARG:HD2	1.90	0.52
1:B:10:ALA:HB2	1:B:186:THR:HA	1.91	0.52
1:B:48:TYR:C	1:B:48:TYR:CD2	2.88	0.52
1:B:119:ALA:HB1	1:B:175:LEU:HA	1.92	0.52
1:A:6:VAL:HG13	1:A:190:TYR:CZ	2.45	0.52
1:A:183:ARG:HG3	1:A:183:ARG:NH1	2.24	0.52
1:A:254:THR:O	1:A:254:THR:HG23	2.09	0.52
1:C:132:ALA:CB	1:C:135:ARG:HH21	2.23	0.52
1:A:133:ILE:O	1:A:133:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.74	0.52
1:C:364:VAL:HG23	1:C:366:THR:CG2	2.32	0.52
1:A:344:TYR:O	1:A:348:VAL:HG23	2.11	0.51
1:B:254:THR:HG23	1:B:254:THR:O	2.09	0.51
1:C:10:ALA:HB2	1:C:186:THR:HA	1.92	0.51
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.75	0.51
1:C:87:GLN:HA	1:C:87:GLN:NE2	2.25	0.51
1:C:2:ASN:O	1:C:6:VAL:HG23	2.10	0.51
1:C:328:ARG:HG2	1:C:328:ARG:NH1	2.26	0.51
1:A:6:VAL:CG1	1:A:186:THR:HG21	2.41	0.51
1:A:364:VAL:HG23	1:A:366:THR:CG2	2.26	0.51
1:A:36:SER:CB	1:A:37:PRO:HD3	2.41	0.51
1:A:200:ASN:N	1:A:200:ASN:HD22	2.09	0.51
1:B:54:TYR:HD2	1:C:282:ASN:ND2	2.08	0.51
1:C:177:ASN:O	1:C:181:GLN:HG2	2.10	0.51
1:C:264:SER:C	1:C:266:THR:H	2.19	0.51
1:A:24:ARG:HA	1:A:94:GLN:CG	2.41	0.50
1:C:417:ASN:N	1:C:417:ASN:ND2	2.60	0.50
1:A:250:LEU:C	1:A:250:LEU:CD2	2.84	0.50
1:B:54:TYR:HD1	1:B:54:TYR:O	1.94	0.50
1:B:132:ALA:HA	1:B:135:ARG:HE	1.75	0.50
1:B:264:SER:O	1:B:266:THR:N	2.45	0.50
1:B:320:HIS:HA	1:B:323:VAL:HG12	1.93	0.50
1:B:230:GLN:HA	1:B:312:ALA:HB1	1.92	0.50
1:B:408:ASN:OD1	1:B:410:GLN:HB2	2.12	0.50
1:C:274:TYR:N	1:C:274:TYR:CD1	2.77	0.50
1:A:53:GLY:HA2	1:B:280:GLY:O	2.11	0.50
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.75	0.50
1:A:294:GLN:CB	1:C:41:GLN:HE22	2.20	0.50
1:A:235:GLU:OE2	1:A:235:GLU:HA	2.11	0.50
1:A:417:ASN:C	1:A:419:LEU:H	2.20	0.50
1:B:39:LEU:HB3	1:B:40:PRO:CD	2.42	0.50
1:A:76:PHE:O	1:A:76:PHE:CD1	2.65	0.50
1:A:417:ASN:HD22	1:A:417:ASN:N	2.08	0.50
1:B:177:ASN:O	1:B:181:GLN:HG2	2.11	0.50
1:C:4:MET:HE2	1:C:412:LEU:C	2.37	0.50
1:A:2:ASN:O	1:A:6:VAL:HG23	2.12	0.49
1:B:368:THR:HG23	1:B:371:ASP:CG	2.36	0.49
1:C:41:GLN:HB2	1:C:72:THR:OG1	2.11	0.49
1:C:137:LEU:HD11	1:C:158:ARG:HG2	1.94	0.49
1:A:279:MET:CE	1:C:57:ALA:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:TYR:C	1:C:48:TYR:CD2	2.89	0.49
1:A:274:TYR:CD1	1:A:274:TYR:N	2.78	0.49
1:B:330:SER:HB3	1:B:400:ILE:CG1	2.40	0.49
1:A:44:LEU:HB2	1:B:292:ILE:HD11	1.94	0.49
1:A:266:THR:HA	1:A:274:TYR:CD2	2.47	0.49
1:B:39:LEU:HB3	1:B:40:PRO:HD2	1.94	0.49
1:C:36:SER:CB	1:C:37:PRO:HD3	2.41	0.49
1:A:302:VAL:O	1:A:306:GLN:HG3	2.12	0.49
1:A:320:HIS:HA	1:A:323:VAL:HG12	1.94	0.49
1:A:146:VAL:O	1:A:148:LEU:HG	2.13	0.49
1:A:398:LEU:CD1	1:A:415:LEU:HD11	2.42	0.49
1:B:274:TYR:CD1	1:B:274:TYR:N	2.78	0.49
1:C:126:THR:HG21	1:C:168:GLU:HA	1.93	0.49
1:B:204:ASP:O	1:B:205:LYS:C	2.55	0.49
1:B:352:GLN:CA	1:B:379:LEU:HD13	2.42	0.49
1:A:126:THR:HG21	1:A:168:GLU:HA	1.94	0.49
1:A:300:SER:OG	1:C:32:ASN:HB2	2.12	0.49
1:C:7:TYR:HB2	1:C:412:LEU:HD21	1.94	0.49
1:A:48:TYR:C	1:A:48:TYR:CD2	2.91	0.48
1:A:81:TRP:O	1:A:82:ARG:C	2.55	0.48
1:A:183:ARG:HA	1:A:188:ASN:O	2.14	0.48
1:A:300:SER:HA	1:C:29:GLU:OE2	2.13	0.48
1:C:320:HIS:HA	1:C:323:VAL:HG12	1.94	0.48
1:A:136:GLN:O	1:A:140:THR:HG23	2.13	0.48
1:C:196:LEU:HD11	1:C:201:PHE:HD1	1.79	0.48
1:A:295:GLY:O	1:C:36:SER:HA	2.14	0.48
1:C:183:ARG:HG2	1:C:189:TYR:CZ	2.48	0.48
1:B:216:ALA:HB2	1:B:404:LEU:CD2	2.38	0.48
1:B:235:GLU:HA	1:B:235:GLU:OE2	2.14	0.48
1:C:24:ARG:HA	1:C:94:GLN:CG	2.44	0.48
1:C:200:ASN:N	1:C:200:ASN:HD22	2.10	0.48
1:B:250:LEU:C	1:B:250:LEU:CD2	2.87	0.48
1:C:198:VAL:HG23	1:C:199:GLU:OE1	2.14	0.48
1:C:408:ASN:OD1	1:C:410:GLN:HB2	2.14	0.48
1:C:420:SER:O	1:C:422:PRO:HD3	2.14	0.48
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.29	0.47
1:B:417:ASN:N	1:B:417:ASN:HD22	2.11	0.47
1:B:237:ILE:HD13	1:B:306:GLN:HG2	1.96	0.47
1:A:84:LEU:O	1:A:88:GLU:HG3	2.13	0.47
1:A:213:LEU:HD21	1:A:324:VAL:HG22	1.95	0.47
1:A:358:MET:HE3	1:A:367:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:SER:O	1:B:422:PRO:HD3	2.14	0.47
1:C:417:ASN:C	1:C:419:LEU:N	2.72	0.47
1:B:132:ALA:CB	1:B:135:ARG:HH21	2.27	0.47
1:C:112:ALA:HB2	1:C:185:ILE:HD12	1.97	0.47
1:A:10:ALA:CB	1:A:186:THR:HA	2.45	0.47
1:A:300:SER:O	1:A:304:GLN:HG3	2.14	0.47
1:B:15:PRO:HB2	1:C:318:SER:OG	2.15	0.47
1:B:24:ARG:HA	1:B:94:GLN:CG	2.45	0.47
1:B:81:TRP:O	1:B:82:ARG:C	2.57	0.47
1:B:266:THR:HA	1:B:274:TYR:CD2	2.47	0.47
1:B:417:ASN:C	1:B:419:LEU:H	2.22	0.47
1:A:58:ASN:OD1	1:A:59:GLY:N	2.47	0.47
1:A:223:LEU:O	1:A:227:ARG:HG3	2.14	0.47
1:B:137:LEU:CD2	1:B:158:ARG:HD2	2.45	0.47
1:A:237:ILE:HD13	1:A:306:GLN:HG2	1.97	0.47
1:C:199:GLU:OE1	1:C:199:GLU:N	2.47	0.47
1:A:11:ARG:O	1:A:11:ARG:HG2	2.16	0.46
1:C:54:TYR:HD1	1:C:54:TYR:O	1.98	0.46
1:A:3:LEU:HD11	1:A:110:ALA:HA	1.97	0.46
1:A:264:SER:O	1:A:266:THR:N	2.48	0.46
1:A:325:GLN:NE2	1:A:329:SER:OG	2.49	0.46
1:B:2:ASN:O	1:B:6:VAL:HG23	2.15	0.46
1:B:324:VAL:HG12	1:B:325:GLN:N	2.29	0.46
1:C:24:ARG:HA	1:C:94:GLN:HG3	1.98	0.46
1:C:235:GLU:OE2	1:C:235:GLU:HA	2.15	0.46
1:B:75:ILE:HB	1:B:248:LEU:O	2.15	0.46
1:C:96:VAL:HG12	1:C:225:GLN:HG3	1.97	0.46
1:C:235:GLU:OE2	1:C:238:ARG:NH1	2.49	0.46
1:A:111:THR:HG22	1:A:115:ASN:ND2	2.30	0.46
1:B:6:VAL:HG13	1:B:190:TYR:CZ	2.51	0.46
1:B:75:ILE:HG21	1:B:248:LEU:HD23	1.98	0.46
1:B:198:VAL:HG12	1:B:390:ARG:CZ	2.45	0.46
1:B:358:MET:HE3	1:B:367:SER:OG	2.15	0.46
1:C:302:VAL:O	1:C:306:GLN:HG3	2.15	0.46
1:A:204:ASP:N	1:A:393:TYR:OH	2.46	0.46
1:B:78:MET:HG3	1:B:245:LEU:CD1	2.46	0.46
1:B:87:GLN:NE2	1:B:87:GLN:HA	2.29	0.46
1:A:237:ILE:HA	1:A:305:ALA:HB1	1.98	0.46
1:A:417:ASN:N	1:A:417:ASN:ND2	2.63	0.46
1:B:24:ARG:HA	1:B:94:GLN:HG3	1.96	0.46
1:B:152:THR:HG22	1:C:357:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:HG3	1:B:183:ARG:NH1	2.27	0.46
1:A:42:LEU:HD23	1:B:292:ILE:CG2	2.44	0.46
1:A:408:ASN:OD1	1:A:410:GLN:HB2	2.16	0.46
1:C:11:ARG:O	1:C:11:ARG:HG2	2.16	0.46
1:C:232:LEU:O	1:C:236:GLN:HG3	2.14	0.46
1:B:60:ILE:C	1:B:61:ASN:ND2	2.72	0.46
1:C:369:ILE:HG23	1:C:370:VAL:N	2.31	0.46
1:A:24:ARG:HA	1:A:94:GLN:HG3	1.97	0.46
1:C:183:ARG:HG3	1:C:183:ARG:NH1	2.27	0.46
1:A:87:GLN:NE2	1:A:87:GLN:HA	2.30	0.45
1:A:280:GLY:O	1:C:53:GLY:HA2	2.16	0.45
1:B:203:THR:HB	1:B:338:ILE:HG12	1.98	0.45
1:A:39:LEU:HB3	1:A:40:PRO:CD	2.46	0.45
1:A:304:GLN:NE2	1:C:30:LYS:HA	2.30	0.45
1:B:331:PHE:O	1:B:334:ILE:HG22	2.16	0.45
1:C:183:ARG:HA	1:C:188:ASN:O	2.16	0.45
1:A:85:THR:HA	1:A:88:GLU:OE1	2.16	0.45
1:C:93:ILE:HG12	1:C:228:LEU:HB3	1.98	0.45
1:C:233:ALA:HB1	1:C:309:PHE:HA	1.98	0.45
1:C:266:THR:HA	1:C:274:TYR:CD2	2.46	0.45
1:A:30:LYS:HA	1:B:304:GLN:NE2	2.32	0.45
1:A:48:TYR:CD1	1:A:65:THR:HG22	2.51	0.45
1:B:369:ILE:HG23	1:B:370:VAL:N	2.31	0.45
1:A:93:ILE:HG12	1:A:228:LEU:HB3	1.98	0.45
1:C:341:ILE:CD1	1:C:390:ARG:HA	2.47	0.45
1:A:196:LEU:HD11	1:A:201:PHE:HD1	1.82	0.45
1:A:233:ALA:HB1	1:A:309:PHE:HA	1.97	0.45
1:B:132:ALA:C	1:B:134:TYR:N	2.75	0.45
1:B:183:ARG:O	1:B:187:GLY:N	2.47	0.45
1:C:129:GLN:HB2	1:C:380:TYR:CD2	2.52	0.45
1:C:133:ILE:O	1:C:133:ILE:CG2	2.64	0.45
1:B:192:GLU:HA	1:B:425:THR:HG23	1.98	0.45
1:C:98:TYR:O	1:C:102:GLN:HG3	2.17	0.45
1:C:250:LEU:C	1:C:250:LEU:CD2	2.86	0.45
1:A:54:TYR:CD1	1:A:55:ARG:HG3	2.52	0.45
1:A:292:ILE:HD11	1:C:44:LEU:HB2	1.98	0.45
1:B:146:VAL:O	1:B:146:VAL:CG1	2.64	0.45
1:C:183:ARG:HD2	1:C:183:ARG:O	2.17	0.45
1:C:54:TYR:HD1	1:C:55:ARG:HG3	1.82	0.45
1:A:54:TYR:HD2	1:B:282:ASN:ND2	2.15	0.44
1:A:192:GLU:OE1	1:A:422:PRO:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:HB3	1:C:40:PRO:CD	2.47	0.44
1:C:45:GLY:O	1:C:67:ALA:HA	2.17	0.44
1:C:132:ALA:C	1:C:134:TYR:H	2.24	0.44
1:A:415:LEU:C	1:A:417:ASN:H	2.26	0.44
1:B:143:ARG:C	1:B:149:VAL:HG22	2.42	0.44
1:C:48:TYR:CD1	1:C:65:THR:HG22	2.52	0.44
1:A:60:ILE:C	1:A:61:ASN:ND2	2.74	0.44
1:B:258:ASP:N	1:B:258:ASP:OD2	2.49	0.44
1:C:81:TRP:O	1:C:82:ARG:C	2.60	0.44
1:C:298:VAL:O	1:C:302:VAL:HG23	2.17	0.44
1:A:57:ALA:HB2	1:B:279:MET:CE	2.47	0.44
1:A:183:ARG:HD2	1:A:183:ARG:O	2.17	0.44
1:B:415:LEU:C	1:B:417:ASN:H	2.26	0.44
1:C:122:VAL:HG22	1:C:384:GLN:OE1	2.17	0.44
1:A:45:GLY:O	1:A:67:ALA:HA	2.17	0.44
1:A:54:TYR:HD1	1:A:54:TYR:O	2.00	0.44
1:A:35:ARG:HB2	1:A:84:LEU:HD22	1.99	0.44
1:A:54:TYR:CD1	1:B:280:GLY:HA3	2.53	0.44
1:B:190:TYR:HA	1:B:191:PRO:HD3	1.87	0.44
1:B:203:THR:CG2	1:B:338:ILE:HG23	2.47	0.44
1:B:341:ILE:CD1	1:B:390:ARG:HA	2.48	0.44
1:C:58:ASN:OD1	1:C:59:GLY:N	2.51	0.44
1:C:358:MET:HE3	1:C:367:SER:OG	2.18	0.44
1:A:29:GLU:OE2	1:B:300:SER:HA	2.18	0.44
1:B:417:ASN:N	1:B:417:ASN:ND2	2.65	0.44
1:C:132:ALA:C	1:C:134:TYR:N	2.76	0.44
1:B:35:ARG:HG2	1:B:35:ARG:HH21	1.83	0.44
1:B:167:ASN:C	1:B:169:LEU:N	2.71	0.44
1:C:84:LEU:O	1:C:88:GLU:HG3	2.16	0.44
1:C:230:GLN:HA	1:C:312:ALA:HB1	2.00	0.44
1:A:28:PHE:CD1	1:A:91:ALA:HB1	2.52	0.44
1:A:54:TYR:HD1	1:A:55:ARG:HG3	1.83	0.43
1:A:369:ILE:HG23	1:A:370:VAL:N	2.32	0.43
1:A:415:LEU:C	1:A:417:ASN:N	2.76	0.43
1:B:11:ARG:HG2	1:B:11:ARG:O	2.17	0.43
1:B:11:ARG:HH21	1:B:12:LEU:HD21	1.83	0.43
1:B:29:GLU:OE2	1:C:300:SER:HA	2.18	0.43
1:B:35:ARG:O	1:B:36:SER:C	2.60	0.43
1:B:325:GLN:CD	1:B:325:GLN:C	2.87	0.43
1:C:223:LEU:O	1:C:227:ARG:HG3	2.18	0.43
1:A:41:GLN:HE22	1:B:294:GLN:CB	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.85	0.43
1:A:230:GLN:HA	1:A:312:ALA:HB1	2.00	0.43
1:B:192:GLU:HB2	1:B:423:VAL:O	2.17	0.43
1:B:266:THR:HG23	1:B:274:TYR:HB3	2.00	0.43
1:C:190:TYR:HA	1:C:191:PRO:HD3	1.89	0.43
1:C:264:SER:O	1:C:266:THR:N	2.50	0.43
1:A:264:SER:C	1:A:266:THR:N	2.76	0.43
1:B:42:LEU:HD23	1:C:292:ILE:HG21	2.00	0.43
1:B:387:ALA:HA	5:B:2013:HOH:O	2.19	0.43
1:C:357:ALA:O	1:C:358:MET:C	2.62	0.43
1:A:39:LEU:HB3	1:A:40:PRO:HD2	1.99	0.43
1:A:116:VAL:O	1:A:120:ILE:HG13	2.18	0.43
1:A:417:ASN:C	1:A:419:LEU:N	2.77	0.43
1:A:420:SER:O	1:A:422:PRO:HD3	2.18	0.43
1:B:54:TYR:CD1	1:B:55:ARG:HG3	2.53	0.43
1:A:368:THR:O	1:A:371:ASP:HB2	2.19	0.43
1:B:136:GLN:O	1:B:140:THR:HG23	2.18	0.43
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.88	0.43
1:A:196:LEU:HD12	1:A:418:ALA:O	2.18	0.43
1:A:331:PHE:O	1:A:334:ILE:HG22	2.19	0.43
1:B:417:ASN:C	1:B:419:LEU:N	2.77	0.43
1:C:58:ASN:O	1:C:265:LYS:HD2	2.18	0.43
1:A:169:LEU:HD11	1:B:339:SER:CB	2.49	0.43
1:B:58:ASN:OD1	1:B:59:GLY:N	2.51	0.43
1:C:196:LEU:HD12	1:C:418:ALA:O	2.18	0.43
1:A:7:TYR:HA	1:A:109:THR:HG21	2.01	0.43
1:A:132:ALA:HA	1:A:135:ARG:HH21	1.83	0.43
1:B:132:ALA:HA	1:B:135:ARG:HH21	1.84	0.43
1:B:169:LEU:CD2	1:B:170:THR:HG22	2.49	0.43
1:C:39:LEU:HB3	1:C:40:PRO:HD2	2.01	0.43
1:C:264:SER:C	1:C:266:THR:N	2.77	0.43
1:C:268:GLY:O	1:C:269:ALA:C	2.60	0.43
1:A:199:GLU:OE1	1:A:199:GLU:N	2.49	0.43
1:A:258:ASP:OD2	1:A:258:ASP:N	2.52	0.42
1:B:415:LEU:C	1:B:417:ASN:N	2.75	0.42
1:C:54:TYR:CD1	1:C:55:ARG:HG3	2.53	0.42
1:C:419:LEU:O	1:C:420:SER:HB2	2.18	0.42
1:C:246:PRO:HB3	1:C:290:LEU:HB2	2.01	0.42
1:A:15:PRO:HB3	1:B:317:GLU:CG	2.50	0.42
1:A:133:ILE:O	1:A:133:ILE:CG2	2.67	0.42
1:A:324:VAL:HG12	1:A:325:GLN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLN:C	1:A:325:GLN:CD	2.88	0.42
1:B:52:ASN:ND2	1:B:52:ASN:C	2.76	0.42
1:A:32:ASN:HB2	1:B:300:SER:OG	2.20	0.42
1:B:50:TYR:CD1	1:B:50:TYR:C	2.97	0.42
1:C:300:SER:O	1:C:304:GLN:HG3	2.20	0.42
1:A:358:MET:HE3	1:A:367:SER:CB	2.49	0.42
1:B:43:GLY:N	3:B:1431:PGE:H2	2.35	0.42
1:B:132:ALA:C	1:B:134:TYR:H	2.27	0.42
1:C:218:LYS:HB2	1:C:218:LYS:HE3	1.85	0.42
1:C:362:TYR:CD1	1:C:367:SER:O	2.71	0.42
1:A:6:VAL:HG13	1:A:190:TYR:OH	2.20	0.42
1:A:132:ALA:C	1:A:134:TYR:N	2.78	0.42
1:A:224:LEU:O	1:A:227:ARG:HB2	2.19	0.42
1:A:303:LYS:HD2	1:C:29:GLU:CD	2.44	0.42
1:A:341:ILE:HD11	1:A:390:ARG:HA	2.01	0.42
1:B:199:GLU:OE1	1:B:199:GLU:N	2.45	0.42
1:B:325:GLN:NE2	1:B:329:SER:OG	2.52	0.42
1:C:368:THR:O	1:C:371:ASP:HB2	2.19	0.42
1:A:98:TYR:O	1:A:102:GLN:HG3	2.20	0.42
1:A:133:ILE:HD12	1:A:164:VAL:HG21	2.00	0.42
1:A:268:GLY:C	1:A:270:ALA:N	2.77	0.42
1:C:132:ALA:HA	1:C:135:ARG:HH21	1.85	0.42
1:B:41:GLN:HE22	1:C:294:GLN:CB	2.24	0.42
1:B:54:TYR:HD1	1:B:55:ARG:HG3	1.84	0.42
1:B:137:LEU:HD21	1:B:158:ARG:CD	2.47	0.42
1:B:224:LEU:O	1:B:227:ARG:HB2	2.20	0.42
1:B:314:GLU:O	1:B:317:GLU:HB3	2.20	0.42
1:C:11:ARG:HH21	1:C:12:LEU:HD21	1.85	0.42
1:A:119:ALA:HB1	1:A:175:LEU:HA	2.02	0.42
1:A:123:LEU:O	1:A:127:GLN:HG3	2.19	0.42
1:C:2:ASN:CG	1:C:416:ASN:OD1	2.63	0.42
1:C:34:ALA:HB1	1:C:84:LEU:HA	2.02	0.42
1:C:50:TYR:CD1	1:C:50:TYR:C	2.98	0.42
1:C:123:LEU:O	1:C:127:GLN:HG3	2.20	0.42
1:C:167:ASN:C	1:C:169:LEU:N	2.76	0.42
1:C:398:LEU:CD1	1:C:415:LEU:HD11	2.49	0.42
1:A:132:ALA:C	1:A:134:TYR:H	2.28	0.42
1:B:133:ILE:O	1:B:133:ILE:CG2	2.67	0.42
1:C:114:PHE:HD2	1:C:395:ILE:CD1	2.28	0.42
1:C:266:THR:HG23	1:C:274:TYR:HB3	2.02	0.42
1:B:103:GLN:NE2	1:B:407:LEU:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:VAL:O	1:C:120:ILE:HG13	2.20	0.41
1:A:34:ALA:HB1	1:A:84:LEU:HA	2.02	0.41
1:A:279:MET:O	1:C:55:ARG:HD3	2.19	0.41
1:C:14:ASN:ND2	1:C:105:LEU:HD13	2.34	0.41
1:A:24:ARG:HA	1:A:94:GLN:HG2	2.02	0.41
1:A:206:PRO:HG3	1:A:334:ILE:CG2	2.49	0.41
1:B:33:GLU:O	1:B:36:SER:HB3	2.20	0.41
1:B:76:PHE:CZ	1:B:78:MET:HG2	2.55	0.41
1:C:35:ARG:HG2	1:C:35:ARG:HH21	1.84	0.41
1:C:227:ARG:HG2	1:C:227:ARG:NH1	2.36	0.41
1:A:292:ILE:CD1	1:C:69:LEU:HD11	2.51	0.41
1:B:76:PHE:CD1	1:B:76:PHE:O	2.73	0.41
1:B:218:LYS:HB2	1:B:218:LYS:HE3	1.74	0.41
1:B:358:MET:HB3	1:B:372:VAL:HA	2.02	0.41
1:A:266:THR:HG23	1:A:274:TYR:HB3	2.01	0.41
1:B:75:ILE:CG2	1:B:248:LEU:HD23	2.50	0.41
1:B:93:ILE:HG12	1:B:228:LEU:HB3	2.03	0.41
1:B:183:ARG:O	1:B:183:ARG:HD2	2.20	0.41
1:C:19:LYS:HD3	1:C:19:LYS:C	2.46	0.41
1:C:28:PHE:CD1	1:C:91:ALA:HB1	2.55	0.41
1:C:196:LEU:HD11	1:C:201:PHE:CD1	2.55	0.41
1:B:85:THR:HA	1:B:88:GLU:OE1	2.19	0.41
1:B:140:THR:HG22	1:B:362:TYR:CZ	2.55	0.41
1:B:337:SER:O	1:B:341:ILE:HG13	2.20	0.41
1:C:10:ALA:CB	1:C:186:THR:HA	2.51	0.41
1:C:204:ASP:O	1:C:205:LYS:C	2.64	0.41
1:C:334:ILE:CD1	1:C:397:GLN:HG2	2.50	0.41
1:A:55:ARG:HD3	1:B:279:MET:O	2.21	0.41
1:A:268:GLY:O	1:A:269:ALA:C	2.64	0.41
1:A:352:GLN:HA	1:A:379:LEU:HD13	2.03	0.41
1:B:246:PRO:HB3	1:B:290:LEU:HB2	2.01	0.41
1:B:302:VAL:O	1:B:306:GLN:HG3	2.21	0.41
1:B:336:ALA:O	1:B:340:SER:HB2	2.21	0.41
1:C:76:PHE:O	1:C:76:PHE:CD1	2.74	0.41
1:C:330:SER:HB3	1:C:400:ILE:CG1	2.47	0.41
1:A:118:ASN:HD21	1:A:388:ASN:ND2	2.19	0.41
1:A:52:ASN:HD22	1:A:61:ASN:ND2	2.19	0.41
1:A:76:PHE:CD1	1:A:76:PHE:C	2.98	0.41
1:A:86:LEU:HD21	1:A:235:GLU:HG3	2.03	0.41
1:A:263:GLY:O	1:A:266:THR:HB	2.21	0.41
1:A:311:GLY:O	1:A:315:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLN:HA	1:A:346:GLN:NE2	2.36	0.41
1:B:76:PHE:CD1	1:B:76:PHE:C	2.99	0.41
1:B:357:ALA:O	1:B:358:MET:C	2.62	0.41
1:C:209:VAL:CG1	1:C:210:ASN:N	2.84	0.41
1:A:190:TYR:HA	1:A:191:PRO:HD3	1.90	0.41
1:B:32:ASN:HD22	1:B:32:ASN:HA	1.67	0.41
1:B:54:TYR:O	1:B:54:TYR:CD1	2.74	0.41
1:B:264:SER:C	1:B:266:THR:N	2.74	0.41
1:A:41:GLN:NE2	1:B:294:GLN:HA	2.36	0.40
1:A:167:ASN:C	1:A:169:LEU:N	2.77	0.40
1:B:330:SER:CB	1:B:400:ILE:HG12	2.49	0.40
1:C:55:ARG:C	1:C:57:ALA:N	2.78	0.40
1:A:290:LEU:HD12	1:A:291:PRO:HD2	2.03	0.40
1:B:34:ALA:HB1	1:B:84:LEU:HA	2.02	0.40
1:B:272:THR:HA	1:B:275:ASP:OD2	2.21	0.40
1:C:52:ASN:HD22	1:C:61:ASN:ND2	2.19	0.40
1:A:180:GLU:OE1	1:B:328:ARG:HD3	2.22	0.40
1:A:358:MET:HE3	1:A:367:SER:HB3	2.03	0.40
1:B:1:GLU:HB3	1:B:5:GLN:HB2	2.04	0.40
1:B:35:ARG:HB2	1:B:84:LEU:HD22	2.04	0.40
1:B:169:LEU:HD11	1:C:340:SER:N	2.35	0.40
1:A:52:ASN:ND2	1:A:52:ASN:C	2.76	0.40
1:A:169:LEU:CD1	1:B:339:SER:OG	2.69	0.40
1:A:334:ILE:HD11	1:A:397:GLN:HG2	2.03	0.40
1:B:30:LYS:HB3	1:B:87:GLN:OE1	2.21	0.40
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.92	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	426/428 (100%)	389 (91%)	32 (8%)	5 (1%)	10	34
1	B	426/428 (100%)	390 (92%)	31 (7%)	5 (1%)	10	34
1	C	426/428 (100%)	392 (92%)	29 (7%)	5 (1%)	10	34
All	All	1278/1284 (100%)	1171 (92%)	92 (7%)	15 (1%)	10	34

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	ALA
1	A	420	SER
1	B	269	ALA
1	B	420	SER
1	C	269	ALA
1	C	420	SER
1	A	265	LYS
1	B	264	SER
1	B	265	LYS
1	C	264	SER
1	C	265	LYS
1	A	264	SER
1	A	147	GLY
1	B	55	ARG
1	C	55	ARG

5.3.2 Protein sidechains ⓘ

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	358/358 (100%)	348 (97%)	10 (3%)	38	72
1	B	358/358 (100%)	347 (97%)	11 (3%)	35	69
1	C	358/358 (100%)	345 (96%)	13 (4%)	31	65
All	All	1074/1074 (100%)	1040 (97%)	34 (3%)	34	68

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	163	THR
1	A	198	VAL
1	A	210	ASN
1	A	213	LEU
1	A	250	LEU
1	A	259	THR
1	A	358	MET
1	A	368	THR
1	A	428	GLU
1	B	71	LEU
1	B	163	THR
1	B	198	VAL
1	B	209	VAL
1	B	210	ASN
1	B	213	LEU
1	B	250	LEU
1	B	340	SER
1	B	358	MET
1	B	368	THR
1	B	428	GLU
1	C	71	LEU
1	C	107	LEU
1	C	163	THR
1	C	198	VAL
1	C	210	ASN
1	C	213	LEU
1	C	250	LEU
1	C	259	THR
1	C	340	SER
1	C	358	MET
1	C	368	THR
1	C	398	LEU
1	C	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	41	GLN
1	A	52	ASN
1	A	61	ASN
1	A	87	GLN

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Mol	Chain	Res	Type
1	A	108	ASN
1	A	115	ASN
1	A	118	ASN
1	A	145	ASN
1	A	155	GLN
1	A	174	ASN
1	A	200	ASN
1	A	207	GLN
1	A	220	ASN
1	A	239	GLN
1	A	278	ASN
1	A	281	GLN
1	A	282	ASN
1	A	301	GLN
1	A	315	GLN
1	A	320	HIS
1	A	325	GLN
1	A	332	ASN
1	A	342	ASN
1	A	346	GLN
1	A	352	GLN
1	A	381	ASN
1	A	392	ASN
1	A	396	ASN
1	A	417	ASN
1	B	9	GLN
1	B	32	ASN
1	B	41	GLN
1	B	52	ASN
1	B	61	ASN
1	B	87	GLN
1	B	103	GLN
1	B	108	ASN
1	B	118	ASN
1	B	136	GLN
1	B	139	GLN
1	B	173	ASN
1	B	174	ASN
1	B	200	ASN
1	B	207	GLN
1	B	220	ASN
1	B	239	GLN

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Mol	Chain	Res	Type
1	B	278	ASN
1	B	281	GLN
1	B	282	ASN
1	B	301	GLN
1	B	315	GLN
1	B	320	HIS
1	B	325	GLN
1	B	342	ASN
1	B	346	GLN
1	B	392	ASN
1	B	396	ASN
1	B	417	ASN
1	C	32	ASN
1	C	41	GLN
1	C	52	ASN
1	C	61	ASN
1	C	108	ASN
1	C	118	ASN
1	C	129	GLN
1	C	136	GLN
1	C	174	ASN
1	C	184	GLN
1	C	200	ASN
1	C	207	GLN
1	C	220	ASN
1	C	225	GLN
1	C	278	ASN
1	C	281	GLN
1	C	282	ASN
1	C	301	GLN
1	C	315	GLN
1	C	325	GLN
1	C	332	ASN
1	C	342	ASN
1	C	346	GLN
1	C	381	ASN
1	C	388	ASN
1	C	392	ASN
1	C	397	GLN
1	C	417	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](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
3	PGE	B	1432	-	9,9,9	0.75	0	8,8,8	0.73	0
3	PGE	B	1431	-	9,9,9	0.75	0	8,8,8	0.63	0
3	PGE	C	1431	-	9,9,9	0.68	0	8,8,8	0.66	0
3	PGE	C	1430	-	9,9,9	0.91	0	8,8,8	0.62	0
3	PGE	A	1430	-	9,9,9	0.66	0	8,8,8	0.68	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	PGE	B	1432	-	-	5/7/7/7	-
3	PGE	B	1431	-	-	6/7/7/7	-
3	PGE	C	1431	-	-	5/7/7/7	-
3	PGE	C	1430	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	A	1430	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1431	PGE	O2-C3-C4-O3
3	B	1432	PGE	O2-C3-C4-O3
3	B	1431	PGE	O2-C3-C4-O3
3	C	1430	PGE	O2-C3-C4-O3
3	B	1432	PGE	O1-C1-C2-O2
3	B	1431	PGE	O1-C1-C2-O2
3	C	1430	PGE	O3-C5-C6-O4
3	C	1431	PGE	O1-C1-C2-O2
3	A	1430	PGE	C3-C4-O3-C5
3	B	1432	PGE	C1-C2-O2-C3
3	B	1432	PGE	C6-C5-O3-C4
3	C	1431	PGE	C4-C3-O2-C2
3	A	1430	PGE	C4-C3-O2-C2
3	B	1432	PGE	O3-C5-C6-O4
3	C	1431	PGE	C6-C5-O3-C4
3	A	1430	PGE	O1-C1-C2-O2
3	B	1431	PGE	C1-C2-O2-C3
3	B	1431	PGE	C4-C3-O2-C2
3	C	1430	PGE	C4-C3-O2-C2
3	A	1430	PGE	C1-C2-O2-C3
3	B	1431	PGE	C6-C5-O3-C4
3	C	1430	PGE	C1-C2-O2-C3
3	B	1431	PGE	C3-C4-O3-C5
3	C	1431	PGE	C3-C4-O3-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1431	PGE	1	0
3	C	1431	PGE	1	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, 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	428/428 (100%)	0.85	44 (10%) 12 10	35, 69, 100, 131	0
1	B	428/428 (100%)	0.31	9 (2%) 63 54	21, 45, 79, 138	0
1	C	428/428 (100%)	0.43	15 (3%) 47 38	22, 55, 95, 159	0
All	All	1284/1284 (100%)	0.53	68 (5%) 32 25	21, 56, 96, 159	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	GLU	4.6
1	A	418	ALA	4.5
1	A	172	ARG	4.3
1	A	140	THR	4.1
1	B	269	ALA	3.8
1	C	131	GLU	3.6
1	C	110	ALA	3.5
1	A	166	ALA	3.4
1	C	270	ALA	3.4
1	A	150	ALA	3.4
1	C	140	THR	3.4
1	A	395	ILE	3.3
1	B	272	THR	3.1
1	A	129	GLN	3.0
1	B	270	ALA	3.0
1	A	146	VAL	3.0
1	A	148	LEU	2.9
1	B	271	GLY	2.9
1	C	64	ALA	2.9
1	A	169	LEU	2.9
1	C	258	ASP	2.8
1	C	178	ALA	2.8
1	A	396	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	412	LEU	2.7
1	A	407	LEU	2.7
1	A	398	LEU	2.7
1	A	133	ILE	2.6
1	A	181	GLN	2.6
1	A	415	LEU	2.5
1	C	112	ALA	2.5
1	A	364	VAL	2.5
1	C	269	ALA	2.4
1	A	109	THR	2.4
1	A	427	PRO	2.4
1	A	130	LYS	2.3
1	A	50	TYR	2.3
1	A	105	LEU	2.3
1	C	191	PRO	2.3
1	A	370	VAL	2.3
1	A	156	ASN	2.3
1	C	139	GLN	2.3
1	A	152	THR	2.3
1	A	392	ASN	2.3
1	A	163	THR	2.3
1	B	198	VAL	2.3
1	A	151	ILE	2.3
1	A	125	TYR	2.3
1	A	201	PHE	2.2
1	A	270	ALA	2.2
1	C	155	GLN	2.2
1	A	175	LEU	2.2
1	B	336	ALA	2.2
1	B	136	GLN	2.2
1	A	128	ALA	2.2
1	A	134	TYR	2.1
1	B	319	ALA	2.1
1	A	160	GLN	2.1
1	C	143	ARG	2.1
1	C	260	SER	2.0
1	A	394	LEU	2.0
1	A	419	LEU	2.0
1	A	11	ARG	2.0
1	A	53	GLY	2.0
1	A	295	GLY	2.0
1	A	77	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	2.0
1	A	380	TYR	2.0
1	C	268	GLY	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($\text{\AA}^2$)	Q<0.9
3	PGE	A	1430	10/10	0.82	0.20	58,70,80,90	0
3	PGE	C	1431	10/10	0.83	0.17	66,73,80,95	0
3	PGE	C	1430	10/10	0.84	0.15	41,52,62,62	0
3	PGE	B	1432	10/10	0.86	0.17	54,74,82,91	0
3	PGE	B	1431	10/10	0.88	0.14	53,73,85,88	0
2	CL	C	1429	1/1	0.91	0.13	55,55,55,55	0
2	CL	A	1429	1/1	0.92	0.09	64,64,64,64	0
2	CL	B	1429	1/1	0.92	0.09	66,66,66,66	0
4	NA	B	1430	1/1	0.97	0.16	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.